

KIM API V2

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Chapter 1

Introduction

The KIM API package is a system-level library that aims to give computer programmers the ability to write atomistic or molecular simulation programs that can seamlessly interface (in a plug-and-play manner) with independent implementations of interatomic models, regardless of the programming language (C, C++, FORTRAN 77, Fortran 90/95/2003, Python, etc.) in which the codes are written.

The KIM API defines standard quantities that must be communicated between the simulation code and the interatomic model, such as the number of particles, the species and position coordinates of each particle, and the forces acting on the particles. This information is communicated via memory pointers so that minimal data copying is necessary. The KIM API provides a "model object" and "compute-arguments object" interface which facilitates and simplifies (as much as possible) the exchange of memory pointers between the simulator and model.

This documentation is organized into the following components:

1. [Features of the KIM API package](#)
2. [Theory](#)
3. [Implementation](#)
4. Example simulators written in C++ ([ex_test_Ar_fcc_cluster_cpp.cpp](#)), C ([ex_test_Ar_fcc_cluster.c](#)), and Fortran ([ex_test_Ar_fcc_cluster_fortran.F90](#)).
5. Example stand-alone models written in C ([ex_model_Ar_P_Morse_07C.c](#)) and Fortran ([ex_model_Ar_P_MLJ_F03.F03](#))
6. Example model drivers written in C++ ([LennardJones612Implementation.hpp](#)), C ([ex_model_driver_P_Morse.c](#)), and Fortran ([ex_model_driver_P_LJ.F90](#)).
7. Example parameterized models ([ex_model_Ar_P_LJ.params](#), [ex_model_Ar_P_Morse.params](#), [LennardJones612_UniversalSh](#))
8. [Summary of Differences Between kim-api-v1 and kim-api-v2](#)
9. [Guide for porting content from KIM API v1 to v2](#)

In addition, all public header files and included example codes are available for [browsing](#).

Chapter 2

Features of the KIM API package

Previous Section: [Introduction](#).

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The current version of the KIM API package supports the following features:

- **Programming Languages:** Currently supported programming languages include C, C++, Fortran.
- **Best Practice API Design:** The guiding design principle for the KIM API has been *simplicity*. In addition to this, general API design *best practices* have been used. These include: implementation hiding (pimpl idiom), loose coupling, minimal-completeness, ease of use (discoverable, difficult to misuse, consistent, orthogonal), static factory methods, use of namespaces, const-correctness, avoiding the use of abbreviations, etc.
- **Language Idiom Support:** Wherever it makes sense and is possible the KIM API supports common idioms of the native language. For example, all C API routines that return an error status do so using the C function return value. For Fortran, all such API routines are SUBROUTINES and have their final argument as an error status.
- **Extensible, Strongly-Typed Enumerations:** The KIM API implements a set of typed constants for each category of entity that it defines (DataType, LanguageName, Numbering, SpeciesName, LengthUnit, EnergyUnit, ChargeUnit, TemperatureUnit, TimeUnit, ComputeArgumentName, ComputeCallbackName, SupportStatus). This allows for backward-compatible additions to the enumerations in future versions of the KIM API. Further, the strong-typing greatly facilitates debugging.
- **Numbering Origin Support:** Support for automatic translation between zero-based numbering of particles (C-style numbering beginning with zero) and one-based numbering (Fortran-style numbering beginning with one).
- **Data Communication:** Communication of an arbitrary number of *arguments* and *callback* routines between a *Model* (interatomic potential) and a *Simulator* (simulation code that uses a Model).
- **Data types:** integer and double.

Each of the data types can be used to create multi-dimensional array arguments that are exchanged between Models and Simulators. The KIM API standard defines the dimension and extent of these arrays for each argument. However, this information is not discoverable at run-time. Thus, it is left to the programmer to ensure that the correct values are used.

Currently, the KIM API does not define any (more complex) data structures. However, in the future (as the need arises, and in consultation with the atomistic and molecular simulation community) additional data types and data structures may be introduced.

- **Physical Units:** The KIM API standard defines the physical units for each argument exchanged between a Model and Simulator. A simulator provides a set of *requested units* to define a unit system and a model either accepts this unit system (and performs appropriate unit conversions for its parameters), or it rejects the request and reports the unit system to be used.
- **Neighbor lists:** Neighbor list routines are expected to be provided by the calling Simulator. All neighbor lists are full, unsorted lists that must contain all particles within the specified cutoff distance (but may contain additional particles). A model must request one or more neighbor lists, each with an associated cutoff distance. (Cutoff distances are typically distinct, but may repeat. Repeated cutoff distances allow a model to simultaneously access the neighbors of multiple particles without needing to make copies of the neighbor list(s).) A simulator must provide all such requested lists and ensure that these lists contain only a small number of particles that are located outside the cutoff distance.
- **Particle Species:** The KIM API provides the ability to designate the physical species of each particle in a simulation. Currently, only one identifier is provided for each element in the periodic table. In the future support for Models that require multiple types of each element may be added.
- **Model Parameters:** The KIM philosophy views a *Model* as a well-defined computational code that includes specific values for all parameters needed to perform an actual computation. However, it is often useful to explore how a Model's predictions vary as the values of its parameters are varied. For this reason, the KIM API allows a Model to (optionally) "publish" its parameters so that a Simulator may modify them during the course of a simulation.
- **Model Drivers:** The KIM API package provides the ability to create Model Driver routines. A Model for a given material can be created which uses an existing Model Driver by providing a file or files with the appropriate parameter values for the material of interest.
- **Logging capabilities:** The KIM API package provides a full-featured logging capability that facilitates the identification and debugging of errors. In addition to built-in support for logging within Model codes, the KIM API also provides access to logging capabilities for general use by Simulator codes.
- **Semantic Versioning:** The KIM API package conforms to the [Semantic Versioning 2.0.0](#) standard. This standard is useful because its version numbers and the way they change convey meaning about the underlying code and what has been modified from one version to the next. In addition, the KIM API provides basic tools for comparing and parsing Semantic Version strings.

Next Section: [Theory](#).

Chapter 3

Theory

Previous Section: [Features of the KIM API package.](#)

At the highest level there are "Simulators" and "Models". Conceptually, a KIM Model is something that defines an energy-per-particle function, E_i , and an "influence distance", r_{infl} , that identifies the particle separation range over which E_i depends on the position of its neighboring particles. (Note, this is not necessarily equal to the neighbor list cutoff radius used by a model.) A KIM Model is defined for a specific material system (a specific set of particle species: e.g., Al, Ni, and Cu) and contains all parameter values necessary for evaluating E_i for any configuration containing particles of the supported species. A KIM Model will, typically, also have the ability to compute other quantities related to the energy-per-particle, such as the force on a particle or the particle's virial.

Conceptually, a KIM Simulator is something that performs a numerical simulation based on the energy, forces, etc. of a set of particles. This could be a molecular dynamics simulation, a monte carlo simulation, or other similar simulation technique. A KIM Simulator treats a KIM Model as a black box. It constructs an atomistic "Configuration" of interest and passes this configuration to a KIM Model along with a list of quantities (energy, force, virial, etc.) to be computed. The model then performs the requested computation and passes the results back to the simulator. Once the simulator has received the model's results it may use these values to advance its simulation and update the atomistic configuration. Typically, this sequence of events is repeated in an iterative process until the simulator determines it has reached convergence or some other stopping condition is achieved.

The purpose of the KIM API is to coordinate the information exchange between KIM Simulators and KIM Models. It does this through the definition of various concepts and quantities, and by providing a set of subroutines that facilitate the necessary communication between simulators and models.

Of central importance to this process is the definition of an atomistic "Configuration", \mathcal{C} . Abstractly, a configuration consists of a set of particles C_p and their associated data. For each particle $i \in C_p$, the following additional data must be defined.

1. The particle's species (H, He, Li, etc.).
2. The particle's position vector $\mathbf{r}^{(i)} = r_j^{(i)} \mathbf{e}_j = r_1^{(i)} \mathbf{e}_1 + r_2^{(i)} \mathbf{e}_2 + r_3^{(i)} \mathbf{e}_3$, where \mathbf{e}_j , $j = 1, 2, 3$ are unit vectors along the global fixed Cartesian coordinate system x , y , and z directions, respectively.
3. The particle's "Contributing Status", which is either "contributing" or "non-contributing". Non-contributing particles exist as part of the configuration only to provide the proper environment for the contributing particles. Thus, non-contributing particles (sometimes called "ghost" or "padding" particles) can be thought of as providing the appropriate boundary conditions for the configuration.

Before proceeding further, introduce the notation $\mathbf{r}^{(i,j)} \equiv \mathbf{r}^{(j)} - \mathbf{r}^{(i)}$ for the relative position vector **from particle i to particle j** , and the notation $r^{(i,j)}$ for the magnitude of the vector $\mathbf{r}^{(i,j)}$. Note that $r^{(j,i)} = r^{(i,j)}$ and these are simply two different notations for the same quantity.

Returning to the definition and description of a configuration, a configuration's set of particles may be partitioned into two disjoint sets: The set of contributing particles C_{cp} , and the set of non-contributing particles C_{ncp} . So that

$$C_p = C_{cp} \cup C_{ncp} \quad \text{and} \quad C_{cp} \cap C_{ncp} = \emptyset.$$

For a particle $i \in C_p$, define the particle's ("punctured") influence neighborhood, $\mathcal{N}_{r_{\text{infl}}}^{(i)}$, as the subset of particles (not including the particle, itself) in the configuration that are located no more than r_{infl} away from particle i . That is,

$$\mathcal{N}_{r_{\text{infl}}}^{(i)} \equiv \{j \in C_p \mid 0 < r^{(i,j)} \leq r_{\text{infl}}\}.$$

Finally, define the closure of the particle's influence neighborhood, $\bar{\mathcal{N}}_{r_{\text{infl}}}^{(i)}$.

$$\bar{\mathcal{N}}_{r_{\text{infl}}}^{(i)} \equiv \mathcal{N}_{r_{\text{infl}}}^{(i)} \cup \{i\}.$$

With the above definitions, it is possible to more specifically identify the functional dependence for a KIM Model's energy-per-particle function, E_i :

$$E_i = \bar{E}_i(\mathbf{r}^{(j)} \mid j \in \bar{\mathcal{N}}_{r_{\text{infl}}}^{(i)}).$$

In fact, due to the principle of material frame indifference, this function can only be a function of the *distances* between these particles:

$$E_i = \tilde{E}_i(r^{(j,k)} \mid j, k \in \bar{\mathcal{N}}_{r_{\text{infl}}}^{(i)}).$$

It is usually most convenient to work with the function of position vectors, $\bar{E}_i(\mathbf{r}^{(j)})$. However, in some cases it is advantageous to work with the function of distances, $\tilde{E}_i(r^{(j,k)})$. When the distinction is unimportant the unaccented notation, E_i , will be used.

Now a configuration's "Partial Energy" may be defined as the sum of its contributing particles' energies:

$$E^C = \sum_{i \in C_{cp}} E_i.$$

From this definition of the configuration's partial energy, a set of additional quantities may be derived that are often of interest in simulations.

First, define formally, the configuration's "Partial Particle Energy" for particle i , E_i^C , as simply the model's energy-per-particle value for contributing particles and zero for non-contributing particles,

$$E_i^C \equiv \begin{cases} E_i, & i \in C_{cp}, \\ 0, & i \in C_{ncp}. \end{cases}$$

Second, the configuration's "Partial Force" on particle j , $\mathbf{f}^C(j)$, is defined as the negative of the derivative of the configuration's partial energy with respect to the particle's position vector:

$$\mathbf{f}^{\mathcal{C}(j)} \equiv -\frac{\partial E^{\mathcal{C}}}{\partial \mathbf{r}^{(j)}}, \quad j \in C_p.$$

Note that, in general, *every* particle (both contributing and non-contributing) has a partial force. As a special case, consider a configuration, \mathcal{C}^i , equivalent to \mathcal{C} except that only particle i is contributing. In this case, the partial forces are

$$\mathbf{f}^{\mathcal{C}^i(j)} = \begin{cases} -\frac{\partial \bar{E}_i}{\partial \mathbf{r}^{(j)}} & j \in \mathcal{N}_{r_{\text{infl}}}^{(i)}, \\ 0, & \text{otherwise.} \end{cases}$$

This can be thought of as the force on particle j due to particle i . With this notation, it is possible to obtain the identity

$$\mathbf{f}^{\mathcal{C}(j)} = \sum_{i \in C_{cp}} \mathbf{f}^{\mathcal{C}^i(j)}.$$

Third, the configuration's "Partial Particle Virial" tensor for contributing particle $i \in C_{cp}$, $\mathbf{V}^{\mathcal{C}(i)}$, is defined in terms of the derivative of its per-particle-energy function:

$$\mathbf{V}^{\mathcal{C}(i)} \equiv \sum_{j \in \mathcal{N}_{r_{\text{infl}}}^{(i)}} \frac{\partial \bar{E}_i}{\partial \mathbf{r}^{(j)}} \otimes \mathbf{r}^{(j)} = \sum_{j \in \mathcal{N}_{r_{\text{infl}}}^{(i)}} -\mathbf{f}^{\mathcal{C}^i(j)} \otimes \mathbf{r}^{(j)} = - \sum_{j \in \mathcal{N}_{r_{\text{infl}}}^{(i)}} \mathbf{f}^{\mathcal{C}^i(j)} \otimes \mathbf{r}^{(j)}.$$

The partial particle virial is zero for non-contributing particles. That is, $\mathbf{V}^{\mathcal{C}(i)} = \mathbf{0}$ for $i \in C_{ncp}$.

Fourth and finally, the configuration's "Partial Virial" tensor, $\mathbf{V}^{\mathcal{C}}$, is the sum of its partial particle virial tensors:

$$\mathbf{V}^{\mathcal{C}} \equiv \sum_{i \in C_p} \mathbf{V}^{\mathcal{C}(i)}.$$

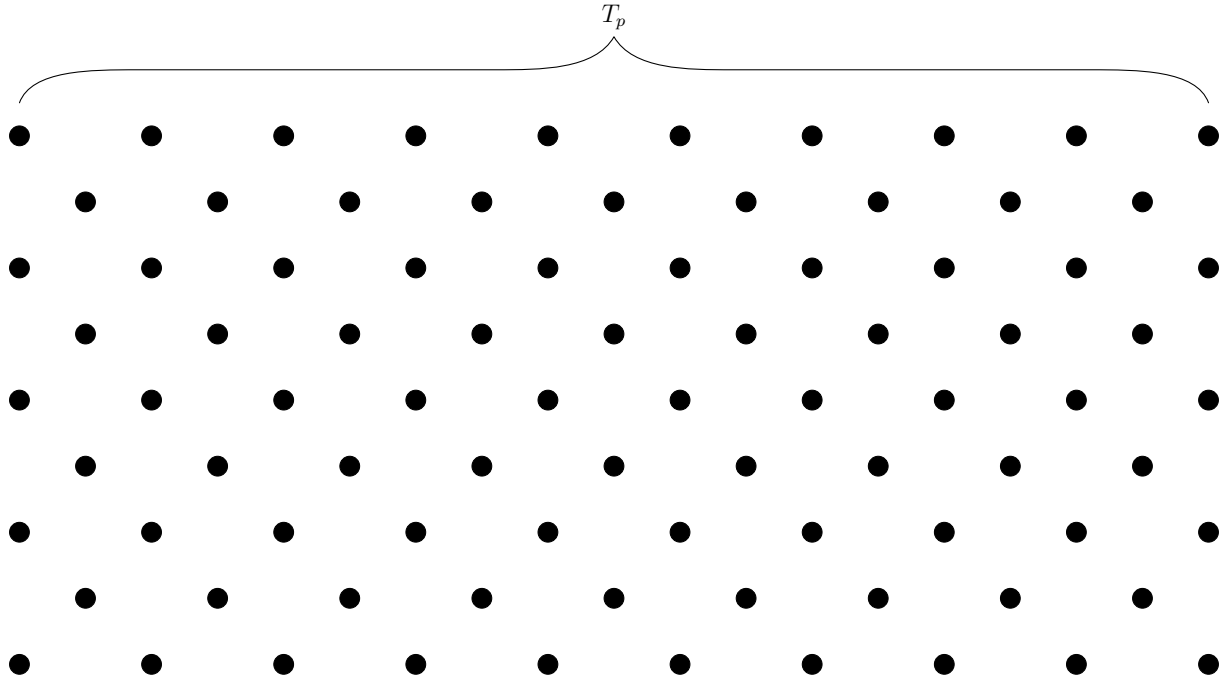
Note that an equivalent expression for the partial virial tensor is given by

$$\mathbf{V}^{\mathcal{C}} = - \sum_{i \in C_p} \mathbf{f}^{\mathcal{C}(i)} \otimes \mathbf{r}^{(i)}.$$

Domain Decomposition

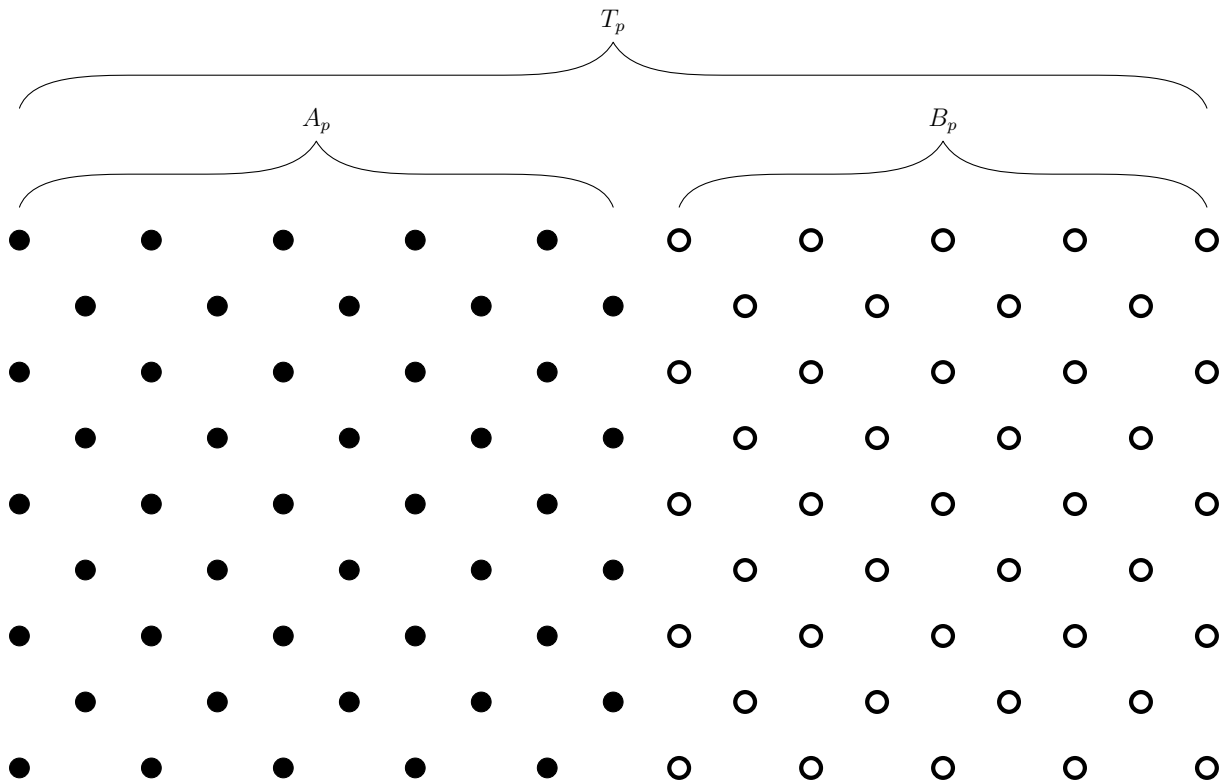
The definitions of a configuration's partial energy, forces, and virial are designed to allow for easy (and low communication) parallel computation via domain decomposition. This section presents a simple example that illustrates how this works.

Start with a configuration of particles corresponding to a finite strip of a centered square lattice.



The total energy of the system and the total force on each particle can be computed using a single configuration. In this case, the configuration is \mathcal{T} , the set of particles is T_p , the set of contributing particles is $T_{cp} = T_p$, and the set of non-contributing particles is $T_{ncp} = \emptyset$. Then, the total energy is $E = E^{\mathcal{T}}$, and the total force on particle $i \in T_p$ is $\mathbf{f}^{(i)} = \mathbf{f}^{\mathcal{T}(i)}$. Next, it is shown how to compute E and $\mathbf{f}^{(i)}$ using a two-domain decomposition.

Partition T_p into two disjoint subsets, A_p and B_p . That is, $A_p \cap B_p = \emptyset$ and $A_p \cup B_p = T_p$.



Next, define configuration \mathcal{C} to have particles $C_p = T_p$ with $C_{cp} = A_p$ and $C_{ncp} = B_p$, and configuration \mathcal{D} to have particles $D_p = T_p$ with $D_{cp} = B_p$ and $D_{ncp} = A_p$. Then,

$$E = E^{\mathcal{C}} + E^{\mathcal{D}},$$

and

$$\mathbf{f}^{(i)} = \mathbf{f}^{\mathcal{C}(i)} + \mathbf{f}^{\mathcal{D}(i)}.$$

In practice, one can get away with including only those non-contributing particles that fall within the "influence distance" of at least one contributing particle.

Next Section: [Implementation](#).

Chapter 4

Implementation

Previous Section: [Theory](#).

In code, a model (or model driver) consists of six routines which perform specific tasks. The first is the *ModelCreate* (or *ModelDriverCreate*) routine, which performs initialization tasks for the model object. The second is the *ModelComputeArgumentsCreate* routine, which performs initialization tasks for a compute-arguments object. The third is the *ModelComputeArgumentsDestroy* routine, which performs finalization tasks for a compute-arguments object. The fourth is the *ModelCompute* routine, which uses the configuration information stored in a compute-arguments object to perform the model's core computational tasks. The fifth is the *ModelRefresh* routine, which performs updates after a simulator makes changes to the model's parameters (if this is supported). The sixth is the *ModelDestroy* routine, which performs finalization tasks for the model object.

To interact with a model, a simulator creates a model object (which, in part, includes execution of the model's *ModelCreate* routine). Using this object, the simulator creates a compute-arguments object (which, in part, includes execution of the model's *ModelComputeArgumentsCreate* routine). Then, the simulator provides a compute-arguments object to the model's *ModelCompute* function. There are input compute-arguments that include the various components that make up a configuration (number of particles, particle position vectors, etc.). And, there are output compute-arguments that include the quantities (like partial energy and partial forces), defined in Section [Theory](#), associated with the configuration. There are also compute-callback functions (such as a function to get a particle's neighbor list) that the simulator provides for use by the model.

The KIM API provides a list of all compute-arguments and compute-callbacks defined as part of the official A↔PI. Each such argument and callback has a "Support Status" which can be one of four values: *requiredByAPI*, *notSupported*, *required*, or *optional*. A model specifies a support status value, as part of its *ModelComputeArgumentsCreate* routine, for every compute-argument and compute-callback defined by the KIM API. It is the responsibility of the simulator to use the compute-arguments object interface to determine the support status of each compute-argument and compute-callback and to use this information to determine if the model is capable of performing the desired computation.

Next, lists of each input compute-argument, output compute-argument, and compute-callback are provided. To be explicit, below zero-based particle numbering is used where necessary.

Input compute-argument table:

Compute Argument Name	Unit	Data Type	Extent	Memory Layout	Valid Support Statuses (bold – default)
numberOfParticles	N/A	integer	1		requiredByAPI
particleSpecies↔Codes	N/A	integer	numberOfParticles	$sc^{(0)}, sc^{(1)}, \dots$	requiredByAPI
particle↔Contributing	N/A	integer	numberOfParticles	$c^{(0)}, c^{(1)}, \dots$	requiredByAPI
coordinates	length	double	numberOfParticles * 3	$r_1^{(0)}, r_2^{(0)}, r_3^{(0)}, r_1^{(1)}, r_2^{(1)}$	requiredByAPI

- numberOfParticles is the number of particles (contributing and non-contributing) in the configuration.
- particleSpeciesCodes contains integer codes (as defined by the model) specifying the species of each particle. For example, if the model defines the mapping $\text{Cu} \leftrightarrow 1$, $\text{Al} \leftrightarrow 2$, and $\text{Ni} \leftrightarrow 3$, then $sc^{(0)} = 3$, $sc^{(1)} = 1$, $sc^{(2)} = 2$, ... means that particle 0 is a nickel atom, particle 1 is a copper atom, particle 2 is an aluminum atom, etc.
- particleContributing contains the contributing/non-contributing status of each particle. Particle i is contributing if $c^{(i)} = 1$ and non-contributing if $c^{(i)} = 0$.
- coordinates contains the Cartesian components of the particles' position vectors, $\mathbf{r}^{(i)} = r_1^{(i)} \mathbf{e}_1 + r_2^{(i)} \mathbf{e}_2 + r_3^{(i)} \mathbf{e}_3$.

Output compute-argument table:

Compute Argument Name	Unit	Data Type	Extent	Memory Layout	Valid Support Statuses (bold – default)
partialEnergy	energy	double	1		required, optional, notSupported
partialForces	force	double	numberOfParticles * 3	$f_1^{C(0)}, f_2^{C(0)}, f_3^{C(0)}, f_1^{C(1)}, f_2^{C(1)}$	required, optional, notSupported
partialParticle \leftrightarrow Energy	energy	double	numberOfParticles	$E^{C(0)}, E^{C(1)}, E^{C(2)}$	required, optional, notSupported
partialVirial	energy	double	6	$V_{11}^C, V_{22}^C, V_{33}^C, V_{23}^C, V_{32}^C$	required, optional, notSupported
partialParticleVirial	energy	double	numberOfParticles * 6	$\mathbf{V}^{C(0)}, \mathbf{V}^{C(1)}, \mathbf{V}^{C(2)}$	required, optional, notSupported

- partialEnergy is the configuration's partial energy E^C .
- partialForces contains the partial force vector for each particle, $\mathbf{f}^{C(i)} = f_1^{C(i)} \mathbf{e}_1 + f_2^{C(i)} \mathbf{e}_2 + f_3^{C(i)} \mathbf{e}_3$.
- partialParticleEnergy contains the partial particle energy for each particle, $E^{C(i)}$.
- partialVirial is the configuration's partial virial tensor, \mathbf{V}^C .
- partialParticleVirial contains the partial particle virial tensor for each particle, $\mathbf{V}^{C(i)}$.

Compute-callback table:

Compute Callback Name	Valid Support Statuses (bold – default)
GetNeighborList	requiredByAPI
ProcessDEDrTerm	required, optional, notSupported
ProcessD2EDr2Term	required, optional, notSupported

- GetNeighborList is a callback function that allows a model to obtain the list of neighbors of a particle. The model may request any number of neighbor lists with different (or equal) cutoff distances. The GetNeighbor \leftrightarrow List callback function must support the return of the appropriate list of neighbors. The returned list of neighbors consists of a contiguous-in-memory list of integers corresponding to an unordered full list of a particle's neighbors. Each such neighbor list must contain at least all particles within the corresponding cutoff distance of the specified particle. (However, the returned list may contain particles beyond the cutoff distance.) Neighbor lists provided by the simulator must be consistent with the configuration coordinates and the model's cutoff values. In particular, the model must, in principle, be able to independently construct its own equivalent

neighbor list using just the particle coordinates. Further, the GetNeighborList callback routine must check to ensure that the neighbor list data (provided, via the Simulator, by the compute-arguments object) is consistent with the model's cutoff values.

CAUTION - SIMULATOR DEVELOPERS: In general, it is important that neighbor lists provided by a simulator are "efficient" in the sense that the list contains only a small number of particles that are located outside the cutoff distance. If the lists are not efficient, then the model computational time may be *severely* impacted. This is especially true for models that request multiple neighbor lists with a wide range of cutoff distances.

- ProcessDEDrTerm is a callback function that allows for access to the derivatives of the configuration's partial energy, E^C , with respect to all pair-distances, $r^{(i,j)}$, $i, j \in C_p$. That is, it allows the model to communicate the values of $\frac{\partial E^C}{\partial r^{(i,j)}}$ to the simulator. Recall that $r^{(i,j)}$ and $r^{(j,i)}$ are just two different notations for the same quantity. Thus, there are only $\frac{\text{numberOfParticles} \cdot (\text{numberOfParticles} + 1)}{2}$ quantities (as opposed to $(\text{numberOfParticles})^2$) referred to by the notation $\frac{\partial E^C}{\partial r^{(i,j)}}$.

These quantities can be used to compute many quantities of interest associated with the configuration. For example, it is possible to independently compute the partial virial from this information using the formula

$$\mathbf{V}^C = \sum_{i \in C_p} \mathbf{V}^{C(i)} = \sum_{i \in C_p} \sum_{j \in \mathcal{N}_{r_{\text{infl}}}^{(i)}} \frac{\bar{E}_i}{\partial \mathbf{r}^{(j)}} \otimes \mathbf{r}^{(j)} = \sum_{i \in C_p} \sum_{j \in \mathcal{N}_{r_{\text{infl}}}^{(i)}} \sum_{k \neq j; k \in \mathcal{N}_{r_{\text{infl}}}^{(i)}} \frac{\partial \bar{E}_i}{\partial r^{(j,k)}} \frac{\partial r^{(j,k)}}{\partial \mathbf{r}^{(j)}} \otimes \mathbf{r}^{(j)}.$$

- ProcessD2EDr2Term is a callback function that allows for access to the second derivatives of the configuration's partial energy, E^C , with respect to all pair-distances, $r^{(i,j)}$, $i, j \in C_p$. That is, it allows the model to communicate the values of $\frac{\partial^2 E^C}{\partial r^{(i,j)} \partial r^{(m,n)}}$ to the simulator.

Next Section: [Summary of Differences Between kim-api-v1 and kim-api-v2.](#)

Chapter 5

Summary of Differences Between kim-api-v1 and kim-api-v2

Previous Section: [Implementation](#).

Experience with using and supporting the kim-api-v1 package has shown that the package's complexity (in terms of the number of different "modes of operation"; e.g., neighbor lists: half, full, iterator, locator; NBCs: cluster, miopbc, neigh_pure, neigh_rvec; etc.) makes it difficult for new users to become competent kim-api-v1 code developers. This also means that KIM Models will only work with KIM-compliant codes that support the same modes of operation, thereby limiting the utility of the kim-api as a standard. Further, the kim-api's complexity results in Model implementations that are convoluted due to developers' desire to support *all* modes of operation. This experience has led us to an approach that gives kim-api-v2 a dramatically simplified form, while still retaining a high degree of flexibility. Thus, in regard to feature design and selection for the kim-api-v2 package, we have taken "simplicity" as a guiding principle.

High-level changes between kim-api-v1 and kim-api-v2

- **NBCs Have Been Eliminated:** kim-api-v2 supports only one type of configuration (as described in Section [Theory](#)). This corresponds, roughly, to the kim-api-v1 NEIGH_PURE_F NBC. Additionally:
 - All neighbor lists in kim-api-v2 are full, unordered, and random-access.
 - Particle Contributing (a.k.a., padding or ghost-atom) status (contributing or non-contributing) is explicitly specified in the *particleContributing* argument. A particle with zero neighbors in (one of) its neighbor lists has no special meaning in kim-api-v2, as opposed to in kim-api-v1 where this indicates the particle is non-contributing.
- **Compute Routine Arguments and Callbacks Have Been Separated From the Model Object:** kim-api-v2 separates the arguments and callbacks of the compute routine from the model object. These items are now stored in a separate compute-arguments object that must be provided to the model's compute routine. This new approach provides a cleaner conceptual distinction between things the model is responsible for (influence distance, cutoffs, parameters, and create / compute / destroy routines), and things that the simulator is responsible for (the configuration, compute-arguments, and compute-callback routines). One practical advantage of this separation occurs for multi-threaded simulators. Such a simulator can use a single model object with multiple compute-arguments objects to compute (energy, forces, etc.) for many different configurations simultaneously. Without the model/compute-arguments separation multiple model objects would be necessary. This would require multiple in-memory copies of the model's parameter set, which can be very wasteful since (in particular, for "machine learning" models) a model's parameter set can be very large.

- **KIM Descriptor Files Have Been Eliminated:** kim-api-v2 does not use *KIM descriptor files*. Instead, kim-api-v2 models register their units, conventions, and parameters in their *ModelCreate* initialization routine, and they register their arguments and callbacks in their *ModelComputeArgumentsCreate* initialization routine. Simulator–Model matching is now the responsibility of the simulator. This is facilitated by kim-api-v2 through the availability of routines for obtaining the model's registered values of all necessary quantities at run-time.

Best practice for kim-api-v2 simulators is to, first create a model object and an associated compute-arguments object (which also execute the model's initialization routines), second interrogate the model's capabilities to determine if the desired computation can be successfully performed with the model, and third, if possible, perform the desired computation.

This scheme for Simulator–Model matching places a larger burden (as compared to kim-api-v1) on the simulator. However, it has been determined that a full-featured "KIM descriptor file"–based matching specification (covering all possibilities) is too complex. Thus, it is best to perform this matching process in the simulator's code at run-time. In the worst-case, a simulator can simply *assume* that it matches with the model and attempt to perform the desired computation. As long as the simulator carefully checks for any and all errors reported by the KIM API, it should detect an error at some point during its processing if the simulator, in fact, does not match with the model.

- **A New Memory Management Scheme:** kim-api-v2 requires the simulator to be responsible for storage memory associated with all input and output compute-arguments communicated between the simulator and the model via a compute-arguments object. Similarly, kim-api-v2 requires the model to be responsible for storage memory associated with its influence distance, its neighbor list cutoff values, and its published parameters.

kim-api-v2 does not provide a routine analogous to the `KIM_API_Allocate()` of kim-api-v1. This routine is now seen as a source of much confusion regarding the memory management model employed in kim-api-v1. Thus, it is best not to provide such a capability as part of kim-api-v2.

- **Language Consistency:** kim-api-v2 aims to conform to standard practice and idioms of the native code language, as opposed to kim-api-v1 which aimed to maintain consistency of the api across languages.

This means that using the kim-api-v2 in your preferred language feels more natural. For example, the C++ api bindings extensively use namespaces, objects, `std::string`, and error codes as function return values. The Fortran api binding provides error codes as arguments to `SUBROUTINES`, uses handles to objects, and hides (as much as possible) the effort of making Fortran interoperable with C and other languages. In particular, the need for explicit use of the intrinsic `C_F_POINTER()` subroutine has been minimized.

Consistent identifier naming schemes have been established within each language binding. Abbreviations have been avoided to make names easier to remember.

- **Explicit Definitions:** Clear definitions for all concepts used by the kim-api-v2 package are provided in [Section Theory](#).

In many cases, these are the same concepts and definitions employed by kim-api-v1. However, they were not explicitly stated in the kim-api-v1 documentation.

- **Improved Logging Facilities and Error Messages:** kim-api-v2 has been redesigned and rewritten from the ground up. Significantly improved facilities for logging events and execution progress have been included. Along with these general enhancements, all error messages have been rewritten with an eye toward improved clarity.

Lower-level changes between kim-api-v2 and kim-api-v1

- **FIXED Parameters Have Been Eliminated:** kim-api-v2 defines only one type of "published" parameters for a model. These are all changeable, and thus, would correspond to the "FREE" parameters of kim-api-v1.

The FIXED parameters of kim-api-v1 must now be stored in the model buffer and are inaccessible to the simulator.

- **Argument Shape and Extent:** For simplicity, explicit api tracking of argument shape and extent has been eliminated from kim-api-v2. These values are defined as part of the api documentation. All arguments must have fixed shape and extent values that are either given numbers or defined in terms of *numberOfParticles*.

Published model parameters are always taken to be one-dimensional arrays with a specified extent that must be defined by the model and communicated to the API through the `get/set` routines for parameters.

Thus, scalar parameters have extent 1. Multidimensional array parameters are treated by the API as one-dimensional arrays with extent equal to the total number of values in the multidimensional array.

- **Extensible Strongly-Typed Enumerations:** kim-api-v2 uses "extensible strongly-typed enumerations" as identifiers for quantities as opposed to kim-api-v1 which uses character arrays (strings) or "index" values. Thus, all "index" values and the associated routines (such as `KIM_API_get_index()`) have been eliminated.
- **Consistent and Descriptive Identifier Names:** The entire set of kim-api-v2 identifier names (namespace, module, object, subroutine, function, enumerations) have been reviewed and selected for clarity and consistency. As a result many of the identifier names from kim-api-v1 have changed in kim-api-v2. Here we provide a complete translation table. The C and Fortran bindings are obtained from the C++ binding by the following transformations (Note: some exceptions to these rules exist):
 - C++ → C: Replace "::" with "_". For example, `KIM::Model::GetNumberOfParameters()` becomes `KIM_Model_GetNumberOfParameters()`.
 - C++ → Fortran: Replace "::" with "_". Where camel-case is used in C++, convert to snake-case. Convert to all lower-case. For example, `KIM::Model::GetNumberOfParameters()` becomes `kim_model_get_number_of_parameters()`.

Routine Identifier Name translation table:

kim-api-v1	kim-api-v2 C++ Binding
<code>KIM_API_file_init()</code>	N/A
<code>KIM_API_string_init()</code>	<code>KIM::Model::Create()</code>
<code>KIM_API_get_version()</code>	<code>KIM::SEM_VER::GetSemVer()</code>
<code>KIM_API_get_version_major()</code>	N/A
<code>KIM_API_get_version_minor()</code>	N/A
<code>KIM_API_get_version_prerelease()</code>	N/A
<code>KIM_API_get_version_build_metadata()</code>	N/A
N/A	<code>KIM::SEM_VER::ParseSemVer()</code>
<code>KIM_API_version_newer()</code>	<code>KIM::SEM_VER::IsLessThan()</code>
<code>KIM_API_model_info()</code>	N/A
<code>KIM_API_allocate()</code>	N/A
<code>KIM_API_c_free()</code>	N/A
<code>KIM_API_free()</code>	<code>KIM::Model::Destroy()</code>
<code>KIM_API_print()</code>	<code>KIM::Model::String()</code> , <code>KIM::ModelCreate::String()</code> , <code>KIM::ModelComputeArgumentsCreate::String()</code> , <code>KIM::ModelComputeArgumentsDestroy::String()</code> , <code>KIM::ModelCompute::String()</code> , <code>KIM::ModelRefresh::String()</code> , <code>KIM::ModelDestroy::String()</code> , <code>KIM::ComputeArguments::String()</code>
<code>KIM_API_model_compute()</code>	<code>KIM::Model::Compute()</code>
<code>KIM_API_model_destroy()</code>	N/A
<code>KIM_API_get_model_index_shift()</code>	N/A
N/A	<code>KIM::ModelCreate::SetModelNumbering()</code> , <code>KIM::ModelDriverCreate::SetModelNumbering()</code>
<code>KIM_API_set_model_buffer()</code>	<code>KIM::ModelCreate::SetModelBufferPointer()</code> , <code>KIM::ModelDriverCreate::SetModelBufferPointer()</code> , <code>KIM::ModelComputeArgumentsCreate::SetModelBufferPointer()</code>
<code>KIM_API_set_sim_buffer()</code>	<code>KIM::Model::SetSimulatorBufferPointer()</code> , <code>KIM::ComputeArguments::SetSimulatorBufferPointer()</code>
<code>KIM_API_get_model_buffer()</code>	<code>KIM::ModelCompute::GetModelBufferPointer()</code> , <code>KIM::ModelDestroy::GetModelBufferPointer()</code> , <code>KIM::ModelRefresh::GetModelBufferPointer()</code> , <code>KIM::ModelComputeArguments::GetModelBufferPointer()</code> , <code>KIM::ModelComputeArgumentsDestroy::GetModelBufferPointer()</code>

kim-api-v1	kim-api-v2 C++ Binding
KIM_API_get_sim_buffer()	KIM::Model::GetSimulatorBufferPointer(), KIM::ComputeArguments::GetSimulatorBufferPointer()
KIM_API_is_half_neighbors()	N/A
KIM_API_set_data()	KIM::ComputeArguments::SetArgumentPointer()
N/A	KIM::ModelComputeArgumentsCreate::SetArgumentSupportStatus()
N/A	KIM::ComputeArguments::GetArgumentSupportStatus()
N/A	KIM::ModelComputeArgumentsCreate::SetCallbackSupportStatus()
N/A	KIM::ComputeArguments::GetCallbackSupportStatus()
KIM_API_set_method()	KIM::ComputeArguments::SetCallbackPointer()
KIM_API_get_data()	KIM::ModelComputeArguments::GetArgumentPointer()
KIM_API_get_method()	N/A
N/A	KIM::ModelComputeArguments::IsCallbackPresent()
N/A	KIM::ComputeArguments::AreAllRequiredArgumentsAndCallbacksPresent()
KIM_API_get_size()	N/A
KIM_API_get_rank()	N/A
KIM_API_get_shape()	N/A
KIM_API_set_shape()	N/A
KIM_API_set_compute()	N/A
KIM_API_get_compute()	N/A
N/A	KIM::ModelCreate::SetInfluenceDistancePointer(), KIM::ModelDriverCreate::SetInfluenceDistancePointer(), KIM::ModelRefresh::SetInfluenceDistancePointer()
N/A	KIM::Model::GetInfluenceDistance()
N/A	KIM::Model::GetNeighborListCutoffsPointer()
N/A	KIM::ModelCreate::SetNeighborListCutoffsPointer(), KIM::ModelDriverCreate::SetNeighborListCutoffsPointer(), KIM::ModelRefresh::SetNeighborListCutoffsPointer()
N/A	KIM::ModelCreate::SetRefreshPointer(), KIM::ModelDriverCreate::SetRefreshPointer()
N/A	KIM::ModelCreate::SetDestroyPointer(), KIM::ModelDriverCreate::SetDestroyPointer()
N/A	KIM::ModelCreate::SetComputeArgumentsCreatePointer(), KIM::ModelDriverCreate::SetComputeArgumentsCreatePointer()
N/A	KIM::ModelCreate::SetComputeArgumentsDestroyPointer(), KIM::ModelDriverCreate::SetComputeArgumentsDestroyPointer()
N/A	KIM::ModelCreate::SetComputePointer(), KIM::ModelDriverCreate::SetComputePointer()
KIM_API_get_index()	N/A
KIM_API_model_init()	N/A
KIM_API_model_reinit()	KIM::Model::ClearInfluenceDistanceAndCutoffsThenRefreshModel()
KIM_API_get_num_model_species()	N/A
KIM_API_get_model_species()	KIM::Model::GetSpeciesSupportAndCode()
KIM_API_get_num_sim_species()	N/A
KIM_API_get_sim_species()	N/A
N/A	KIM::ModelDriverCreate::GetNumberOfParameterFiles()
N/A	KIM::ModelDriverCreate::GetParameterFileName()
KIM_API_get_num_params()	KIM::Model::GetNumberOfParameters()
KIM_API_get_parameter()	KIM::Model::GetParameter()
N/A	KIM::Model::SetParameter()
N/A	KIM::Model::GetParameterDataTypeExtentAndDescription()

kim-api-v1	kim-api-v2 C++ Binding
N/A	KIM::ModelCreate::SetParameterPointer() , KIM::ModelDriverCreate::SetParameterPointer()
KIM_API_get_num_free_params()	N/A
KIM_API_get_free_parameter()	N/A
KIM_API_get_num_fixed_params()	N/A
KIM_API_get_fixed_parameter()	N/A
KIM_API_get_NBC_method()	N/A
KIM_API_get_species_code()	KIM::Model::GetSpeciesSupportAndCode()
KIM_API_set_species_code()	KIM::ModelCreate::SetSpeciesCode() , KIM::ModelDriverCreate::SetSpeciesCode()
KIM_API_get_model_kim_str_len()	N/A
KIM_API_get_model_kim_str()	N/A
KIM_API_get_neigh_mode()	N/A
KIM_API_get_neigh()	KIM::ModelComputeArguments::GetNeighborList()
KIM_API_process_dEdr()	KIM::ModelComputeArguments::ProcessDEDrTerm()
KIM_API_process_d2Edr2()	KIM::ModelComputeArguments::ProcessD2EDr2Term()
KIM_API_get_status_msg()	N/A
KIM_API_report_error()	KIM::Log::LogEntry() , KIM::ModelCreate::LogEntry() , KIM::ModelCompute::LogEntry() , KIM::ModelRefresh::LogEntry() , KIM::ModelDestroy::LogEntry() , KIM::ModelComputeArguments::LogEntry() , KIM::ModelComputeArgumentsCreate::LogEntry() , KIM::ModelComputeArgumentsDestroy::LogEntry()
N/A	KIM::Model::SetLogID() , KIM::ComputeArguments::SetLogID()
N/A	KIM::Model::PushLogVerbosity() , KIM::ComputeArguments::PushLogVerbosity()
N/A	KIM::Model::PopLogVerbosity() , KIM::ComputeArguments::PopLogVerbosity()
KIM_API_get_scale_conversion()	KIM::ModelCreate::ConvertUnit() , KIM::ModelDriverCreate::ConvertUnit()
KIM_API_get_unit_handling()	N/A
KIM_API_get_unit_length()	KIM::Model::GetUnits()
KIM_API_get_unit_energy()	KIM::Model::GetUnits()
KIM_API_get_unit_charge()	KIM::Model::GetUnits()
KIM_API_get_unit_temperature()	KIM::Model::GetUnits()
KIM_API_get_unit_time()	KIM::Model::GetUnits()
N/A	KIM::ModelCreate::SetUnits() , KIM::ModelDriverCreate::SetUnits()
KIM_API_convert_to_act_unit()	N/A
KIM_API_set_data_by_index()	N/A
KIM_API_set_method_by_index()	N/A
KIM_API_get_data_by_index()	N/A
KIM_API_get_method_by_index()	N/A
KIM_API_get_size_by_index()	N/A
KIM_API_get_rank_by_index()	N/A
KIM_API_get_shape_by_index()	N/A
KIM_API_set_compute_by_index()	N/A
KIM_API_get_compute_by_index()	N/A
KIM_API_getm_compute()	N/A
KIM_API_setm_compute()	N/A
KIM_API_getm_compute_by_index()	N/A
KIM_API_setm_compute_by_index()	N/A
KIM_API_getm_data()	N/A
KIM_API_getm_method()	N/A
KIM_API_setm_data()	N/A

kim-api-v1	kim-api-v2 C++ Binding
KIM_API_setm_method()	N/A
KIM_API_getm_data_by_index()	N/A
KIM_API_getm_method_by_index()	N/A
KIM_API_setm_data_by_index()	N/A
KIM_API_setm_method_by_index()	N/A
KIM_API_getm_index()	N/A

Extensible enumeration Identifier Name translation table:

kim-api-v1	kim-api-v2 C++ Binding
"numberOfParticles"	KIM::COMPUTE_ARGUMENT_NAME::numberOfParticles
"particleSpecies"	KIM::COMPUTE_ARGUMENT_NAME::particleSpeciesCodes
N/A	KIM::COMPUTE_ARGUMENT_NAME::particleContributing
"coordinates"	KIM::COMPUTE_ARGUMENT_NAME::coordinates
"energy"	KIM::COMPUTE_ARGUMENT_NAME::partialEnergy
"forces"	KIM::COMPUTE_ARGUMENT_NAME::partialForces
"particleEnergy"	KIM::COMPUTE_ARGUMENT_NAME::partialParticleEnergy
"virial"	KIM::COMPUTE_ARGUMENT_NAME::partialVirial
"particleVirial"	KIM::COMPUTE_ARGUMENT_NAME::partialParticleVirial
"cutoff"	N/A
"numberContributingParticles"	N/A
"numberOfSpecies"	N/A
"particleCharge"	N/A
"particleSize"	N/A
"neighObject"	N/A
"boxSideLengths"	N/A
"temperature"	N/A
"hessian"	N/A
"PARAM_FREE_cutoff"	N/A
"get_neigh"	KIM::COMPUTE_CALLBACK_NAME::GetNeighborList
"process_dEdr"	KIM::COMPUTE_CALLBACK_NAME::ProcessDEDrTerm
"process_d2Edr2"	KIM::COMPUTE_CALLBACK_NAME::ProcessD2EDr2Term
"ZeroBasedLists"	KIM::NUMBERING::zeroBased
"OneBasedLists"	KIM::NUMBERING::oneBased
"Neigh_IterAccess"	N/A
"Neigh_LocaAccess"	N/A
"Neigh_BothAccess"	N/A
"CLUSTER"	N/A
"NEIGH_PURE_H"	N/A
"NEIGH_PURE_F"	N/A
"NEIGH_RVEC_H"	N/A
"NEIGH_RVEC_F"	N/A
"MI_OPBC_H"	N/A
"MI_OPBC_F"	N/A
"electron"	KIM::SPECIES_NAME::electron
"H"	KIM::SPECIES_NAME::H
"He"	KIM::SPECIES_NAME::He
etc.	etc.

kim-api-v1	kim-api-v2 C++ Binding
"user20"	KIM::SPECIES_NAME::user20
"C"	KIM::CHARGE_UNIT::C
"e"	KIM::CHARGE_UNIT::e
"statC"	KIM::CHARGE_UNIT::statC
N/A	KIM::CHARGE_UNIT::unused
"amu_A2_per_ps2"	KIM::ENERGY_UNIT::amu_A2_per_ps2
"erg"	KIM::ENERGY_UNIT::erg
"eV"	KIM::ENERGY_UNIT::eV
"Hartree"	KIM::ENERGY_UNIT::Hartree
"J"	KIM::ENERGY_UNIT::J
"kcal_mol"	KIM::ENERGY_UNIT::kcal_mol
N/A	KIM::ENERGY_UNIT::unused
"A"	KIM::LENGTH_UNIT::A
"Bohr"	KIM::LENGTH_UNIT::Bohr
"cm"	KIM::LENGTH_UNIT::cm
"m"	KIM::LENGTH_UNIT::m
"nm"	KIM::LENGTH_UNIT::nm
N/A	KIM::LENGTH_UNIT::unused
"K"	KIM::TEMPERATURE_UNIT::K
N/A	KIM::TEMPERATURE_UNIT::unused
"fs"	KIM::TIME_UNIT::fs
"ps"	KIM::TIME_UNIT::ps
"ns"	KIM::TIME_UNIT::ns
"s"	KIM::TIME_UNIT::s
N/A	KIM::TIME_UNIT::unused

Each of the extensible enumerations in kim-api-v2 has an interface for discovering all of the members of the enumeration. This is implemented using two functions. One provides the number of members in the enumeration, and the other provides a copy of the *i*-th enumeration member. (The ordering is undefined, but guaranteed to be stable during any single run-time program execution using the KIM API.) For example, the [KIM::ChargeUnit](#) enumeration has the [KIM::CHARGE_UNIT::GetNumberOfChargeUnits\(\)](#) and the [KIM::CHARGE_UNIT::GetChargeUnit\(\)](#) functions.

In addition, the [KIM::ComputeArgumentName](#) enumeration also has the [KIM::COMPUTE_ARGUMENT_NAME::GetComputeArgumentName\(\)](#) function.

Next Section: [Guide for porting content from KIM API v1 to v2.](#)

Chapter 6

Guide for porting content from KIM API v1 to v2

Previous Section: [Summary of Differences Between kim-api-v1 and kim-api-v2](#).

Version 2 of the KIM API constitutes a major rewrite with a simplified interface, best practice design, and new capabilities. For more details, see the [Features of the KIM API package](#) page.

Version 2 is *NOT* backward compatible and therefore requires significant modifications to existing code (Model Drivers, Models, Test Drivers, and Tests) to work. The purpose of this document is to provide step-by-step instructions on how to transition content from version 1 to 2.

A complete translation table of v1 and v2 identifier names is available on the [Summary of Differences Between kim-api-v1 and kim-api-v2](#) page.

This page includes instructions for [Porting Models and Model Drivers](#) and for [Porting Simulators](#).

6.1 Porting Models and Model Drivers

Model drivers and stand-alone models compatible with version 1 of the KIM API will need to be modified to conform to version 2. A step-by-step process for doing so is described below. (In what follows the generic term "model" will be used to refer to both Model Drivers and Models. The only difference between the two cases is that Model Drivers have these two additional functions: [KIM::ModelDriverCreate::GetNumberOfParameterFiles\(\)](#) and [KIM::ModelDriverCreate::GetParameterFileName\(\)](#).)

6.1.1 Step 0

- Setup your machine to perform the conversion. We suggest that you create a local installation of kim-api-v1 and kim-api-v2 in your home directory so that you can work with everything simultaneously.

```
$ cd ${HOME}
$ mkdir kim-api-porting
$ cd kim-api-porting

$ wget https://s3.openkim.org/kim-api/kim-api-v1.9.5.txz
$ tar Jxf kim-api-v1.9.5.txz
$ rm kim-api-v1.9.5.txz
$ cd kim-api-v1.9.5
$ ./configure --prefix=${HOME}/kim-api-porting/kim-api-installed
$ make
$ make install
$ cd ..

$ wget https://s3.openkim.org/kim-api/kim-api-v2.0.0-beta.0.txz
$ tar Jxf kim-api-v2.0.0-beta.0.txz
$ rm kim-api-v2.0.0-beta.0.txz
$ cd kim-api-v2.0.0-beta.0
$ ./configure --prefix=${HOME}/kim-api-porting/kim-api-installed
$ make
$ make install
$ cd ..
```

- Now, "activate" (update the PATH variable and set up tab-completion) both versions of the KIM API within your bash shell

```
$ source ${HOME}/kim-api-porting/kim-api-installed/bin/kim-api-v1-activate
$ source ${HOME}/kim-api-porting/kim-api-installed/bin/kim-api-v2-activate
```

Now, you can use the `kim-api-v#-build-config` and `kim-api-v#-collections-management` utilities as you perform your work.

When you are done working on this activity, you can deactivate the KIM API with

```
$ source kim-api-v1-deactivate
$ source kim-api-v2-deactivate
```

Or, simply exit the shell.

- Next, copy the example codes associated with these instructions

```
$ cp -r ./kim-api-v2.0.0-beta-0/docs/porting-content-from-v1-to-v2-examples v1-v2-porting
```

The [porting-content-from-v1-to-v2-examples](#) codes include two models (one in C and one in Fortran) and three simulators (one each in C, C++, and Fortran). Links to these codes are provided for each step in the instructions below (where changes occur). These can be compared to see a specific example of the code changes described below.

To start, the kim-api-v1 compatible versions of the models can be installed

```
$ kim-api-v1-collections-management install system ./v1-v2-porting/models/step0/ex_model_Ar_P_MLJ_F03
$ kim-api-v1-collections-management install system ./v1-v2-porting/models/step0/ex_model_Ar_P_Morse_07C
```

It will be useful to know the output of these models generated by the example simulator. This can be generated as follows:

```
$ cp -r v1-v2-porting/simulators/step0/ex_test_Ar_fcc_cluster ./v1-ex_test_Ar_fcc_cluster
$ cd v1-ex_test_Ar_fcc_cluster
$ make
```

```
$ printf ex_model_Ar_P_MLJ_F03 | ./ex_test_Ar_fcc_cluster
```

```
Please enter valid KIM Model name:
This is Test : ex_test_Ar_fcc_cluster
```

```
-----
Results for KIM Model : ex_model_Ar_P_MLJ_F03
      Energy,      Force Norm,      Lattice Spacing
2.6568305947e+01,  1.2671877978e+01,  4.2080000000e+00
1.5269225751e+01,  7.9639127468e+00,  4.3395000000e+00
8.1940651929e+00,  4.9863838571e+00,  4.4710000000e+00
3.7947024307e+00,  3.0924620572e+00,  4.6025000000e+00
1.0980474405e+00,  1.8835116189e+00,  4.7340000000e+00
-5.1288233270e-01,  1.1111343811e+00,  4.8655000000e+00
-1.4321763817e+00,  6.1892128072e-01,  4.9970000000e+00
-1.9129769394e+00,  3.0756389059e-01,  5.1285000000e+00
-2.1185529279e+00,  1.1421905922e-01,  5.2600000000e+00
-2.1545585638e+00,  2.4987808283e-02,  5.3915000000e+00
-2.0893135757e+00,  8.1104969450e-02,  5.5230000000e+00
-1.9668026189e+00,  1.1844534144e-01,  5.6545000000e+00
-1.8151243558e+00,  1.3646818860e-01,  5.7860000000e+00
-1.6520140667e+00,  1.4203290937e-01,  5.9175000000e+00
-1.4884681605e+00,  1.3991074278e-01,  6.0490000000e+00
-1.3310358744e+00,  1.3327798308e-01,  6.1805000000e+00
```

```
$ printf ex_model_Ar_P_Morse_07C | ./ex_test_Ar_fcc_cluster
```

```
Please enter valid KIM Model name:
This is Test : ex_test_Ar_fcc_cluster
```

```
-----
Results for KIM Model : ex_model_Ar_P_Morse_07C
      Energy,      Force Norm,      Lattice Spacing
1.4703219623e+01,  6.9678657557e+00,  4.2080000000e+00
8.2453550705e+00,  4.8650873812e+00,  4.3395000000e+00
3.7883556879e+00,  3.3409407134e+00,  4.4710000000e+00
7.7810749699e-01,  2.2399352517e+00,  4.6025000000e+00
-1.1944148939e+00,  1.4518130136e+00,  4.7340000000e+00
-2.4291941022e+00,  8.9239060716e-01,  4.8655000000e+00
-3.1445433206e+00,  5.0063786968e-01,  4.9970000000e+00
```



```

-3.4996095359e+00,    2.3199479279e-01,    5.1285000000e+00
-3.6112724693e+00,    6.3687021777e-02,    5.2600000000e+00
-3.5604853404e+00,    8.7536239707e-02,    5.3915000000e+00
-3.4059878193e+00,    1.5700051389e-01,    5.5230000000e+00
-3.1896247548e+00,    1.9909723852e-01,    5.6545000000e+00
-2.9407853637e+00,    2.1928061006e-01,    5.7860000000e+00
-2.6800661721e+00,    2.2574027063e-01,    5.9175000000e+00
-2.4197463013e+00,    2.2234487833e-01,    6.0490000000e+00
-2.1685167432e+00,    2.1265537489e-01,    6.1805000000e+00

```

\$ cd ..

- You can see the corresponding example codes by following these links: [Step0~Fortan~Model](#), [Step0~C~Model](#), [Step0~C~Simulator](#).

6.1.2 Step 1

- Working with v1 of the model, strip out all supported neighbor list and boundary conditions (NBCs) *except* for NEIGH_PURE_F, which is the only one supported by v2. If the model does not support this NBC, add it.
- Next, strip out all supported neighbor list methods except for Neigh_LocaAccess. If the model does not support this method, add it.
- In the Makefile, append "_step1" to the model name. This will allow you to install the updated model alongside the original version and check that they give the same output.
- When ready, install the new model. For the example codes, do

```

$ kim-api-v1-collections-management install system ./v1-v2-porting/models/step1/ex_model_Ar_P_MLJ_F03
$ kim-api-v1-collections-management install system ./v1-v2-porting/models/step1/ex_model_Ar_P_Morse_07C

```

If you make further changes to the code, you can reinstall (remove and install) the model with commands such as

```

$ kim-api-v1-collections-management reinstall ./v1-v2-porting/models/step1/ex_model_Ar_P_MLJ_F03
$ kim-api-v1-collections-management reinstall ./v1-v2-porting/models/step1/ex_model_Ar_P_Morse_07C

```

(The above commands will fail if the model was not previously *successfully* installed. Alternatively, you can use the commands

```

$ kim-api-v1-collections-management install --force system
./v1-v2-porting/models/step1/ex_model_Ar_P_MLJ_F03
$ kim-api-v1-collections-management install --force system
./v1-v2-porting/models/step1/ex_model_Ar_P_Morse_07C

```

These commands will work even if the model is not currently installed.)

You can see the installed models using the kim-api-v1-collections-managment utility:

```

$ kim-api-v1-collections-management list

Knowledgebase of Interatomic Models (KIM) --- Model Collections Listing
=====

kim-api library:
  /.../kim-api-porting/lib/kim-api-v1/libkim-api-v1.9.5.GCC.linux.64bit.dynamic-load.so
.
.
.

System Collection
-----
Drivers: /.../kim-api-porting/lib/kim-api-v1/model_drivers
--empty--

Models: /.../kim-api-porting/lib/kim-api-v1/models
  ex_model_Ar_P_MLJ_F03
  ex_model_Ar_P_MLJ_F03_step1
  ex_model_Ar_P_Morse_07C
  ex_model_Ar_P_Morse_07C_step1

$

```

- Execute the model using the example test `ex_test_Ar_fcc_cluster` to generate output that can be compared with the original model. For example:

```
$ cd v1-ex_test_Ar_fcc_cluster
$ printf ex_model_Ar_P_MLJ_F03_step1 | ./ex_test_Ar_fcc_cluster

Please enter valid KIM Model name:
This is Test : ex_test_Ar_fcc_cluster
-----
Results for KIM Model : ex_model_Ar_P_MLJ_F03_step1
      Energy,      Force Norm,      Lattice Spacing
2.6568305947e+01, 1.2671877978e+01, 4.2080000000e+00
1.5269225751e+01, 7.9639127468e+00, 4.3395000000e+00
8.1940651929e+00, 4.9863838571e+00, 4.4710000000e+00
3.7947024307e+00, 3.0924620572e+00, 4.6025000000e+00
1.0980474405e+00, 1.8835116189e+00, 4.7340000000e+00
-5.1288233270e-01, 1.1111343811e+00, 4.8655000000e+00
-1.4321763817e+00, 6.1892128072e-01, 4.9970000000e+00
-1.9129769394e+00, 3.0756389059e-01, 5.1285000000e+00
-2.1185529279e+00, 1.1421905922e-01, 5.2600000000e+00
-2.1545585638e+00, 2.4987808283e-02, 5.3915000000e+00
-2.0893135757e+00, 8.1104969450e-02, 5.5230000000e+00
-1.9668026189e+00, 1.1844534144e-01, 5.6545000000e+00
-1.8151243558e+00, 1.3646818860e-01, 5.7860000000e+00
-1.6520140667e+00, 1.4203290937e-01, 5.9175000000e+00
-1.4884681605e+00, 1.3991074278e-01, 6.0490000000e+00
-1.3310358744e+00, 1.3327798308e-01, 6.1805000000e+00

$ cd ..
```

- You can see the corresponding example codes by following these links: [Step1~Fortran~Model](#), [Step1~C~Model](#).

6.1.3 Step 2

Become familiar with v2 by reading the [documentation](#), and reviewing the example Model Drivers and/or Models. (The examples are under "Files" in the documentation. The `ex_model_Ar_P_MLJ_F03.F03` and `ex_model_Ar_P_Morse_07C.c` examples are the same codes found in the [Guide for porting content from KIM API v1 to v2](#) examples used in these instructions.)

As you review the material, if you have any questions, post them to the OpenKIM Google Group forum by emailing openkim@googlegroups.com or by visiting the [group](#). This will help others with similar questions. Continue using the forum for support in the next steps.

6.1.4 Step 3

You are now ready to make the modifications to the code needed for it to be compatible with v2.

Start with the `ModelDriverCreate` or `ModelCreate` routine. Since KIM descriptor files no longer exist in v2, the information encoded in these files must be incorporated into this routine (and the `ModelCompute`↔`ArgumentsCreate` routine described in the next step) to make it available to the API.

- Update the Makefile to use new pre/post-amble and to provide kim-api-v2 variables. For Paramaterized Models, remove the `SPECIES_###_NAME` variables and convert `PARAM_FILE_###_NAME` variables to `PARAM_FILE_#_NAME` (numbering should start from 1 and be in sequence without any gaps). Also, update the model name to end in "`_step3`" so that it can be installed alongside the previous versions.
- Update source files to use new v2 header file (module) as opposed to old v1 versions.
- Comment out the v1 versions of the model's `compute`, `reinit`, and `destroy` functions.
- Update the v1 `model_init` routine to a v2 `ModelDriverCreate` of `ModelCreate` routine:
- Change the prototype to match the v2 requirements (see examples).

- Translate the model's v1 KIM descriptor file into appropriate code within the new routine:
 - First, a list of things in the descriptor file that will be simply discarded:
 - * The `KIM_API_Version` value
 - * `Neigh_LocaAccess`
 - * `NEIGH_PURE_F`
 - Set the base units to be used by the model. If the v1 model has flexible-units, simply make a call to `KIM::ModelCreate::SetUnits()` and pass in the "requested" unit values (Although, be careful to convert any "unused" values to appropriate unit values as necessary). Update the model's parameters to the requested units with call(s) to `KIM::ModelCreate::ConvertUnit()`. If the v1 model has fixed-units, simply make a call to `KIM::ModelCreate::SetUnits()` with the desired values. Make sure to specify the new "unused" value where appropriate.
 - Register the model's supported species and their codes with call(s) to `KIM::ModelCreate::SetSpeciesCode()`. (By default no species are supported.)
 - Set the model's numbering with a call to `KIM::ModelCreate::SetModelNumbering()`.
 - Register the model's `ComputeArgumentsCreate` function pointer with a call to `KIM::ModelCreate::SetComputeArgumentsC` (Use 2 for now (for Fortran, use `c_funloc(kim_model_compute_string)`) as a placeholder. We'll implement this function and update this call in a later step.)
 - Register the model's `ComputeArgumentsDestroy` function pointer with a call to `KIM::ModelCreate::SetComputeArgumentsD` (Use 2 for now (for Fortran, use `c_funloc(kim_model_compute_string)`) as a placeholder. We'll implement this function and update this call in a later step.)
 - Register the model's `Compute` function pointer with a call to `KIM::ModelCreate::SetComputePointer()`. (Use 2 for now (for Fortran, use `c_funloc(kim_model_compute_string)`) as a placeholder. We'll implement this function and update this call in a later step.)
 - Register the model's `Destroy` function pointer with a call to `KIM::ModelCreate::SetDestroyPointer()`. (Use 2 for now (for Fortran, use `c_funloc(kim_model_compute_string)`) as a placeholder. We'll implement this function and update this call in a later step.)
 - Register the model's `Refresh` function pointer with a call to `KIM::ModelCreate::SetRefreshPointer()`. (Use 2 for now (for Fortran, use `c_funloc(kim_model_compute_string)`) as a placeholder. We'll implement this function and update this call in a later step.)
 - The last set of items in the v1 KIM descriptor file is the model's parameters. These will be registered with call(s) to `KIM::ModelCreate::SetParameterPointer()`. However, before doing this, you will need to setup and register the model's buffer memory space (See below items).
 - Update/Create the model buffer structure that will contain the model's influence distance value, the model's neighbor list cutoff value(s), and the model's parameters (if any). In the `ModelCreate` routine, allocate memory for this structure and register the buffer with a call to `KIM::ModelCreate::SetModelBufferPointer()`. Next, set the values to be stored in the buffer (remember to perform unit conversion, if necessary, using call(s) to `KIM::ModelCreate::ConvertUnit()`).
 - Register the model's influence distance pointer with a call to `KIM::ModelCreate::SetInfluenceDistancePointer()`.
 - Register the model's neighbor list cutoff values pointer with a call to `KIM::ModelCreate::SetNeighborListCutoffsPointer()`.
 - Register the parameters with call(s) to `KIM::ModelCreate::SetParameterPointer()`, if necessary.
- Make sure to update all error codes from the v1 codes to the v2 codes. v2 has just two error codes `error = 1` (true, an error has occurred) and `error = 0` (false, no error has occurred).
- At the end of the `ModelCreate` routine, just before a successful return, print out the content of the model object to verify the settings. See the examples provided below for the necessary code.
- Build the model and use a simulator to execute it. You will receive a segmentation fault due to the missing compute routine (etc.), but you should also see a print out of all the data registered by the `ModelCreate` routine. Make updates to the code until this data is all correct.

```
$ kim-api-v2-collections-management install system ./v1-v2-porting/models/step3/ex_model_Ar_P_MLJ_F03
$ kim-api-v2-collections-management install system ./v1-v2-porting/models/step3/ex_model_Ar_P_Morse_07C
```

Note that the v2 collections management utility is now used. If build errors are reported for the model being updated, correct the reported compiler errors and try again. To test the model, a v2 version of the simulator is needed:

```
$ cp -r v1-v2-porting/simulators/step5/ex_test_Ar_fcc_cluster v2-ex_test_Ar_fcc_cluster
$ cd v2-ex_test_Ar_fcc_cluster
$ make
```

Now the new ModelCreate routine can be tested to verify it is performing correctly. For example, the ex_model_Ar_P_Morse_07C_step3 produces

```
$ printf ex_model_Ar_P_Morse_07C_step3 | ./ex_test_Ar_fcc_cluster

Please enter valid KIM Model name:
=====

Model object
-----

Model Name : ex_model_Ar_P_Morse_07C_step3
Log ID : 0x79624090

Model Supplied Functions :
  Function Name          Language  Pointer (1-set / 0-unset)
  -----
  Refresh                c          1
  Destroy                c          1
  ComputeArgumentsCreate c          1
  ComputeArgumentsDestroy c         1
  Compute                c          1

Numbering : zeroBased

Units :
  Length Unit      : A
  Energy Unit      : eV
  Charge Unit      : unused
  Temperature Unit : unused
  Time Unit        : unused

Influence Distance : 8.1500000000e+00

Number Of Neighbor List Cutoffs : 1
Neighbor List Cutoffs :
  0 : 8.1500000000e+00

Supported Species :
  Species  Code
  -----

  Ar       1

Number Of Parameters : 0
  index  Data Type Extent  Pointer  Description
  -----

Buffers
  Buffer      Pointer
  -----

  Model      0x7a81fb00
  Simulator   0

=====

Segmentation fault: 11

$ cd ..
```

- You can see the corresponding example codes by following these links: [Step3~Fortran~Model](#), [Step3~C~Model](#). Compare these with the versions from [Step 1](#) to see the changes associated with this step.

6.1.5 Step 4

Next you will implement the ModelComputeArgumentsCreate and ModelComputeArguments↔Destroy routines. The create routine registers the model's supported compute arguments and compute

callbacks. The destroy routine allows the model to clean up the memory (if any) it stored at the compute-arguments object's model buffer pointer.

- Modify the Makefile to update the model name to end in "_step4".
- Create the `ModelComputeArgumentsCreate` routine to conform to the v2 specifications.
 - Register the model's compute argument support status with call(s) to `KIM::ModelComputeArgumentsCreate::SetArgument` (By default all arguments are either `requiredByAPI` or `notSupported` as defined on the [Implementation](#) page.)
 - Register the model's compute callback support status with call(s) to `KIM::ModelComputeArgumentsCreate::SetCallbackSu` (By default all callbacks are either `requiredByAPI` or `notSupported` as defined on the [Implementation](#) page.)
 - At the end of the `ModelComputeArgumentsCreate` routine, just before a successful return, print out the content of the compute arguments object to verify the settings. See the examples provided below for the necessary code.
- Create the `ModelComputeArgumentsDestroy` routine to conform to the v1 specifications. In many cases this routine will be empty. See the examples provided below for the necessary code.
- Finally, go back to the `ModelCreate` routine:
 - Update the call to `KIM::ModelCreate::SetComputeArgumentsCreatePointer()` to reference the new `ModelComputeArgumentsCreate` routine.
 - Update the call to `KIM::ModelCreate::SetComputeArgumentsDestroyPointer()` to reference the new `ModelComputeArgumentsDestroy` routine.
- Build the model and use a simulator to execute it. You will receive a segmentation fault due to the missing compute routine (etc.), but you should also see a print out of all the data registered by the `ModelComputeArgumentsCreate` routine. Make updates to the code until this data is all correct.

```
$ kim-api-v2-collections-management install --force system
./v1-v2-porting/models/step4/ex_model_Ar_P_MLJ_F03
$ kim-api-v2-collections-management install --force system
./v1-v2-porting/models/step4/ex_model_Ar_P_Morse_07C
```

Now the new `ModelComputeArgumentsCreate` routine can be tested to verify it is performing correctly. For example, the `ex_model_Ar_P_Morse_07C_step4` produces

```
$ cd v2-ex_test_Ar_fcc_cluster
$ printf ex_model_Ar_P_Morse_07C_step4 | ./ex_test_Ar_fcc_cluster

Please enter valid KIM Model name:
=====

Model object
-----

Model Name : ex_model_Ar_P_Morse_07C_step4
Log ID : 0x7b6724a0

Model Supplied Functions :
Function Name      Language  Pointer (1-set / 0-unset)
-----
Refresh            c          1
Destroy            c          1
ComputeArgumentsCreate c          1
ComputeArgumentsDestroy c          1
Compute            c          1

Numbering : zeroBased

Units :
Length Unit      : A
Energy Unit      : eV
Charge Unit      : unused
Temperature Unit : unused
Time Unit        : unused
```

```

Influence Distance : 8.1500000000e+00

Number Of Neighbor List Cutoffs : 1
Neighbor List Cutoffs :
  0 : 8.1500000000e+00

Supported Species :
Species   Code
-----
Ar        1

Number Of Parameters : 0
index    Data Type Extent   Pointer   Description
-----

Buffers
Buffer      Pointer
-----

Model       0x7c86df00
Simulator   0

=====

ComputeArguments object
-----

Model Name : ex_model_Ar_P_Morse_07C_step4
Log ID : 0x7b6724a0_0x7b76e590

Compute Arguments :
Compute Argument Name   SupportStatus   Pointer
-----
numberOfParticles       requiredByAPI   0
particleSpeciesCodes    requiredByAPI   0
particleContributing     requiredByAPI   0
coordinates              requiredByAPI   0
partialEnergy            optional        0
partialForces             optional        0
partialParticleEnergy     optional        0
partialVirial            notSupported    N/A
partialParticleVirial     notSupported    N/A

Compute Callback Functions :
Compute Callback Name   SupportStatus   Language   Data Pointer   Pointer (1-set / 0-unset)
-----
GetNeighborList         requiredByAPI   cpp        0              0
ProcessDEDrTerm         optional       cpp        0              0
ProcessD2EDr2Term       optional       cpp        0              0

Buffers
Buffer      Pointer
-----

Model       0
Simulator   0

=====

This is Test : ex_test_Ar_fcc_cluster
-----
Results for KIM Model : ex_model_Ar_P_Morse_07C_step4
Energy, Force Norm, Lattice Spacing
Segmentation fault: 11

$ cd ..

```

- You can see the corresponding example codes by following these links: [Step4~Fortran~Model](#), [Step4~C~Model](#). Compare these with the versions from [Step 3](#) to see the changes associated with this step.

6.1.6 Step 5

- Modify/create the `ModelRefresh` and `ModelDestroy` routines to conform to v2.

- The `ModelRefresh` routine is used to allow the model to refresh the values of private data in its model buffer based on changes to the published parameter values in the model buffer which have been changed by the simulator. Additionally, at the end of the `ModelRefresh` routine, the model must re-register pointers to its influence distance and cutoffs data (since, generally, these values will change due to the changes made to the published parameters by the simulator).
 - * Create the `ModelRefresh` routine (or convert the v1 `reinit` function)
 - * Get the model buffer pointer with a call to `KIM::ModelRefresh::GetModelBufferPointer()`.
 - * Update any private data and, if necessary, the influence distance and cutoffs.
 - * Register the influence distance with a call to `KIM::ModelRefresh::SetInfluenceDistancePointer()`.
 - * Register the cutoff values pointer with a call to `KIM::ModelRefresh::SetNeighborListCutoffsPointer()`.
- The `ModelDestroy` routine is used to clean up the model buffer memory when the model is being destroyed.
 - * Create the `ModelDestroy` routine (or convert the v1 `destroy` function)
 - * Get the model buffer pointer with a call to `KIM::ModelDestroy::GetModelBufferPointer()`.
 - * Deallocate memory associated with the buffer.
- Go back to the `ModelCreate` routine:
 - Update the call to `KIM::ModelCreate::SetRefreshPointer()` to reference the new `ModelRefresh` routine.
 - Update the call to `KIM::ModelCreate::SetDestroyPointer()` to reference the new `ModelDestroy` routine.
- Finally, remove the code that prints the model object and the code that prints the compute arguments object.
- Build the model to ensure no compiler errors are generated. It is probably not worth executing a simulator with this version as it will simply give a segmentation fault due to the `ModelCompute` routine still being missing.

```
$ kim-api-v2-collections-management install --force system
./v1-v2-porting/models/step5/ex_model_Ar_P_MLJ_F03
$ kim-api-v2-collections-management install --force system
./v1-v2-porting/models/step5/ex_model_Ar_P_Morse_07C
```

- You can see the corresponding example codes by following these links: [Step5~Fortran~Model](#), [Step5~C~Model](#). Compare these with the versions from [Step 4](#) to see the changes associated with this step.

6.1.7 Step 6

- Modify the Makefile to have the final v2 model name. (This may be the same as the v1 model name since the v1 model cannot be used with kim-api-v2.)
- Update the `ModelCompute` routine to get everything working.
 - Update the `ModelCompute` routine prototype (for Fortran, this also includes changing from a `FUNCTION` to a `SUBROUTINE`).
 - For Fortran codes, remove `type(c_ptr)` variables, they will not be needed in the v2 version of the compute routine. This also means that the `C_F_POINTER` intrinsic function should not be needed.
 - Make changes to the code to use one of the `LOG_*` macros or the `KIM::ModelCompute::LogEntry()` routine as opposed to the v1 `KIM_API_report_error()` routine.

- Make changes to the code that determines what computations have been requested and unpacking the arguments. In v1 this is associated with calls to `KIM_API_get(m)_compute()`, and `KIM_API_get(m)_data()`. In v2, these should be replaced with calls to `KIM::ModelComputeArguments::IsCallbackPresent()`, and `KIM::ModelComputeArguments::GetArgumentPointer()` (in C there are `KIM_ModelComputeArguments_GetArgumentPointerInteger()` and `KIM_ModelComputeArguments_GetArgumentPointerDouble()`, and C++ and Fortran use function overloading and have only `KIM::ModelComputeArguments::GetArgumentPointer()`). The `KIM::COMPUTE_CALLBACK_NAME::GetNeighborList()` callback is `requiredByAPI` so it will always be present, and it is not necessary to check explicitly with a call to `KIM::ModelComputeArguments::IsCallbackPresent()`. In v2, an argument is present if its pointer value is not `NULL` (zero). Thus, once the pointer values have been unpacked with a call to `KIM::ModelComputeArguments::GetArgumentPointer()` a comparison of the pointer to `NULL` (for Fortran, use the intrinsic function `ASSOCIATED`) will determine if the argument is present or not.
- Make changes to the code so that it gets the neighbor list cutoff, not from the cutoff argument as in v1, but from the value(s) stored in the model buffer. This will require a call to the `KIM::ModelCompute::GetModelBufferPointer()` routine.
- Make changes to the code to use the `particleContributing` argument values to identify contributing or non-contributing particles, as opposed to the approach in v1 where the number of neighbors for a particle is used.
- Make changes to the code to use the v2 `KIM::ModelComputeArguments::GetNeighborList()` routine as opposed to the v1 `KIM_API_get_neigh` routine.
- Make changes to the code to use the v2 `KIM::ModelComputeArguments::ProcessDEDrTerm()` and `KIM::ModelComputeArguments::ProcessD2EDr2Term()` routines as opposed to the v1 `KIM_API_process_dEdr()` and `KIM_API_process_d2EDr2()` routines, if necessary.
- Make sure to update all error codes from the v1 codes to the v2 codes. v2 has just two error codes `error = 1` (true, an error has occurred) and `error = 0` (false, no error has occurred).
- Finally, go back to the `ModelCreate` routine:
 - Update the call to `KIM::ModelCreate::SetComputePointer()` to reference the new `ModelCompute` routine.
- Build and install the final updated model.

```
$ kim-api-v2-collections-management install --force system
./v1-v2-porting/models/step6/ex_model_Ar_P_MLJ_F03
$ kim-api-v2-collections-management install --force system
./v1-v2-porting/models/step6/ex_model_Ar_P_Morse_07C
```

If build errors are reported for the model being updated, correct the reported compiler errors and try again.

- You can see the corresponding example codes by following these links: [Step6~Fortran~Model](#), [Step6~C~Model](#). Compare these with the versions from [Step 5](#) to see the changes associated with this step.

6.1.8 Step 7

Now the new model can be used with the v2 simulator and the output compared with the original output from [Step 1](#).

```
$ cd v2-ex_test_Ar_fcc_cluster
$ printf ex_model_Ar_P_MLJ_F03 | ./ex_test_Ar_fcc_cluster
```

```
Please enter valid KIM Model name:
This is Test : ex_test_Ar_fcc_cluster
```

```
-----
Results for KIM Model : ex_model_Ar_P_MLJ_F03
      Energy,          Force Norm,      Lattice Spacing
2.6568305947e+01,    1.2671877978e+01,    4.2080000000e+00
1.5269225751e+01,    7.9639127468e+00,    4.3395000000e+00
8.1940651929e+00,    4.9863838571e+00,    4.4710000000e+00
3.7947024307e+00,    3.0924620572e+00,    4.6025000000e+00
1.0980474405e+00,    1.8835116189e+00,    4.7340000000e+00
```



```

-5.1288233270e-01,    1.1111343811e+00,    4.8655000000e+00
-1.4321763817e+00,    6.1892128072e-01,    4.9970000000e+00
-1.9129769394e+00,    3.0756389059e-01,    5.1285000000e+00
-2.1185529279e+00,    1.1421905922e-01,    5.2600000000e+00
-2.1545585638e+00,    2.4987808283e-02,    5.3915000000e+00
-2.0893135757e+00,    8.1104969450e-02,    5.5230000000e+00
-1.9668026189e+00,    1.1844534144e-01,    5.6545000000e+00
-1.8151243558e+00,    1.3646818860e-01,    5.7860000000e+00
-1.6520140667e+00,    1.4203290937e-01,    5.9175000000e+00
-1.4884681605e+00,    1.3991074278e-01,    6.0490000000e+00
-1.3310358744e+00,    1.3327798308e-01,    6.1805000000e+00

$ printf ex_model_Ar_P_Morse_07C | ./ex_test_Ar_fcc_cluster

Please enter valid KIM Model name:
This is Test : ex_test_Ar_fcc_cluster
-----
Results for KIM Model : ex_model_Ar_P_Morse_07C
      Energy,           Force Norm,      Lattice Spacing
1.4703219623e+01,    6.9678657557e+00,    4.2080000000e+00
8.2453550705e+00,    4.8650873812e+00,    4.3395000000e+00
3.7883556879e+00,    3.3409407134e+00,    4.4710000000e+00
7.7810749699e-01,    2.2399352517e+00,    4.6025000000e+00
-1.1944148939e+00,    1.4518130136e+00,    4.7340000000e+00
-2.4291941022e+00,    8.9239060716e-01,    4.8655000000e+00
-3.1445433206e+00,    5.0063786968e-01,    4.9970000000e+00
-3.4996095359e+00,    2.3199479279e-01,    5.1285000000e+00
-3.6112724693e+00,    6.3687021777e-02,    5.2600000000e+00
-3.5604853404e+00,    8.7536239707e-02,    5.3915000000e+00
-3.4059878193e+00,    1.5700051389e-01,    5.5230000000e+00
-3.1896247548e+00,    1.9909723852e-01,    5.6545000000e+00
-2.9407853637e+00,    2.1928061006e-01,    5.7860000000e+00
-2.6800661721e+00,    2.2574027063e-01,    5.9175000000e+00
-2.4197463013e+00,    2.2234487833e-01,    6.0490000000e+00
-2.1685167432e+00,    2.1265537489e-01,    6.1805000000e+00

$ cd ..

```

6.2 Porting Simulators

6.2.1 Step 0

- See [Porting Models: Step 0](#), above.
- You can see the corresponding example codes by following these links: [Step0~C~Simulator](#), [Step0~C++~Simulator](#), and [Step0~Fortran~Simulator](#).

6.2.2 Step 1

- Working with v1 of the simulator, strip out all supported neighbor list and boundary conditions (NBCs) *except* for NEIGH_PURE_F, which is the only one supported by v2. If the simulator does not support this NBC, add it.
- Next, strip out all supported neighbor list methods except for Neigh_LocaAccess. If the simulator does not support this method, add it.
- When ready, build the simulator and test it with the v1 models you installed in [Porting Models: Step 0](#).

```

$ cp -r ./v1-v2-porting/simulators/step1/ex_test_Ar_fcc_cluster v1-ex_test_Ar_fcc_cluster-step1
$ cd v1-ex_test_Ar_fcc_cluster-step1
$ make

$ printf ex_model_Ar_P_MLJ_F03 | ./ex_test_Ar_fcc_cluster

Please enter valid KIM Model name:
This is Test : ex_test_Ar_fcc_cluster
-----
Results for KIM Model : ex_model_Ar_P_MLJ_F03
      Energy,           Force Norm,      Lattice Spacing
2.6568305947e+01,    1.2671877978e+01,    4.2080000000e+00

```

```

1.5269225751e+01, 7.9639127468e+00, 4.3395000000e+00
8.1940651929e+00, 4.9863838571e+00, 4.4710000000e+00
3.7947024307e+00, 3.0924620572e+00, 4.6025000000e+00
1.0980474405e+00, 1.8835116189e+00, 4.7340000000e+00
-5.1288233270e-01, 1.1111343811e+00, 4.8655000000e+00
-1.4321763817e+00, 6.1892128072e-01, 4.9970000000e+00
-1.9129769394e+00, 3.0756389059e-01, 5.1285000000e+00
-2.1185529279e+00, 1.1421905922e-01, 5.2600000000e+00
-2.1545585638e+00, 2.4987808283e-02, 5.3915000000e+00
-2.0893135757e+00, 8.1104969450e-02, 5.5230000000e+00
-1.9668026189e+00, 1.1844534144e-01, 5.6545000000e+00
-1.8151243558e+00, 1.3646818860e-01, 5.7860000000e+00
-1.6520140667e+00, 1.4203290937e-01, 5.9175000000e+00
-1.4884681605e+00, 1.3991074278e-01, 6.0490000000e+00
-1.3310358744e+00, 1.3327798308e-01, 6.1805000000e+00

```

\$ cd ..

- You can see the corresponding example codes by following these links: [Step1~C~Simulator](#), [Step1~C++~Simulator](#), and [Step1~Fortran~Simulator](#). Compare these with the versions from [Step 0](#) to see the changes associated with this step.

6.2.3 Step 2

See [Step 2](#) for Models, above.

6.2.4 Step 3

You are now ready to make the modifications to the code needed to make it compatible with v2.

- Update the Makefile to use new preamble build-config variables.
- Update the source files to use new v2 header file (module) as opposed to old v1 version.
- Change any error messages using the `KIM_API_report_error`, as v2 does not provide a similar capability. If desired, v2 does provide access to its logging facility (see the [KIM::Log](#) documentation) which places messages in the `kim.log` file.
- Change the simulator's neighbor list data structure to include any needed values (such as the number of cutoffs, cutoff values, and number of particles), as the KIM Model object is not available within the `GetNeighborList` function in v2. Also, v2 now requires that the `GetNeighborList` callback routine verifies that the neighbor list cutoff values used to generate the neighbor lists are compatible with the model's cutoffs. Next, change the prototype of the simulator's `GetNeighborList` routine to match the v2 specification. Update the `GetNeighborList` function to conform to the v2 specification.
- If appropriate, change the simulator's `ProcessDEDrTerm` and `ProcessD2EDr2Term` callbacks in a manner similar to the changes needed for the previous item.
- You can see the corresponding example codes online by following these links: [Step3~C~Simulator](#), [Step3~C++~Simulator](#), and [Step3~Fortran~Simulator](#). Compare these with the versions from [Step 1](#) to see the changes associated with this step.

6.2.5 Step 4

- Translate the simulator's v1 KIM descriptor file into appropriate code within the new Simulator's main routine:
 - First, a list of things in the descriptor file that will be simply discarded:
 - * `KIM_API_Version` value
 - * `Neigh_LocaAccess`
 - * `NEIGH_PURE_F`
 - Provide the simulator's numbering and requested base units as part of the call to `KIM::Model::Create()`. Be sure to use "unused" values as appropriate. After the `KIM::Model::Create()` routine returns, check to see if the units request was accepted. If not, adjust the simulator's behavior appropriately, or exit with an error message.
 - Check to see that the model supports the simulator's required species with call(s) to `KIM::Model::GetSpeciesSupportAndC`.
 - Use the model object to create an associated compute-arguments object that will be used to communicate data between the simulator and model. Use a call to `KIM::Model::ComputeArgumentsCreate()`.
 - Check (with call(s) to `KIM::COMPUTE_ARGUMENT_NAME::GetNumberOfComputeArgumentNames()`, `KIM::COMPUTE_ARGUMENT_NAME::GetComputeArgumentName()`, and `KIM::ComputeArguments::GetArgumentSupport` to see that the model supports the arguments (with the appropriate `SupportStatus: required` or `optional`) that the simulator will use. Also, check to see that the model does not have any other required arguments not supported by the simulator.
 - Check (with call(s) to `KIM::COMPUTE_CALLBACK_NAME::GetNumberOfComputeCallbackNames()`, `KIM::COMPUTE_CALLBACK_NAME::GetComputeCallbackName()`, and `KIM::ComputeArguments::GetCallbackSupport` to see that the model supports the callbacks (with the appropriate `SupportStatus: required` or `optional`) that the simulator will use. Also, check to see that the model does not have any other required callbacks not supported by the simulator.
 - If the v1 simulator used the `KIM_API_file_init()` routine, remove the `descriptor.kim` file. If it used the `KIM_API_string_init()` routine, remove the associated string and/or routine.
- You can see the corresponding example codes by following these links: [Step4~C~Simulator](#), [Step4~C++~Simulator](#), and [Step4~Fortran~Simulator](#). Compare these with the versions from [Step 3](#) to see the changes associated with this step.

6.2.6 Step 5

- Remove the v1 `numberOfSpecies` argument, which is not needed in v2.
- Register the simulator's arguments memory pointers with call(s) to `KIM::ComputeArguments::SetArgumentPointer()` (in C there are `KIM_ComputeArguments_SetArgumentPointerInteger()` and `KIM_ComputeArguments_SetArgumentPointerDouble()`; C++ and Fortran use function overloading and have only `KIM::ComputeArguments::SetArgumentPointer()`).
- Register the simulator's callback memory pointers and data object pointers with call(s) to `KIM::ComputeArguments::SetCallback`.
- Update the simulator code to work with the v2 model's influence distance and multiple cutoffs features.
- Update the simulator code to populate the `particleSpeciesCode` array.
- Add code to the simulator to populate the `particleContributing` array.
- Update call(s) to `KIM::Model::Compute()`.
- Add call(s) to `KIM::Model::ComputeArgumentsDestroy()` to clean up and release memory associated with the compute-arguments object(s).
- Update call(s) to `KIM::Model::Destroy()`. Note, the single v2 call to `KIM::Model::Destroy()` covers the two v1 calls to `KIM_API_model_destroy()` and `KIM_API_free()`.

- When ready, build the simulator and test it with the v2 models installed as part of [Step 6](#) for porting models. (If you have not already copied the example simulator as part of [Porting Models: Step 3](#), do the following)

```
$ cp -r ./v1-v2-porting/simulators/step5/ex_test_Ar_fcc_cluster v2-ex_test_Ar_fcc_cluster
```

Now, execute your simulator

```
$ cd v2-ex_test_Ar_fcc_cluster
$ make

$ printf ex_model_Ar_P_MLJ_F03 | ./ex_test_Ar_fcc_cluster
Please enter valid KIM Model name:
This is Test : ex_test_Ar_fcc_cluster
-----
Results for KIM Model : ex_model_Ar_P_MLJ_F03
      Energy,      Force Norm,      Lattice Spacing
2.6568305947e+01, 1.2671877978e+01, 4.2080000000e+00
1.5269225751e+01, 7.9639127468e+00, 4.3395000000e+00
8.1940651929e+00, 4.9863838571e+00, 4.4710000000e+00
3.7947024307e+00, 3.0924620572e+00, 4.6025000000e+00
1.0980474405e+00, 1.8835116189e+00, 4.7340000000e+00
-5.1288233270e-01, 1.111343811e+00, 4.8655000000e+00
-1.4321763817e+00, 6.1892128072e-01, 4.9970000000e+00
-1.9129769394e+00, 3.0756389059e-01, 5.1285000000e+00
-2.1185529279e+00, 1.1421905922e-01, 5.2600000000e+00
-2.1545585638e+00, 2.4987808283e-02, 5.3915000000e+00
-2.0893135757e+00, 8.1104969450e-02, 5.5230000000e+00
-1.9668026189e+00, 1.1844534144e-01, 5.6545000000e+00
-1.8151243558e+00, 1.3646818860e-01, 5.7860000000e+00
-1.6520140667e+00, 1.4203290937e-01, 5.9175000000e+00
-1.4884681605e+00, 1.3991074278e-01, 6.0490000000e+00
-1.3310358744e+00, 1.3327798308e-01, 6.1805000000e+00

$ cd ..
```

You can also try the C++ and Fortran examples.

```
$ cp -r ./v1-v2-porting/simulators/step5/ex_test_Ar_fcc_cluster_cpp v2-ex_test_Ar_fcc_cluster_cpp
$ cp -r ./v1-v2-porting/simulators/step5/ex_test_Ar_fcc_cluster_fortran v2-ex_test_Ar_fcc_cluster_fortran

$ cd v2-ex_test_Ar_fcc_cluster_cpp
$ make

$ printf ex_model_Ar_P_Morse_07C | ./ex_test_Ar_fcc_cluster_cpp

Please enter valid KIM Model name:
LengthUnit is "A"
EnergyUnit is "eV"
ChargeUnit is "unused"
TemperatureUnit is "unused"
TimeUnit is "unused"
ComputeArgument Name "numberOfParticles" is of type "Integer" and has supportStatus "requiredByAPI"
ComputeArgument Name "particleSpeciesCodes" is of type "Integer" and has supportStatus "requiredByAPI"
ComputeArgument Name "particleContributing" is of type "Integer" and has supportStatus "requiredByAPI"
ComputeArgument Name "coordinates" is of type "Double" and has supportStatus "requiredByAPI"
ComputeArgument Name "partialEnergy" is of type "Double" and has supportStatus "optional"
ComputeArgument Name "partialForces" is of type "Double" and has supportStatus "optional"
ComputeArgument Name "partialParticleEnergy" is of type "Double" and has supportStatus "optional"
ComputeArgument Name "partialVirial" is of type "Double" and has supportStatus "notSupported"
ComputeArgument Name "partialParticleVirial" is of type "Double" and has supportStatus "notSupported"
ComputeCallback Name "GetNeighborList" has supportStatus "requiredByAPI"
ComputeCallback Name "ProcessDEDrTerm" has supportStatus "optional"
ComputeCallback Name "ProcessD2EDr2Term" has supportStatus "optional"
This is Test : ex_test_Ar_fcc_cluster_cpp
-----
Results for KIM Model : ex_model_Ar_P_Morse_07C
      Energy      Force Norm      Lattice Spacing
1.4703219623e+01 6.9678657557e+00 4.2080000000e+00
8.2453550705e+00 4.8650873812e+00 4.3395000000e+00
3.7883556879e+00 3.3409407134e+00 4.4710000000e+00
7.7810749699e-01 2.2399352517e+00 4.6025000000e+00
-1.1944148939e+00 1.4518130136e+00 4.7340000000e+00
-2.4291941022e+00 8.9239060716e-01 4.8655000000e+00
-3.1445433206e+00 5.0063786968e-01 4.9970000000e+00
-3.4996095359e+00 2.3199479279e-01 5.1285000000e+00
-3.6112724693e+00 6.3687021777e-02 5.2600000000e+00
-3.5604853404e+00 8.7536239707e-02 5.3915000000e+00
-3.4059878193e+00 1.5700051389e-01 5.5230000000e+00
-3.1896247548e+00 1.9909723852e-01 5.6545000000e+00
-2.9407853637e+00 2.1928061006e-01 5.7860000000e+00
-2.6800661721e+00 2.2574027063e-01 5.9175000000e+00
```

```

-2.4197463013e+00    2.2234487833e-01    6.0490000000e+00
-2.1685167432e+00    2.1265537489e-01    6.1805000000e+00

$ cd ..
$ cd v2-ex_test_Ar_fcc_cluster_fortran
$ make

$ printf ex_model_Ar_P_Morse_07C | ./ex_test_Ar_fcc_cluster_fortran

Please enter a valid KIM model name:

This is Test : ex_test_Ar_fcc_cluster_fortran
-----
Results for KIM Model : ex_model_Ar_P_Morse_07C
      Energy      Force Norm      Lattice Spacing
1.4703215955E+01    6.9678645853E+00    4.2080000627E+00
8.2453524404E+00    4.8650865034E+00    4.3395000647E+00
3.7883538362E+00    3.3409400589E+00    4.4710000666E+00
7.7810622791E-01    2.2399347674E+00    4.6025000686E+00
-1.1944157316E+00    1.4518126584E+00    4.7340000705E+00
-2.4291946228E+00    8.9239034976E-01    4.8655000725E+00
-3.1445436110E+00    5.0063768619E-01    4.9970000745E+00
-3.4996096616E+00    2.3199466611E-01    5.1285000764E+00
-3.6112724807E+00    6.3686958966E-02    5.2600000784E+00
-3.5604852727E+00    8.7536289674E-02    5.3915000803E+00
-3.4059876997E+00    1.5700054839E-01    5.5230000823E+00
-3.1896246031E+00    1.9909725795E-01    5.6545000843E+00
-2.9407851953E+00    2.1928061852E-01    5.7860000862E+00
-2.6800659962E+00    2.2574027119E-01    5.9175000882E+00
-2.4197461252E+00    2.2234487350E-01    6.0490000901E+00
-2.1685165719E+00    2.1265536654E-01    6.1805000921E+00
-1.9316933369E+00    1.9920520002E-01    6.3120000941E+00

$ cd ..

```

- You can see the corresponding example codes by following these links: [Step5~C~Simulator](#), [Step5~C++~Simulator](#), and [Step5~Fortran~Simulator](#). Compare these with the versions from [Step 4](#) to see the changes associated with this step.

Next Section: [Browse files](#).

Chapter 7

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7.1 Namespace List

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Chapter 8

Class Index

8.1 Class List

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Chapter 9

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Chapter 10

Namespace Documentation

10.1 error Module Reference

Functions/Subroutines

- subroutine [my_error](#) (message, line, file)
- subroutine [my_warning](#) (message, line, file)

10.1.1 Function/Subroutine Documentation

10.1.1.1 [my_error\(\)](#)

```
subroutine error::my_error (  
    character(len=*, kind=c_char), intent(in) message,  
    integer, intent(in) line,  
    character(len=*, kind=c_char), intent(in) file )
```

Definition at line 37 of file `ex_test_Ar_fcc_cluster_fortran.F90`.

10.1.1.2 [my_warning\(\)](#)

```
subroutine error::my_warning (  
    character(len=*, kind=c_char), intent(in) message,  
    integer, intent(in) line,  
    character(len=*, kind=c_char), intent(in) file )
```

Definition at line 48 of file `ex_test_Ar_fcc_cluster_fortran.F90`.

10.2 ex_model_ar_p_ml_j_f03 Module Reference

Functions/Subroutines

- integer(c_int) function, public [compute_energy_forces](#) (pkim)
- subroutine, public [model_compute_arguments_create](#) (model_compute_handle, model_compute_↵arguments_create_handle, ierr)
- subroutine, public [model_compute_arguments_destroy](#) (model_compute_handle, model_compute_↵arguments_destroy_handle, ierr)
- subroutine, public [model_destroy_func](#) (model_destroy_handle, ierr)
- subroutine, public [model_refresh_func](#) (model_refresh_handle, ierr)
- subroutine, public [compute_energy_forces](#) (model_compute_handle, model_compute_arguments_handle, ierr)

Variables

- real(c_double), parameter, public [model_cutoff](#) = 8.15_cd

10.2.1 Function/Subroutine Documentation

10.2.1.1 compute_energy_forces() [1/2]

```
integer(c_int) function, public ex_model_ar_p_ml_j_f03::compute_energy_forces (
    type(c_ptr), intent(in) pkim )
```

Definition at line 162 of file ex_model_Ar_P_MLJ_F03.F03.

10.2.1.2 compute_energy_forces() [2/2]

```
subroutine public ex_model_ar_p_ml_j_f03::compute_energy_forces (
    type(kim_model_compute_handle_type), intent(in) model_compute_handle,
    type(kim_model_compute_arguments_handle_type), intent(in) model_compute_arguments↵
_handle,
    integer(c_int), intent(out) ierr )
```

Definition at line 171 of file ex_model_Ar_P_MLJ_F03.F03.

10.2.1.3 model_compute_arguments_create()

```
subroutine public ex_model_ar_p_ml_j_f03::model_compute_arguments_create (
    type(kim_model_compute_handle_type), intent(in) model_compute_handle,
    type(kim_model_compute_arguments_create_handle_type), intent(inout) model_↵
compute_arguments_create_handle,
    integer(c_int), intent(out) ierr )
```

Definition at line 344 of file ex_model_Ar_P_MLJ_F03.F03.

10.2.1.4 model_compute_arguments_destroy()

```
subroutine public ex_model_ar_p_ml_j_f03::model_compute_arguments_destroy (
    type(kim_model_compute_handle_type), intent(in) model_compute_handle,
    type(kim_model_compute_arguments_destroy_handle_type), intent(inout) model_↵
compute_arguments_destroy_handle,
    integer(c_int), intent(out) ierr )
```

Definition at line 407 of file ex_model_Ar_P_MLJ_F03.F03.

10.2.1.5 model_destroy_func()

```
subroutine public ex_model_ar_p_ml_j_f03::model_destroy_func (
    type(kim_model_destroy_handle_type), intent(inout) model_destroy_handle,
    integer(c_int), intent(out) ierr )
```

Definition at line 345 of file ex_model_Ar_P_MLJ_F03.F03.

10.2.1.6 model_refresh_func()

```
subroutine public ex_model_ar_p_ml_j_f03::model_refresh_func (
    type(kim_model_refresh_handle_type), intent(inout) model_refresh_handle,
    integer(c_int), intent(out) ierr )
```

Definition at line 371 of file ex_model_Ar_P_MLJ_F03.F03.

10.2.2 Variable Documentation

10.2.2.1 model_cutoff

```
real(c_double), parameter, public ex_model_ar_p_ml_j_f03::model_cutoff = 8.15_cd
```

Definition at line 64 of file ex_model_Ar_P_MLJ_F03.F03.

10.3 ex_model_driver_p_lj Module Reference

Functions/Subroutines

- subroutine, public [calc_phi](#) (model_epsilon, model_sigma, model_shift, model_cutoff, r, phi)
- subroutine, public [calc_phi_dphi](#) (model_epsilon, model_sigma, model_shift, model_cutoff, r, phi, dphi)
- subroutine, public [calc_phi_dphi_d2phi](#) (model_epsilon, model_sigma, model_shift, model_cutoff, r, phi, dphi, d2phi)
- subroutine, public [compute_energy_forces](#) (model_compute_handle, model_compute_arguments_handle, ierr)
- subroutine, public [refresh](#) (model_refresh_handle, ierr)
- subroutine, public [destroy](#) (model_destroy_handle, ierr)
- subroutine, public [compute_arguments_create](#) (model_compute_handle, model_compute_arguments_↵ create_handle, ierr)
- subroutine, public [compute_arguments_destroy](#) (model_compute_handle, model_compute_arguments_↵ destroy_handle, ierr)

Variables

- integer(c_int), parameter, public `speccode` = 1

10.3.1 Function/Subroutine Documentation

10.3.1.1 `calc_phi()`

```
subroutine, public ex_model_driver_p_lj::calc_phi (
    real(c_double), intent(in) model_epsilon,
    real(c_double), intent(in) model_sigma,
    real(c_double), intent(in) model_shift,
    real(c_double), intent(in) model_cutoff,
    real(c_double), intent(in) r,
    real(c_double), intent(out) phi )
```

Definition at line 94 of file `ex_model_driver_P_LJ.F90`.

10.3.1.2 `calc_phi_dphi()`

```
subroutine, public ex_model_driver_p_lj::calc_phi_dphi (
    real(c_double), intent(in) model_epsilon,
    real(c_double), intent(in) model_sigma,
    real(c_double), intent(in) model_shift,
    real(c_double), intent(in) model_cutoff,
    real(c_double), intent(in) r,
    real(c_double), intent(out) phi,
    real(c_double), intent(out) dphi )
```

Definition at line 130 of file `ex_model_driver_P_LJ.F90`.

10.3.1.3 `calc_phi_dphi_d2phi()`

```
subroutine, public ex_model_driver_p_lj::calc_phi_dphi_d2phi (
    real(c_double), intent(in) model_epsilon,
    real(c_double), intent(in) model_sigma,
    real(c_double), intent(in) model_shift,
    real(c_double), intent(in) model_cutoff,
    real(c_double), intent(in) r,
    real(c_double), intent(out) phi,
    real(c_double), intent(out) dphi,
    real(c_double), intent(out) d2phi )
```

Definition at line 168 of file `ex_model_driver_P_LJ.F90`.

10.3.1.4 compute_arguments_create()

```

subroutine, public ex_model_driver_p_lj::compute_arguments_create (
    type(kim_model_compute_handle_type), intent(in) model_compute_handle,
    type(kim_model_compute_arguments_create_handle_type), intent(inout) model_↵
compute_arguments_create_handle,
    integer(c_int), intent(out) ierr )

```

Definition at line 554 of file ex_model_driver_P_LJ.F90.

10.3.1.5 compute_arguments_destroy()

```

subroutine, public ex_model_driver_p_lj::compute_arguments_destroy (
    type(kim_model_compute_handle_type), intent(in) model_compute_handle,
    type(kim_model_compute_arguments_destroy_handle_type), intent(inout) model_↵
compute_arguments_destroy_handle,
    integer(c_int), intent(out) ierr )

```

Definition at line 620 of file ex_model_driver_P_LJ.F90.

10.3.1.6 compute_energy_forces()

```

subroutine, public ex_model_driver_p_lj::compute_energy_forces (
    type(kim_model_compute_handle_type), intent(in) model_compute_handle,
    type(kim_model_compute_arguments_handle_type), intent(in) model_compute_arguments↵
_handle,
    integer(c_int), intent(out) ierr )

```

Definition at line 207 of file ex_model_driver_P_LJ.F90.

10.3.1.7 destroy()

```

subroutine, public ex_model_driver_p_lj::destroy (
    type(kim_model_destroy_handle_type), intent(inout) model_destroy_handle,
    integer(c_int), intent(out) ierr )

```

Definition at line 526 of file ex_model_driver_P_LJ.F90.

10.3.1.8 refresh()

```

subroutine, public ex_model_driver_p_lj::refresh (
    type(kim_model_refresh_handle_type), intent(inout) model_refresh_handle,
    integer(c_int), intent(out) ierr )

```

Definition at line 484 of file ex_model_driver_P_LJ.F90.

10.3.2 Variable Documentation

10.3.2.1 speccode

```
integer(c_int), parameter, public ex_model_driver_p_lj::speccode = 1
```

Definition at line 66 of file ex_model_driver_P_LJ.F90.

10.4 KIM Namespace Reference

Namespaces

- [CHARGE_UNIT](#)
- [COMPUTE_ARGUMENT_NAME](#)
- [COMPUTE_CALLBACK_NAME](#)
- [DATA_TYPE](#)
- [ENERGY_UNIT](#)
- [LANGUAGE_NAME](#)
- [LENGTH_UNIT](#)
- [LOG_VERBOSITY](#)
- [NUMBERING](#)
- [SEM_VER](#)
- [SPECIES_NAME](#)
- [SUPPORT_STATUS](#)
- [TEMPERATURE_UNIT](#)
- [TIME_UNIT](#)

Classes

- class [ChargeUnit](#)
- class [ComputeArgumentName](#)
- class [ComputeArguments](#)
- class [ComputeCallbackName](#)
- class [DataType](#)
- class [EnergyUnit](#)
- class [LanguageName](#)
- class [LengthUnit](#)
- class [Log](#)
- class [LogVerbosity](#)
- class [Model](#)
- class [ModelCompute](#)
- class [ModelComputeArguments](#)
- class [ModelComputeArgumentsCreate](#)
- class [ModelComputeArgumentsDestroy](#)
- class [ModelCreate](#)
- class [ModelDestroy](#)
- class [ModelDriverCreate](#)
- class [ModelRefresh](#)
- class [Numbering](#)
- class [SpeciesName](#)
- class [SupportStatus](#)
- class [TemperatureUnit](#)
- class [TimeUnit](#)

Typedefs

- typedef void() [func](#)()

10.4.1 Typedef Documentation

10.4.1.1 func

```
typedef void() KIM::func()
```

Definition at line 40 of file KIM_func.hpp.

10.5 KIM::CHARGE_UNIT Namespace Reference

Classes

- struct [Comparator](#)

Functions

- void [GetNumberOfChargeUnits](#) (int *const numberOfChargeUnits)
- int [GetChargeUnit](#) (int const index, [ChargeUnit](#) *const chargeUnit)

Variables

- [ChargeUnit](#) const [unused](#)
- [ChargeUnit](#) const [C](#)
- [ChargeUnit](#) const [e](#)
- [ChargeUnit](#) const [statC](#)

10.5.1 Function Documentation

10.5.1.1 GetChargeUnit()

```
int KIM::CHARGE_UNIT::GetChargeUnit (
    int const index,
    ChargeUnit *const chargeUnit )
```

10.5.1.2 GetNumberOfChargeUnits()

```
void KIM::CHARGE_UNIT::GetNumberOfChargeUnits (
    int *const numberOfChargeUnits )
```

10.5.2 Variable Documentation

10.5.2.1 C

```
ChargeUnit const KIM::CHARGE_UNIT::C
```

10.5.2.2 e

```
ChargeUnit const KIM::CHARGE_UNIT::e
```

10.5.2.3 statC

```
ChargeUnit const KIM::CHARGE_UNIT::statC
```

10.5.2.4 unused

```
ChargeUnit const KIM::CHARGE_UNIT::unused
```

10.6 KIM::COMPUTE_ARGUMENT_NAME Namespace Reference

Classes

- struct [Comparator](#)

Functions

- void [GetNumberOfComputeArgumentNames](#) (int *const numberOfComputeArgumentNames)
- int [GetComputeArgumentName](#) (int const index, [ComputeArgumentName](#) *const computeArgumentName)
- int [GetComputeArgumentDataType](#) ([ComputeArgumentName](#) const computeArgumentName, [DataType](#) *const dataType)

Variables

- [ComputeArgumentName](#) const [numberOfParticles](#)
- [ComputeArgumentName](#) const [particleSpeciesCodes](#)
- [ComputeArgumentName](#) const [particleContributing](#)
- [ComputeArgumentName](#) const [coordinates](#)
- [ComputeArgumentName](#) const [partialEnergy](#)
- [ComputeArgumentName](#) const [partialForces](#)
- [ComputeArgumentName](#) const [partialParticleEnergy](#)
- [ComputeArgumentName](#) const [partialVirial](#)
- [ComputeArgumentName](#) const [partialParticleVirial](#)

10.6.1 Function Documentation

10.6.1.1 GetComputeArgumentDataType()

```
int KIM::COMPUTE_ARGUMENT_NAME::GetComputeArgumentDataType (
    ComputeArgumentName const computeArgumentName,
    DataType *const dataType )
```

10.6.1.2 GetComputeArgumentName()

```
int KIM::COMPUTE_ARGUMENT_NAME::GetComputeArgumentName (
    int const index,
    ComputeArgumentName *const computeArgumentName )
```

10.6.1.3 GetNumberOfComputeArgumentNames()

```
void KIM::COMPUTE_ARGUMENT_NAME::GetNumberOfComputeArgumentNames (
    int *const numberOfComputeArgumentNames )
```

10.6.2 Variable Documentation

10.6.2.1 coordinates

```
ComputeArgumentName const KIM::COMPUTE_ARGUMENT_NAME::coordinates
```

10.6.2.2 numberOfParticles

`ComputeArgumentName` const KIM::COMPUTE_ARGUMENT_NAME::numberOfParticles

10.6.2.3 partialEnergy

`ComputeArgumentName` const KIM::COMPUTE_ARGUMENT_NAME::partialEnergy

10.6.2.4 partialForces

`ComputeArgumentName` const KIM::COMPUTE_ARGUMENT_NAME::partialForces

10.6.2.5 partialParticleEnergy

`ComputeArgumentName` const KIM::COMPUTE_ARGUMENT_NAME::partialParticleEnergy

10.6.2.6 partialParticleVirial

`ComputeArgumentName` const KIM::COMPUTE_ARGUMENT_NAME::partialParticleVirial

10.6.2.7 partialVirial

`ComputeArgumentName` const KIM::COMPUTE_ARGUMENT_NAME::partialVirial

10.6.2.8 particleContributing

`ComputeArgumentName` const KIM::COMPUTE_ARGUMENT_NAME::particleContributing

10.6.2.9 particleSpeciesCodes

`ComputeArgumentName` const KIM::COMPUTE_ARGUMENT_NAME::particleSpeciesCodes

10.7 KIM::COMPUTE_CALLBACK_NAME Namespace Reference

Classes

- struct [Comparator](#)

Functions

- void [GetNumberOfComputeCallbackNames](#) (int *const numberOfComputeCallbackNames)
- int [GetComputeCallbackName](#) (int const index, [ComputeCallbackName](#) *const computeCallbackName)

Variables

- [ComputeCallbackName](#) const [GetNeighborList](#)
- [ComputeCallbackName](#) const [ProcessDEDrTerm](#)
- [ComputeCallbackName](#) const [ProcessD2EDr2Term](#)

10.7.1 Function Documentation

10.7.1.1 GetComputeCallbackName()

```
int KIM::COMPUTE_CALLBACK_NAME::GetComputeCallbackName (
    int const index,
    ComputeCallbackName *const computeCallbackName )
```

10.7.1.2 GetNumberOfComputeCallbackNames()

```
void KIM::COMPUTE_CALLBACK_NAME::GetNumberOfComputeCallbackNames (
    int *const numberOfComputeCallbackNames )
```

10.7.2 Variable Documentation

10.7.2.1 GetNeighborList

```
ComputeCallbackName const KIM::COMPUTE_CALLBACK_NAME::GetNeighborList
```

10.7.2.2 ProcessD2EDr2Term

`ComputeCallbackName` const KIM::COMPUTE_CALLBACK_NAME::ProcessD2EDr2Term

10.7.2.3 ProcessDEDrTerm

`ComputeCallbackName` const KIM::COMPUTE_CALLBACK_NAME::ProcessDEDrTerm

10.8 KIM::DATA_TYPE Namespace Reference

Classes

- struct [Comparator](#)

Functions

- void [GetNumberOfDataTypes](#) (int *const numberOfDataTypes)
- int [GetDataType](#) (int const index, [DataType](#) *const dataType)

Variables

- [DataType](#) const [Integer](#)
- [DataType](#) const [Double](#)

10.8.1 Function Documentation

10.8.1.1 GetDataType()

```
int KIM::DATA_TYPE::GetDataType (
    int const index,
    DataType *const dataType )
```

10.8.1.2 GetNumberOfDataTypes()

```
void KIM::DATA_TYPE::GetNumberOfDataTypes (
    int *const numberOfDataTypes )
```

10.8.2 Variable Documentation

10.8.2.1 Double

`DataType` const KIM::DATA_TYPE::Double

10.8.2.2 Integer

`DataType` const KIM::DATA_TYPE::Integer

10.9 KIM::ENERGY_UNIT Namespace Reference

Classes

- struct [Comparator](#)

Functions

- void [GetNumberOfEnergyUnits](#) (int *const numberOfEnergyUnits)
- int [GetEnergyUnit](#) (int const index, [EnergyUnit](#) *const energyUnit)

Variables

- [EnergyUnit](#) const [unused](#)
- [EnergyUnit](#) const [amu_A2_per_ps2](#)
- [EnergyUnit](#) const [erg](#)
- [EnergyUnit](#) const [eV](#)
- [EnergyUnit](#) const [Hartree](#)
- [EnergyUnit](#) const [J](#)
- [EnergyUnit](#) const [kcal_mol](#)

10.9.1 Function Documentation

10.9.1.1 GetEnergyUnit()

```
int KIM::ENERGY_UNIT::GetEnergyUnit (
    int const index,
    EnergyUnit *const energyUnit )
```

10.9.1.2 GetNumberOfEnergyUnits()

```
void KIM::ENERGY_UNIT::GetNumberOfEnergyUnits (
    int *const numberOfEnergyUnits )
```

10.9.2 Variable Documentation

10.9.2.1 amu_A2_per_ps2

```
EnergyUnit const KIM::ENERGY_UNIT::amu_A2_per_ps2
```

10.9.2.2 erg

```
EnergyUnit const KIM::ENERGY_UNIT::erg
```

10.9.2.3 eV

```
EnergyUnit const KIM::ENERGY_UNIT::eV
```

10.9.2.4 Hartree

```
EnergyUnit const KIM::ENERGY_UNIT::Hartree
```

10.9.2.5 J

```
EnergyUnit const KIM::ENERGY_UNIT::J
```

10.9.2.6 kcal_mol

```
EnergyUnit const KIM::ENERGY_UNIT::kcal_mol
```


10.9.2.7 unused

```
EnergyUnit const KIM::ENERGY_UNIT::unused
```

10.10 KIM::LANGUAGE_NAME Namespace Reference

Classes

- struct [Comparator](#)

Functions

- void [GetNumberOfLanguageNames](#) (int *const numberOfLanguageNames)
- int [GetLanguageName](#) (int const index, [LanguageName](#) *const languageName)

Variables

- [LanguageName](#) const [cpp](#)
- [LanguageName](#) const [c](#)
- [LanguageName](#) const [fortran](#)

10.10.1 Function Documentation

10.10.1.1 [GetLanguageName\(\)](#)

```
int KIM::LANGUAGE_NAME::GetLanguageName (
    int const index,
    LanguageName *const languageName )
```

10.10.1.2 [GetNumberOfLanguageNames\(\)](#)

```
void KIM::LANGUAGE_NAME::GetNumberOfLanguageNames (
    int *const numberOfLanguageNames )
```

10.10.2 Variable Documentation

10.10.2.1 c

[LanguageName](#) const KIM::LANGUAGE_NAME::c

10.10.2.2 cpp

[LanguageName](#) const KIM::LANGUAGE_NAME::cpp

10.10.2.3 fortran

[LanguageName](#) const KIM::LANGUAGE_NAME::fortran

10.11 KIM::LENGTH_UNIT Namespace Reference

Classes

- struct [Comparator](#)

Functions

- void [GetNumberOfLengthUnits](#) (int *const numberOfLengthUnits)
- int [GetLengthUnit](#) (int const index, [LengthUnit](#) *const lengthUnit)

Variables

- [LengthUnit](#) const [unused](#)
- [LengthUnit](#) const [A](#)
- [LengthUnit](#) const [Bohr](#)
- [LengthUnit](#) const [cm](#)
- [LengthUnit](#) const [m](#)
- [LengthUnit](#) const [nm](#)

10.11.1 Function Documentation

10.11.1.1 GetLengthUnit()

```
int KIM::LENGTH_UNIT::GetLengthUnit (
    int const index,
    LengthUnit *const lengthUnit )
```

10.11.1.2 GetNumberOfLengthUnits()

```
void KIM::LENGTH_UNIT::GetNumberOfLengthUnits (
    int *const numberOfLengthUnits )
```

10.11.2 Variable Documentation

10.11.2.1 A

```
LengthUnit const KIM::LENGTH_UNIT::A
```

10.11.2.2 Bohr

```
LengthUnit const KIM::LENGTH_UNIT::Bohr
```

10.11.2.3 cm

```
LengthUnit const KIM::LENGTH_UNIT::cm
```

10.11.2.4 m

```
LengthUnit const KIM::LENGTH_UNIT::m
```

10.11.2.5 nm

```
LengthUnit const KIM::LENGTH_UNIT::nm
```

10.11.2.6 unused

```
LengthUnit const KIM::LENGTH_UNIT::unused
```

10.12 KIM::LOG_VERBOSITY Namespace Reference

Classes

- struct [Comparator](#)

Functions

- void [GetNumberOfLogVerbosities](#) (int *const numberOfLogVerbosities)
- int [GetLogVerbosity](#) (int const index, [LogVerbosity](#) *const logVerbosity)

Variables

- [LogVerbosity](#) const [silent](#)
- [LogVerbosity](#) const [fatal](#)
- [LogVerbosity](#) const [error](#)
- [LogVerbosity](#) const [warning](#)
- [LogVerbosity](#) const [information](#)
- [LogVerbosity](#) const [debug](#)

10.12.1 Function Documentation

10.12.1.1 [GetLogVerbosity\(\)](#)

```
int KIM::LOG_VERBOSITY::GetLogVerbosity (
    int const index,
    LogVerbosity *const logVerbosity )
```

10.12.1.2 [GetNumberOfLogVerbosities\(\)](#)

```
void KIM::LOG_VERBOSITY::GetNumberOfLogVerbosities (
    int *const numberOfLogVerbosities )
```

10.12.2 Variable Documentation

10.12.2.1 [debug](#)

[LogVerbosity](#) const KIM::LOG_VERBOSITY::debug

10.12.2.2 error

`LogVerbosity` const KIM::LOG_VERBOSITY::error

10.12.2.3 fatal

`LogVerbosity` const KIM::LOG_VERBOSITY::fatal

10.12.2.4 information

`LogVerbosity` const KIM::LOG_VERBOSITY::information

10.12.2.5 silent

`LogVerbosity` const KIM::LOG_VERBOSITY::silent

10.12.2.6 warning

`LogVerbosity` const KIM::LOG_VERBOSITY::warning

10.13 KIM::NUMBERING Namespace Reference

Classes

- struct [Comparator](#)

Functions

- void [GetNumberOfNumberings](#) (int *const numberOfNumberings)
- int [GetNumbering](#) (int const index, [Numbering](#) *const numbering)

Variables

- [Numbering](#) const [zeroBased](#)
- [Numbering](#) const [oneBased](#)

10.13.1 Function Documentation

10.13.1.1 `GetNumbering()`

```
int KIM::NUMBERING::GetNumbering (
    int const index,
    Numbering *const numbering )
```

10.13.1.2 `GetNumberOfNumberings()`

```
void KIM::NUMBERING::GetNumberOfNumberings (
    int *const numberOfNumberings )
```

10.13.2 Variable Documentation

10.13.2.1 `oneBased`

```
Numbering const KIM::NUMBERING::oneBased
```

10.13.2.2 `zeroBased`

```
Numbering const KIM::NUMBERING::zeroBased
```

10.14 KIM::SEM_VER Namespace Reference

Functions

- void `GetSemVer` (std::string const &&const version)
- int `IsLessThan` (std::string const &versionA, std::string const &versionB, int *const isLessThan)
- int `ParseSemVer` (std::string const &version, int *const major, int *const minor, int *const patch, std::string *const prerelease, std::string *const buildMetadata)

10.14.1 Function Documentation

10.14.1.1 GetSemVer()

```
void KIM::SEM_VER::GetSemVer (
    std::string const &version )
```

10.14.1.2 IsLessThan()

```
int KIM::SEM_VER::IsLessThan (
    std::string const &versionA,
    std::string const &versionB,
    int *const isLessThan )
```

10.14.1.3 ParseSemVer()

```
int KIM::SEM_VER::ParseSemVer (
    std::string const &version,
    int *const major,
    int *const minor,
    int *const patch,
    std::string *const prerelease,
    std::string *const buildMetadata )
```

10.15 KIM::SPECIES_NAME Namespace Reference

Classes

- struct [Comparator](#)

Functions

- void [GetNumberOfSpeciesNames](#) (int *const numberOfSpeciesNames)
- int [GetSpeciesName](#) (int const index, [SpeciesName](#) *const speciesName)

Variables

- [SpeciesName](#) const [electron](#)
- [SpeciesName](#) const [H](#)
- [SpeciesName](#) const [He](#)
- [SpeciesName](#) const [Li](#)
- [SpeciesName](#) const [Be](#)
- [SpeciesName](#) const [B](#)
- [SpeciesName](#) const [C](#)
- [SpeciesName](#) const [N](#)
- [SpeciesName](#) const [O](#)
- [SpeciesName](#) const [F](#)
- [SpeciesName](#) const [Ne](#)
- [SpeciesName](#) const [Na](#)
- [SpeciesName](#) const [Mg](#)
- [SpeciesName](#) const [Al](#)
- [SpeciesName](#) const [Si](#)
- [SpeciesName](#) const [P](#)
- [SpeciesName](#) const [S](#)
- [SpeciesName](#) const [Cl](#)
- [SpeciesName](#) const [Ar](#)
- [SpeciesName](#) const [K](#)
- [SpeciesName](#) const [Ca](#)
- [SpeciesName](#) const [Sc](#)
- [SpeciesName](#) const [Ti](#)
- [SpeciesName](#) const [V](#)
- [SpeciesName](#) const [Cr](#)
- [SpeciesName](#) const [Mn](#)
- [SpeciesName](#) const [Fe](#)
- [SpeciesName](#) const [Co](#)
- [SpeciesName](#) const [Ni](#)
- [SpeciesName](#) const [Cu](#)
- [SpeciesName](#) const [Zn](#)
- [SpeciesName](#) const [Ga](#)
- [SpeciesName](#) const [Ge](#)
- [SpeciesName](#) const [As](#)
- [SpeciesName](#) const [Se](#)
- [SpeciesName](#) const [Br](#)
- [SpeciesName](#) const [Kr](#)
- [SpeciesName](#) const [Rb](#)
- [SpeciesName](#) const [Sr](#)
- [SpeciesName](#) const [Y](#)
- [SpeciesName](#) const [Zr](#)
- [SpeciesName](#) const [Nb](#)
- [SpeciesName](#) const [Mo](#)
- [SpeciesName](#) const [Tc](#)
- [SpeciesName](#) const [Ru](#)
- [SpeciesName](#) const [Rh](#)
- [SpeciesName](#) const [Pd](#)
- [SpeciesName](#) const [Ag](#)
- [SpeciesName](#) const [Cd](#)
- [SpeciesName](#) const [In](#)
- [SpeciesName](#) const [Sn](#)
- [SpeciesName](#) const [Sb](#)
- [SpeciesName](#) const [Te](#)

- [SpeciesName](#) const [I](#)
- [SpeciesName](#) const [Xe](#)
- [SpeciesName](#) const [Cs](#)
- [SpeciesName](#) const [Ba](#)
- [SpeciesName](#) const [La](#)
- [SpeciesName](#) const [Ce](#)
- [SpeciesName](#) const [Pr](#)
- [SpeciesName](#) const [Nd](#)
- [SpeciesName](#) const [Pm](#)
- [SpeciesName](#) const [Sm](#)
- [SpeciesName](#) const [Eu](#)
- [SpeciesName](#) const [Gd](#)
- [SpeciesName](#) const [Tb](#)
- [SpeciesName](#) const [Dy](#)
- [SpeciesName](#) const [Ho](#)
- [SpeciesName](#) const [Er](#)
- [SpeciesName](#) const [Tm](#)
- [SpeciesName](#) const [Yb](#)
- [SpeciesName](#) const [Lu](#)
- [SpeciesName](#) const [Hf](#)
- [SpeciesName](#) const [Ta](#)
- [SpeciesName](#) const [W](#)
- [SpeciesName](#) const [Re](#)
- [SpeciesName](#) const [Os](#)
- [SpeciesName](#) const [Ir](#)
- [SpeciesName](#) const [Pt](#)
- [SpeciesName](#) const [Au](#)
- [SpeciesName](#) const [Hg](#)
- [SpeciesName](#) const [Tl](#)
- [SpeciesName](#) const [Pb](#)
- [SpeciesName](#) const [Bi](#)
- [SpeciesName](#) const [Po](#)
- [SpeciesName](#) const [At](#)
- [SpeciesName](#) const [Rn](#)
- [SpeciesName](#) const [Fr](#)
- [SpeciesName](#) const [Ra](#)
- [SpeciesName](#) const [Ac](#)
- [SpeciesName](#) const [Th](#)
- [SpeciesName](#) const [Pa](#)
- [SpeciesName](#) const [U](#)
- [SpeciesName](#) const [Np](#)
- [SpeciesName](#) const [Pu](#)
- [SpeciesName](#) const [Am](#)
- [SpeciesName](#) const [Cm](#)
- [SpeciesName](#) const [Bk](#)
- [SpeciesName](#) const [Cf](#)
- [SpeciesName](#) const [Es](#)
- [SpeciesName](#) const [Fm](#)
- [SpeciesName](#) const [Md](#)
- [SpeciesName](#) const [No](#)
- [SpeciesName](#) const [Lr](#)
- [SpeciesName](#) const [Rf](#)
- [SpeciesName](#) const [Db](#)
- [SpeciesName](#) const [Sg](#)
- [SpeciesName](#) const [Bh](#)

- [SpeciesName](#) const [Hs](#)
- [SpeciesName](#) const [Mt](#)
- [SpeciesName](#) const [Ds](#)
- [SpeciesName](#) const [Rg](#)
- [SpeciesName](#) const [Cn](#)
- [SpeciesName](#) const [Uut](#)
- [SpeciesName](#) const [Fl](#)
- [SpeciesName](#) const [Uup](#)
- [SpeciesName](#) const [Lv](#)
- [SpeciesName](#) const [Uus](#)
- [SpeciesName](#) const [Uuo](#)
- [SpeciesName](#) const [user01](#)
- [SpeciesName](#) const [user02](#)
- [SpeciesName](#) const [user03](#)
- [SpeciesName](#) const [user04](#)
- [SpeciesName](#) const [user05](#)
- [SpeciesName](#) const [user06](#)
- [SpeciesName](#) const [user07](#)
- [SpeciesName](#) const [user08](#)
- [SpeciesName](#) const [user09](#)
- [SpeciesName](#) const [user10](#)
- [SpeciesName](#) const [user11](#)
- [SpeciesName](#) const [user12](#)
- [SpeciesName](#) const [user13](#)
- [SpeciesName](#) const [user14](#)
- [SpeciesName](#) const [user15](#)
- [SpeciesName](#) const [user16](#)
- [SpeciesName](#) const [user17](#)
- [SpeciesName](#) const [user18](#)
- [SpeciesName](#) const [user19](#)
- [SpeciesName](#) const [user20](#)

10.15.1 Function Documentation

10.15.1.1 GetNumberOfSpeciesNames()

```
void KIM::SPECIES_NAME::GetNumberOfSpeciesNames (
    int *const numberOfSpeciesNames )
```

10.15.1.2 GetSpeciesName()

```
int KIM::SPECIES_NAME::GetSpeciesName (
    int const index,
    SpeciesName *const speciesName )
```

10.15.2 Variable Documentation

10.15.2.1 Ac

`SpeciesName` const KIM::SPECIES_NAME::Ac

10.15.2.2 Ag

`SpeciesName` const KIM::SPECIES_NAME::Ag

10.15.2.3 Al

`SpeciesName` const KIM::SPECIES_NAME::Al

10.15.2.4 Am

`SpeciesName` const KIM::SPECIES_NAME::Am

10.15.2.5 Ar

`SpeciesName` const KIM::SPECIES_NAME::Ar

10.15.2.6 As

`SpeciesName` const KIM::SPECIES_NAME::As

10.15.2.7 At

`SpeciesName` const KIM::SPECIES_NAME::At

10.15.2.8 Au

`SpeciesName` const KIM::SPECIES_NAME::Au

10.15.2.9 B

`SpeciesName` const KIM::SPECIES_NAME::B

10.15.2.10 Ba

`SpeciesName` const KIM::SPECIES_NAME::Ba

10.15.2.11 Be

`SpeciesName` const KIM::SPECIES_NAME::Be

10.15.2.12 Bh

`SpeciesName` const KIM::SPECIES_NAME::Bh

10.15.2.13 Bi

`SpeciesName` const KIM::SPECIES_NAME::Bi

10.15.2.14 Bk

`SpeciesName` const KIM::SPECIES_NAME::Bk

10.15.2.15 Br

`SpeciesName` const KIM::SPECIES_NAME::Br

10.15.2.16 C

`SpeciesName` const KIM::SPECIES_NAME::C

10.15.2.17 Ca

`SpeciesName` const KIM::SPECIES_NAME::Ca

10.15.2.18 Cd

`SpeciesName` const KIM::SPECIES_NAME::Cd

10.15.2.19 Ce

`SpeciesName` const KIM::SPECIES_NAME::Ce

10.15.2.20 Cf

`SpeciesName` const KIM::SPECIES_NAME::Cf

10.15.2.21 Cl

`SpeciesName` const KIM::SPECIES_NAME::Cl

10.15.2.22 Cm

`SpeciesName` const KIM::SPECIES_NAME::Cm

10.15.2.23 Cn

`SpeciesName` const KIM::SPECIES_NAME::Cn

10.15.2.24 Co

`SpeciesName` const KIM::SPECIES_NAME::Co

10.15.2.25 Cr

`SpeciesName` const KIM::SPECIES_NAME::Cr

10.15.2.26 Cs

`SpeciesName` const KIM::SPECIES_NAME::Cs

10.15.2.27 Cu

`SpeciesName` const KIM::SPECIES_NAME::Cu

10.15.2.28 Db

`SpeciesName` const KIM::SPECIES_NAME::Db

10.15.2.29 Ds

`SpeciesName` const KIM::SPECIES_NAME::Ds

10.15.2.30 Dy

`SpeciesName` const KIM::SPECIES_NAME::Dy

10.15.2.31 electron

`SpeciesName` const KIM::SPECIES_NAME::electron

10.15.2.32 Er

`SpeciesName` const KIM::SPECIES_NAME::Er

10.15.2.33 Es

`SpeciesName` const KIM::SPECIES_NAME::Es

10.15.2.34 Eu

`SpeciesName` const KIM::SPECIES_NAME::Eu

10.15.2.35 F

`SpeciesName` const KIM::SPECIES_NAME::F

10.15.2.36 Fe

`SpeciesName` const KIM::SPECIES_NAME::Fe

10.15.2.37 Fl

`SpeciesName` const KIM::SPECIES_NAME::Fl

10.15.2.38 Fm

`SpeciesName` const KIM::SPECIES_NAME::Fm

10.15.2.39 Fr

`SpeciesName` const KIM::SPECIES_NAME::Fr

10.15.2.40 Ga

`SpeciesName` const KIM::SPECIES_NAME::Ga

10.15.2.41 Gd

`SpeciesName` const KIM::SPECIES_NAME::Gd

10.15.2.42 Ge

`SpeciesName` const KIM::SPECIES_NAME::Ge

10.15.2.43 H

`SpeciesName` const KIM::SPECIES_NAME::H

10.15.2.44 He

`SpeciesName` const KIM::SPECIES_NAME::He

10.15.2.45 Hf

`SpeciesName` const KIM::SPECIES_NAME::Hf

10.15.2.46 Hg

`SpeciesName` const KIM::SPECIES_NAME::Hg

10.15.2.47 Ho

`SpeciesName` const KIM::SPECIES_NAME::Ho

10.15.2.48 Hs

`SpeciesName` const KIM::SPECIES_NAME::Hs

10.15.2.49 I

`SpeciesName` const KIM::SPECIES_NAME::I

10.15.2.50 In

`SpeciesName` const KIM::SPECIES_NAME::In

10.15.2.51 Ir

`SpeciesName` const KIM::SPECIES_NAME::Ir

10.15.2.52 K

`SpeciesName` const KIM::SPECIES_NAME::K

10.15.2.53 Kr

`SpeciesName` const KIM::SPECIES_NAME::Kr

10.15.2.54 La

`SpeciesName` const KIM::SPECIES_NAME::La

10.15.2.55 Li

`SpeciesName` const KIM::SPECIES_NAME::Li

10.15.2.56 Lr

`SpeciesName` const KIM::SPECIES_NAME::Lr

10.15.2.57 Lu

`SpeciesName` const KIM::SPECIES_NAME::Lu

10.15.2.58 Lv

`SpeciesName` const KIM::SPECIES_NAME::Lv

10.15.2.59 Md

`SpeciesName` const KIM::SPECIES_NAME::Md

10.15.2.60 Mg

`SpeciesName` const KIM::SPECIES_NAME::Mg

10.15.2.61 Mn

`SpeciesName` const KIM::SPECIES_NAME::Mn

10.15.2.62 Mo

`SpeciesName` const KIM::SPECIES_NAME::Mo

10.15.2.63 Mt

`SpeciesName` const KIM::SPECIES_NAME::Mt

10.15.2.64 N

`SpeciesName` const KIM::SPECIES_NAME::N

10.15.2.65 Na

`SpeciesName` const KIM::SPECIES_NAME::Na

10.15.2.66 Nb

`SpeciesName` const KIM::SPECIES_NAME::Nb

10.15.2.67 Nd

`SpeciesName` const KIM::SPECIES_NAME::Nd

10.15.2.68 Ne

`SpeciesName` const KIM::SPECIES_NAME::Ne

10.15.2.69 Ni

`SpeciesName` const KIM::SPECIES_NAME::Ni

10.15.2.70 No

`SpeciesName` const KIM::SPECIES_NAME::No

10.15.2.71 Np

`SpeciesName` const KIM::SPECIES_NAME::Np

10.15.2.72 O

`SpeciesName` const KIM::SPECIES_NAME::O

10.15.2.73 Os

`SpeciesName` const KIM::SPECIES_NAME::Os

10.15.2.74 P

`SpeciesName` const KIM::SPECIES_NAME::P

10.15.2.75 Pa

`SpeciesName` const KIM::SPECIES_NAME::Pa

10.15.2.76 Pb

`SpeciesName` const KIM::SPECIES_NAME::Pb

10.15.2.77 Pd

`SpeciesName` const KIM::SPECIES_NAME::Pd

10.15.2.78 Pm

`SpeciesName` const KIM::SPECIES_NAME::Pm

10.15.2.79 Po

`SpeciesName` const KIM::SPECIES_NAME::Po

10.15.2.80 Pr

`SpeciesName` const KIM::SPECIES_NAME::Pr

10.15.2.81 Pt

`SpeciesName` const KIM::SPECIES_NAME::Pt

10.15.2.82 Pu

`SpeciesName` const KIM::SPECIES_NAME::Pu

10.15.2.83 Ra

`SpeciesName` const KIM::SPECIES_NAME::Ra

10.15.2.84 Rb

`SpeciesName` const KIM::SPECIES_NAME::Rb

10.15.2.85 Re

`SpeciesName` const KIM::SPECIES_NAME::Re

10.15.2.86 Rf

`SpeciesName` const KIM::SPECIES_NAME::Rf

10.15.2.87 Rg

`SpeciesName` const KIM::SPECIES_NAME::Rg

10.15.2.88 Rh

`SpeciesName` const KIM::SPECIES_NAME::Rh

10.15.2.89 Rn

`SpeciesName` const KIM::SPECIES_NAME::Rn

10.15.2.90 Ru

`SpeciesName` const KIM::SPECIES_NAME::Ru

10.15.2.91 S

`SpeciesName` const KIM::SPECIES_NAME::S

10.15.2.92 Sb

`SpeciesName` const KIM::SPECIES_NAME::Sb

10.15.2.93 Sc

`SpeciesName` const KIM::SPECIES_NAME::Sc

10.15.2.94 Se

`SpeciesName` const KIM::SPECIES_NAME::Se

10.15.2.95 Sg

`SpeciesName` const KIM::SPECIES_NAME::Sg

10.15.2.96 Si

`SpeciesName` const KIM::SPECIES_NAME::Si

10.15.2.97 Sm

`SpeciesName` const KIM::SPECIES_NAME::Sm

10.15.2.98 Sn

`SpeciesName` const KIM::SPECIES_NAME::Sn

10.15.2.99 Sr

`SpeciesName` const KIM::SPECIES_NAME::Sr

10.15.2.100 Ta

`SpeciesName` const KIM::SPECIES_NAME::Ta

10.15.2.101 Tb

`SpeciesName` const KIM::SPECIES_NAME::Tb

10.15.2.102 Tc

`SpeciesName` const KIM::SPECIES_NAME::Tc

10.15.2.103 Te

`SpeciesName` const KIM::SPECIES_NAME::Te

10.15.2.104 Th

`SpeciesName` const KIM::SPECIES_NAME::Th

10.15.2.105 Ti

`SpeciesName` const KIM::SPECIES_NAME::Ti

10.15.2.106 Tl

`SpeciesName` const KIM::SPECIES_NAME::Tl

10.15.2.107 Tm

`SpeciesName` const KIM::SPECIES_NAME::Tm

10.15.2.108 U

`SpeciesName` const KIM::SPECIES_NAME::U

10.15.2.109 user01

`SpeciesName` const KIM::SPECIES_NAME::user01

10.15.2.110 user02

`SpeciesName` const KIM::SPECIES_NAME::user02

10.15.2.111 user03

`SpeciesName` const KIM::SPECIES_NAME::user03

10.15.2.112 user04

`SpeciesName` const KIM::SPECIES_NAME::user04

10.15.2.113 user05

`SpeciesName` const KIM::SPECIES_NAME::user05

10.15.2.114 user06

`SpeciesName` const KIM::SPECIES_NAME::user06

10.15.2.115 user07

`SpeciesName` const KIM::SPECIES_NAME::user07

10.15.2.116 user08

`SpeciesName` const KIM::SPECIES_NAME::user08

10.15.2.117 user09

`SpeciesName` const KIM::SPECIES_NAME::user09

10.15.2.118 user10

`SpeciesName` const KIM::SPECIES_NAME::user10

10.15.2.119 user11

`SpeciesName` const KIM::SPECIES_NAME::user11

10.15.2.120 user12

`SpeciesName` const KIM::SPECIES_NAME::user12

10.15.2.121 user13

`SpeciesName` const KIM::SPECIES_NAME::user13

10.15.2.122 user14

`SpeciesName` const KIM::SPECIES_NAME::user14

10.15.2.123 user15

`SpeciesName` const KIM::SPECIES_NAME::user15

10.15.2.124 user16

`SpeciesName` const KIM::SPECIES_NAME::user16

10.15.2.125 user17

`SpeciesName` const KIM::SPECIES_NAME::user17

10.15.2.126 user18

`SpeciesName` const KIM::SPECIES_NAME::user18

10.15.2.127 user19

`SpeciesName` const KIM::SPECIES_NAME::user19

10.15.2.128 user20

`SpeciesName` const KIM::SPECIES_NAME::user20

10.15.2.129 Uuo

`SpeciesName` const KIM::SPECIES_NAME::Uuo

10.15.2.130 Uup

`SpeciesName` const KIM::SPECIES_NAME::Uup

10.15.2.131 Uus

`SpeciesName` const KIM::SPECIES_NAME::Uus

10.15.2.132 Uut

`SpeciesName` const KIM::SPECIES_NAME::Uut

10.15.2.133 V

`SpeciesName` const KIM::SPECIES_NAME::V

10.15.2.134 W

`SpeciesName` const KIM::SPECIES_NAME::W

10.15.2.135 Xe

`SpeciesName` const KIM::SPECIES_NAME::Xe

10.15.2.136 Y

`SpeciesName` const KIM::SPECIES_NAME::Y

10.15.2.137 Yb

`SpeciesName` const KIM::SPECIES_NAME::Yb

10.15.2.138 Zn

`SpeciesName` const KIM::SPECIES_NAME::Zn

10.15.2.139 Zr

`SpeciesName` const KIM::SPECIES_NAME::Zr

10.16 KIM::SUPPORT_STATUS Namespace Reference

Classes

- struct [Comparator](#)

Functions

- void [GetNumberOfSupportStatuses](#) (int *const numberOfSupportStatuses)
- int [GetSupportStatus](#) (int const index, [SupportStatus](#) *const supportStatus)

Variables

- [SupportStatus](#) const [requiredByAPI](#)
- [SupportStatus](#) const [notSupported](#)
- [SupportStatus](#) const [required](#)
- [SupportStatus](#) const [optional](#)

10.16.1 Function Documentation

10.16.1.1 GetNumberOfSupportStatuses()

```
void KIM::SUPPORT_STATUS::GetNumberOfSupportStatuses (
    int *const numberOfSupportStatuses )
```

10.16.1.2 GetSupportStatus()

```
int KIM::SUPPORT_STATUS::GetSupportStatus (
    int const index,
    SupportStatus *const supportStatus )
```

10.16.2 Variable Documentation

10.16.2.1 notSupported

```
SupportStatus const KIM::SUPPORT_STATUS::notSupported
```

10.16.2.2 optional

```
SupportStatus const KIM::SUPPORT_STATUS::optional
```

10.16.2.3 required

```
SupportStatus const KIM::SUPPORT_STATUS::required
```

10.16.2.4 requiredByAPI

```
SupportStatus const KIM::SUPPORT_STATUS::requiredByAPI
```

10.17 KIM::TEMPERATURE_UNIT Namespace Reference

Classes

- struct [Comparator](#)

Functions

- void [GetNumberOfTemperatureUnits](#) (int *const numberOfTemperatureUnits)
- int [GetTemperatureUnit](#) (int const index, [TemperatureUnit](#) *const temperatureUnit)

Variables

- [TemperatureUnit](#) const [unused](#)
- [TemperatureUnit](#) const [K](#)

10.17.1 Function Documentation

10.17.1.1 [GetNumberOfTemperatureUnits\(\)](#)

```
void KIM::TEMPERATURE_UNIT::GetNumberOfTemperatureUnits (  
    int *const numberOfTemperatureUnits )
```

10.17.1.2 [GetTemperatureUnit\(\)](#)

```
int KIM::TEMPERATURE_UNIT::GetTemperatureUnit (  
    int const index,  
    TemperatureUnit *const temperatureUnit )
```

10.17.2 Variable Documentation

10.17.2.1 [K](#)

```
TemperatureUnit const KIM::TEMPERATURE_UNIT::K
```

10.17.2.2 [unused](#)

```
TemperatureUnit const KIM::TEMPERATURE_UNIT::unused
```

10.18 KIM::TIME_UNIT Namespace Reference

Classes

- struct [Comparator](#)

Functions

- void [GetNumberOfTimeUnits](#) (int *const numberOfTimeUnits)
- int [GetTimeUnit](#) (int const index, [TimeUnit](#) *const timeUnit)

Variables

- [TimeUnit](#) const [unused](#)
- [TimeUnit](#) const [fs](#)
- [TimeUnit](#) const [ps](#)
- [TimeUnit](#) const [ns](#)
- [TimeUnit](#) const [s](#)

10.18.1 Function Documentation

10.18.1.1 GetNumberOfTimeUnits()

```
void KIM::TIME_UNIT::GetNumberOfTimeUnits (  
    int *const numberOfTimeUnits )
```

10.18.1.2 GetTimeUnit()

```
int KIM::TIME_UNIT::GetTimeUnit (  
    int const index,  
    TimeUnit *const timeUnit )
```

10.18.2 Variable Documentation

10.18.2.1 fs

```
TimeUnit const KIM::TIME_UNIT::fs
```

10.18.2.2 ns

`TimeUnit` const KIM::TIME_UNIT::ns

10.18.2.3 ps

`TimeUnit` const KIM::TIME_UNIT::ps

10.18.2.4 s

`TimeUnit` const KIM::TIME_UNIT::s

10.18.2.5 unused

`TimeUnit` const KIM::TIME_UNIT::unused

10.19 kim_charge_unit_module Module Reference

Variables

- type(kim_charge_unit_type), public, protected [kim_charge_unit_unused](#)
- type(kim_charge_unit_type), public, protected [kim_charge_unit_c](#)
- type(kim_charge_unit_type), public, protected [kim_charge_unit_e](#)
- type(kim_charge_unit_type), public, protected [kim_charge_unit_statc](#)

10.19.1 Variable Documentation

10.19.1.1 kim_charge_unit_c

type(kim_charge_unit_type), public, protected kim_charge_unit_module::kim_charge_unit_c

Definition at line 62 of file kim_charge_unit_module.f90.

10.19.1.2 kim_charge_unit_e

```
type(kim_charge_unit_type), public, protected kim_charge_unit_module::kim_charge_unit_e
```

Definition at line 65 of file kim_charge_unit_module.f90.

10.19.1.3 kim_charge_unit_statc

```
type(kim_charge_unit_type), public, protected kim_charge_unit_module::kim_charge_unit_statc
```

Definition at line 68 of file kim_charge_unit_module.f90.

10.19.1.4 kim_charge_unit_unused

```
type(kim_charge_unit_type), public, protected kim_charge_unit_module::kim_charge_unit_unused
```

Definition at line 59 of file kim_charge_unit_module.f90.

10.20 kim_compute_argument_name_module Module Reference**Variables**

- type(kim_compute_argument_name_type), public, protected [kim_compute_argument_name_number_of_particles](#)
- type(kim_compute_argument_name_type), public, protected [kim_compute_argument_name_particle_species_codes](#)
- type(kim_compute_argument_name_type), public, protected [kim_compute_argument_name_particle_contributing](#)
- type(kim_compute_argument_name_type), public, protected [kim_compute_argument_name_coordinates](#)
- type(kim_compute_argument_name_type), public, protected [kim_compute_argument_name_partial_energy](#)
- type(kim_compute_argument_name_type), public, protected [kim_compute_argument_name_partial_forces](#)
- type(kim_compute_argument_name_type), public, protected [kim_compute_argument_name_partial_particle_energy](#)
- type(kim_compute_argument_name_type), public, protected [kim_compute_argument_name_partial_virial](#)
- type(kim_compute_argument_name_type), public, protected [kim_compute_argument_name_partial_particle_virial](#)

10.20.1 Variable Documentation**10.20.1.1 kim_compute_argument_name_coordinates**

```
type(kim_compute_argument_name_type), public, protected kim_compute_argument_name_module↵  
::kim_compute_argument_name_coordinates
```

Definition at line 74 of file kim_compute_argument_name_module.f90.

10.20.1.2 kim_compute_argument_name_number_of_particles

```
type(kim_compute_argument_name_type), public, protected kim_compute_argument_name_module↔  
::kim_compute_argument_name_number_of_particles
```

Definition at line 65 of file kim_compute_argument_name_module.f90.

10.20.1.3 kim_compute_argument_name_partial_energy

```
type(kim_compute_argument_name_type), public, protected kim_compute_argument_name_module↔  
::kim_compute_argument_name_partial_energy
```

Definition at line 77 of file kim_compute_argument_name_module.f90.

10.20.1.4 kim_compute_argument_name_partial_forces

```
type(kim_compute_argument_name_type), public, protected kim_compute_argument_name_module↔  
::kim_compute_argument_name_partial_forces
```

Definition at line 80 of file kim_compute_argument_name_module.f90.

10.20.1.5 kim_compute_argument_name_partial_particle_energy

```
type(kim_compute_argument_name_type), public, protected kim_compute_argument_name_module↔  
::kim_compute_argument_name_partial_particle_energy
```

Definition at line 83 of file kim_compute_argument_name_module.f90.

10.20.1.6 kim_compute_argument_name_partial_particle_virial

```
type(kim_compute_argument_name_type), public, protected kim_compute_argument_name_module↔  
::kim_compute_argument_name_partial_particle_virial
```

Definition at line 89 of file kim_compute_argument_name_module.f90.

10.20.1.7 kim_compute_argument_name_partial_virial

```
type(kim_compute_argument_name_type), public, protected kim_compute_argument_name_module↔  
::kim_compute_argument_name_partial_virial
```

Definition at line 86 of file kim_compute_argument_name_module.f90.

10.20.1.8 kim_compute_argument_name_particle_contributing

```
type(kim_compute_argument_name_type), public, protected kim_compute_argument_name_module↔
::kim_compute_argument_name_particle_contributing
```

Definition at line 71 of file kim_compute_argument_name_module.f90.

10.20.1.9 kim_compute_argument_name_particle_species_codes

```
type(kim_compute_argument_name_type), public, protected kim_compute_argument_name_module↔
::kim_compute_argument_name_particle_species_codes
```

Definition at line 68 of file kim_compute_argument_name_module.f90.

10.21 kim_compute_arguments_module Module Reference

Data Types

- interface [kim_compute_arguments_are_all_required_present](#)
- interface [kim_compute_arguments_get_argument_support_status](#)
- interface [kim_compute_arguments_get_callback_support_status](#)
- interface [kim_compute_arguments_pop_log_verbosity](#)
- interface [kim_compute_arguments_set_callback_pointer](#)

Variables

- type(kim_compute_arguments_handle_type), public, protected [kim_compute_arguments_null_handle](#)

10.21.1 Variable Documentation

10.21.1.1 kim_compute_arguments_null_handle

```
type(kim_compute_arguments_handle_type), public, protected kim_compute_arguments_module::kim↔
_compute_arguments_null_handle
```

Definition at line 60 of file kim_compute_arguments_module.f90.

10.22 kim_compute_callback_name_module Module Reference

Variables

- type(kim_compute_callback_name_type), public, protected [kim_compute_callback_name_get_neighbor_list](#)
- type(kim_compute_callback_name_type), public, protected [kim_compute_callback_name_process_dedr_term](#)
- type(kim_compute_callback_name_type), public, protected [kim_compute_callback_name_process_d2edr2_term](#)

10.22.1 Variable Documentation

10.22.1.1 kim_compute_callback_name_get_neighbor_list

```
type(kim_compute_callback_name_type), public, protected kim_compute_callback_name_module↔  
::kim_compute_callback_name_get_neighbor_list
```

Definition at line 58 of file kim_compute_callback_name_module.f90.

10.22.1.2 kim_compute_callback_name_process_d2edr2_term

```
type(kim_compute_callback_name_type), public, protected kim_compute_callback_name_module↔  
::kim_compute_callback_name_process_d2edr2_term
```

Definition at line 64 of file kim_compute_callback_name_module.f90.

10.22.1.3 kim_compute_callback_name_process_dedr_term

```
type(kim_compute_callback_name_type), public, protected kim_compute_callback_name_module↔  
::kim_compute_callback_name_process_dedr_term
```

Definition at line 61 of file kim_compute_callback_name_module.f90.

10.23 kim_data_type_module Module Reference

Variables

- type(kim_data_type_type), public, protected [kim_data_type_integer](#)
- type(kim_data_type_type), public, protected [kim_data_type_double](#)

10.23.1 Variable Documentation

10.23.1.1 kim_data_type_double

```
type(kim_data_type_type), public, protected kim_data_type_module::kim_data_type_double
```

Definition at line 60 of file kim_data_type_module.f90.

10.23.1.2 kim_data_type_integer

```
type(kim_data_type_type), public, protected kim_data_type_module::kim_data_type_integer
```

Definition at line 57 of file kim_data_type_module.f90.

10.24 kim_energy_unit_module Module Reference

Variables

- type(kim_energy_unit_type), public, protected [kim_energy_unit_unused](#)
- type(kim_energy_unit_type), public, protected [kim_energy_unit_amu_a2_per_ps2](#)
- type(kim_energy_unit_type), public, protected [kim_energy_unit_erg](#)
- type(kim_energy_unit_type), public, protected [kim_energy_unit_ev](#)
- type(kim_energy_unit_type), public, protected [kim_energy_unit_hartree](#)
- type(kim_energy_unit_type), public, protected [kim_energy_unit_j](#)
- type(kim_energy_unit_type), public, protected [kim_energy_unit_kcal_mol](#)

10.24.1 Variable Documentation

10.24.1.1 kim_energy_unit_amu_a2_per_ps2

```
type(kim_energy_unit_type), public, protected kim_energy_unit_module::kim_energy_unit_amu_a2↵_per_ps2
```

Definition at line 65 of file kim_energy_unit_module.f90.

10.24.1.2 kim_energy_unit_erg

```
type(kim_energy_unit_type), public, protected kim_energy_unit_module::kim_energy_unit_erg
```

Definition at line 68 of file kim_energy_unit_module.f90.

10.24.1.3 kim_energy_unit_ev

```
type(kim_energy_unit_type), public, protected kim_energy_unit_module::kim_energy_unit_ev
```

Definition at line 71 of file kim_energy_unit_module.f90.

10.24.1.4 kim_energy_unit_hartree

```
type(kim_energy_unit_type), public, protected kim_energy_unit_module::kim_energy_unit_hartree
```

Definition at line 74 of file kim_energy_unit_module.f90.

10.24.1.5 kim_energy_unit_j

```
type(kim_energy_unit_type), public, protected kim_energy_unit_module::kim_energy_unit_j
```

Definition at line 77 of file kim_energy_unit_module.f90.

10.24.1.6 kim_energy_unit_kcal_mol

```
type(kim_energy_unit_type), public, protected kim_energy_unit_module::kim_energy_unit_kcal_mol
```

Definition at line 80 of file kim_energy_unit_module.f90.

10.24.1.7 kim_energy_unit_unused

```
type(kim_energy_unit_type), public, protected kim_energy_unit_module::kim_energy_unit_unused
```

Definition at line 62 of file kim_energy_unit_module.f90.

10.25 kim_language_name_module Module Reference

Variables

- type(kim_language_name_type), public, protected [kim_language_name_cpp](#)
- type(kim_language_name_type), public, protected [kim_language_name_c](#)
- type(kim_language_name_type), public, protected [kim_language_name_fortran](#)

10.25.1 Variable Documentation

10.25.1.1 kim_language_name_c

```
type(kim_language_name_type), public, protected kim_language_name_module::kim_language_name_c
```

Definition at line 61 of file kim_language_name_module.f90.

10.25.1.2 kim_language_name_cpp

```
type(kim_language_name_type), public, protected kim_language_name_module::kim_language_name_↵  
cpp
```

Definition at line 58 of file kim_language_name_module.f90.

10.25.1.3 kim_language_name_fortran

```
type(kim_language_name_type), public, protected kim_language_name_module::kim_language_name_↵  
fortran
```

Definition at line 64 of file kim_language_name_module.f90.

10.26 kim_length_unit_module Module Reference

Variables

- type(kim_length_unit_type), public, protected [kim_length_unit_unused](#)
- type(kim_length_unit_type), public, protected [kim_length_unit_a](#)
- type(kim_length_unit_type), public, protected [kim_length_unit_bohr](#)
- type(kim_length_unit_type), public, protected [kim_length_unit_cm](#)
- type(kim_length_unit_type), public, protected [kim_length_unit_m](#)
- type(kim_length_unit_type), public, protected [kim_length_unit_nm](#)

10.26.1 Variable Documentation

10.26.1.1 kim_length_unit_a

```
type(kim_length_unit_type), public, protected kim_length_unit_module::kim_length_unit_a
```

Definition at line 64 of file kim_length_unit_module.f90.

10.26.1.2 kim_length_unit_bohr

```
type(kim_length_unit_type), public, protected kim_length_unit_module::kim_length_unit_bohr
```

Definition at line 67 of file kim_length_unit_module.f90.

10.26.1.3 kim_length_unit_cm

```
type(kim_length_unit_type), public, protected kim_length_unit_module::kim_length_unit_cm
```

Definition at line 70 of file kim_length_unit_module.f90.

10.26.1.4 kim_length_unit_m

```
type(kim_length_unit_type), public, protected kim_length_unit_module::kim_length_unit_m
```

Definition at line 73 of file kim_length_unit_module.f90.

10.26.1.5 kim_length_unit_nm

```
type(kim_length_unit_type), public, protected kim_length_unit_module::kim_length_unit_nm
```

Definition at line 76 of file kim_length_unit_module.f90.

10.26.1.6 kim_length_unit_unused

```
type(kim_length_unit_type), public, protected kim_length_unit_module::kim_length_unit_unused
```

Definition at line 61 of file kim_length_unit_module.f90.

10.27 kim_log_module Module Reference

Data Types

- interface [kim_log_pop_verbosity](#)

Variables

- type(kim_log_handle_type), public, protected [kim_log_null_handle](#)

10.27.1 Variable Documentation

10.27.1.1 kim_log_null_handle

```
type(kim_log_handle_type), public, protected kim_log_module::kim_log_null_handle
```

Definition at line 56 of file kim_log_module.f90.

10.28 kim_log_verbosity_module Module Reference

Variables

- type(kim_log_verbosity_type), public, protected [kim_log_verbosity_silent](#)
- type(kim_log_verbosity_type), public, protected [kim_log_verbosity_fatal](#)
- type(kim_log_verbosity_type), public, protected [kim_log_verbosity_error](#)
- type(kim_log_verbosity_type), public, protected [kim_log_verbosity_warning](#)
- type(kim_log_verbosity_type), public, protected [kim_log_verbosity_information](#)
- type(kim_log_verbosity_type), public, protected [kim_log_verbosity_debug](#)
- character(len=4096, kind=c_char), public [kim_log_file](#)
- character(len=65536, kind=c_char), public [kim_log_message](#)

10.28.1 Variable Documentation

10.28.1.1 kim_log_file

```
character(len=4096, kind=c_char), public kim_log_verbosity_module::kim_log_file
```

Definition at line 181 of file kim_log_verbosity_module.f90.

10.28.1.2 kim_log_message

```
character(len=65536, kind=c_char), public kim_log_verbosity_module::kim_log_message
```

Definition at line 182 of file kim_log_verbosity_module.f90.

10.28.1.3 kim_log_verbosity_debug

```
type(kim_log_verbosity_type), public, protected kim_log_verbosity_module::kim_log_verbosity_↔  
debug
```

Definition at line 83 of file kim_log_verbosity_module.f90.

10.28.1.4 kim_log_verbosity_error

```
type(kim_log_verbosity_type), public, protected kim_log_verbosity_module::kim_log_verbosity_↵  
error
```

Definition at line 74 of file kim_log_verbosity_module.f90.

10.28.1.5 kim_log_verbosity_fatal

```
type(kim_log_verbosity_type), public, protected kim_log_verbosity_module::kim_log_verbosity_↵  
fatal
```

Definition at line 71 of file kim_log_verbosity_module.f90.

10.28.1.6 kim_log_verbosity_information

```
type(kim_log_verbosity_type), public, protected kim_log_verbosity_module::kim_log_verbosity_↵  
information
```

Definition at line 80 of file kim_log_verbosity_module.f90.

10.28.1.7 kim_log_verbosity_silent

```
type(kim_log_verbosity_type), public, protected kim_log_verbosity_module::kim_log_verbosity_↵  
silent
```

Definition at line 68 of file kim_log_verbosity_module.f90.

10.28.1.8 kim_log_verbosity_warning

```
type(kim_log_verbosity_type), public, protected kim_log_verbosity_module::kim_log_verbosity_↵  
warning
```

Definition at line 77 of file kim_log_verbosity_module.f90.

10.29 kim_model_compute_arguments_create_module Module Reference

Data Types

- interface [kim_model_compute_arguments_create_set_callback_support_status](#)
- interface [kim_model_compute_arguments_create_set_model_buffer_pointer](#)
- interface [kim_model_compute_arguments_create_string](#)

Variables

- type(kim_model_compute_arguments_create_handle_type), public, protected [kim_model_compute_arguments_create_null_handle](#)

10.29.1 Variable Documentation

10.29.1.1 kim_model_compute_arguments_create_null_handle

```
type(kim_model_compute_arguments_create_handle_type), public, protected kim_model_compute_↵
arguments_create_module::kim_model_compute_arguments_create_null_handle
```

Definition at line 54 of file kim_model_compute_arguments_create_module.f90.

10.30 kim_model_compute_arguments_destroy_module Module Reference

Data Types

- interface [kim_model_compute_arguments_destroy_string](#)

Variables

- type(kim_model_compute_arguments_destroy_handle_type), public, protected [kim_model_compute_arguments_destroy_null_handle](#)

10.30.1 Variable Documentation

10.30.1.1 kim_model_compute_arguments_destroy_null_handle

```
type(kim_model_compute_arguments_destroy_handle_type), public, protected kim_model_compute_↵
arguments_destroy_module::kim_model_compute_arguments_destroy_null_handle
```

Definition at line 52 of file kim_model_compute_arguments_destroy_module.f90.

10.31 kim_model_compute_arguments_module Module Reference

Data Types

- interface [kim_model_compute_arguments_get_neighbor_list](#)
- interface [kim_model_compute_arguments_set_model_buffer_pointer](#)
- interface [kim_model_compute_arguments_string](#)

Variables

- type(kim_model_compute_arguments_handle_type), public, protected [kim_model_compute_arguments_null_handle](#)

10.31.1 Variable Documentation

10.31.1.1 kim_model_compute_arguments_null_handle

```
type(kim_model_compute_arguments_handle_type), public, protected kim_model_compute_arguments↔  
_module::kim_model_compute_arguments_null_handle
```

Definition at line 58 of file kim_model_compute_arguments_module.f90.

10.32 kim_model_compute_module Module Reference

Data Types

- interface [kim_model_compute_string](#)

Variables

- type(kim_model_compute_handle_type), public, protected [kim_model_compute_null_handle](#)

10.32.1 Variable Documentation

10.32.1.1 kim_model_compute_null_handle

```
type(kim_model_compute_handle_type), public, protected kim_model_compute_module::kim_model↔  
compute_null_handle
```

Definition at line 52 of file kim_model_compute_module.f90.

10.33 kim_model_create_module Module Reference

Data Types

- interface [kim_model_create_convert_unit](#)
- interface [kim_model_create_log_entry](#)
- interface [kim_model_create_set_compute_arguments_create_pointer](#)
- interface [kim_model_create_set_compute_arguments_destroy_pointer](#)
- interface [kim_model_create_set_compute_pointer](#)
- interface [kim_model_create_set_destroy_pointer](#)
- interface [kim_model_create_set_influence_distance_pointer](#)
- interface [kim_model_create_set_model_buffer_pointer](#)
- interface [kim_model_create_set_species_code](#)
- interface [kim_model_create_string](#)

Variables

- type(kim_model_create_handle_type), public, protected [kim_model_create_null_handle](#)

10.33.1 Variable Documentation

10.33.1.1 kim_model_create_null_handle

```
type(kim_model_create_handle_type), public, protected kim_model_create_module::kim_model_create_null_handle
```

Definition at line 64 of file kim_model_create_module.f90.

10.34 kim_model_destroy_module Module Reference

Data Types

- interface [kim_model_destroy_string](#)

Variables

- type(kim_model_destroy_handle_type), public, protected [kim_model_destroy_null_handle](#)

10.34.1 Variable Documentation

10.34.1.1 kim_model_destroy_null_handle

```
type(kim_model_destroy_handle_type), public, protected kim_model_destroy_module::kim_model_destroy_null_handle
```

Definition at line 52 of file kim_model_destroy_module.f90.

10.35 kim_model_driver_create_module Module Reference

Data Types

- interface [kim_model_driver_create_convert_unit](#)
- interface [kim_model_driver_create_log_entry](#)
- interface [kim_model_driver_create_set_compute_arguments_create_pointer](#)
- interface [kim_model_driver_create_set_compute_arguments_destroy_pointer](#)
- interface [kim_model_driver_create_set_compute_pointer](#)
- interface [kim_model_driver_create_set_destroy_pointer](#)
- interface [kim_model_driver_create_set_influence_distance_pointer](#)
- interface [kim_model_driver_create_set_model_buffer_pointer](#)
- interface [kim_model_driver_create_set_species_code](#)
- interface [kim_model_driver_create_string](#)

Variables

- `type(kim_model_driver_create_handle_type)`, public, protected [kim_model_driver_create_null_handle](#)

10.35.1 Variable Documentation

10.35.1.1 kim_model_driver_create_null_handle

```
type(kim_model_driver_create_handle_type), public, protected kim_model_driver_create_module↔
::kim_model_driver_create_null_handle
```

Definition at line 66 of file `kim_model_driver_create_module.f90`.

10.36 kim_model_driver_headers_module Module Reference

10.37 kim_model_headers_module Module Reference

10.38 kim_model_module Module Reference

Data Types

- interface [kim_model_clear_influence_dist_and_cutoffs_then_refresh_model](#)
- interface [kim_model_compute](#)
- interface [kim_model_compute_arguments_create](#)
- interface [kim_model_compute_arguments_destroy](#)
- interface [kim_model_destroy](#)
- interface [kim_model_get_number_of_parameters](#)
- interface [kim_model_pop_log_verbosity](#)
- interface [kim_model_set_simulator_buffer_pointer](#)

Variables

- `type(kim_model_handle_type)`, public, protected [kim_model_null_handle](#)

10.38.1 Variable Documentation

10.38.1.1 kim_model_null_handle

```
type(kim_model_handle_type), public, protected kim_model_module::kim_model_null_handle
```

Definition at line 71 of file `kim_model_module.f90`.

10.39 kim_model_refresh_module Module Reference

Data Types

- interface [kim_model_refresh_string](#)

Variables

- type(kim_model_refresh_handle_type), public, protected [kim_model_refresh_null_handle](#)

10.39.1 Variable Documentation

10.39.1.1 kim_model_refresh_null_handle

```
type(kim_model_refresh_handle_type), public, protected kim_model_refresh_module::kim_model_↵  
refresh_null_handle
```

Definition at line 54 of file kim_model_refresh_module.f90.

10.40 kim_numbering_module Module Reference

Variables

- type(kim_numbering_type), public, protected [kim_numbering_zero_based](#)
- type(kim_numbering_type), public, protected [kim_numbering_one_based](#)

10.40.1 Variable Documentation

10.40.1.1 kim_numbering_one_based

```
type(kim_numbering_type), public, protected kim_numbering_module::kim_numbering_one_based
```

Definition at line 60 of file kim_numbering_module.f90.

10.40.1.2 kim_numbering_zero_based

```
type(kim_numbering_type), public, protected kim_numbering_module::kim_numbering_zero_based
```

Definition at line 57 of file kim_numbering_module.f90.

10.41 kim_sem_ver_module Module Reference

10.42 kim_simulator_headers_module Module Reference

10.43 kim_species_name_module Module Reference

Variables

- type(kim_species_name_type), public, protected [kim_species_name_electron](#)
- type(kim_species_name_type), public, protected [kim_species_name_h](#)
- type(kim_species_name_type), public, protected [kim_species_name_he](#)
- type(kim_species_name_type), public, protected [kim_species_name_li](#)
- type(kim_species_name_type), public, protected [kim_species_name_be](#)
- type(kim_species_name_type), public, protected [kim_species_name_b](#)
- type(kim_species_name_type), public, protected [kim_species_name_c](#)
- type(kim_species_name_type), public, protected [kim_species_name_n](#)
- type(kim_species_name_type), public, protected [kim_species_name_o](#)
- type(kim_species_name_type), public, protected [kim_species_name_f](#)
- type(kim_species_name_type), public, protected [kim_species_name_ne](#)
- type(kim_species_name_type), public, protected [kim_species_name_na](#)
- type(kim_species_name_type), public, protected [kim_species_name_mg](#)
- type(kim_species_name_type), public, protected [kim_species_name_al](#)
- type(kim_species_name_type), public, protected [kim_species_name_si](#)
- type(kim_species_name_type), public, protected [kim_species_name_p](#)
- type(kim_species_name_type), public, protected [kim_species_name_s](#)
- type(kim_species_name_type), public, protected [kim_species_name_cl](#)
- type(kim_species_name_type), public, protected [kim_species_name_ar](#)
- type(kim_species_name_type), public, protected [kim_species_name_k](#)
- type(kim_species_name_type), public, protected [kim_species_name_ca](#)
- type(kim_species_name_type), public, protected [kim_species_name_sc](#)
- type(kim_species_name_type), public, protected [kim_species_name_ti](#)
- type(kim_species_name_type), public, protected [kim_species_name_v](#)
- type(kim_species_name_type), public, protected [kim_species_name_cr](#)
- type(kim_species_name_type), public, protected [kim_species_name_mn](#)
- type(kim_species_name_type), public, protected [kim_species_name_fe](#)
- type(kim_species_name_type), public, protected [kim_species_name_co](#)
- type(kim_species_name_type), public, protected [kim_species_name_ni](#)
- type(kim_species_name_type), public, protected [kim_species_name_cu](#)
- type(kim_species_name_type), public, protected [kim_species_name_zn](#)
- type(kim_species_name_type), public, protected [kim_species_name_ga](#)
- type(kim_species_name_type), public, protected [kim_species_name_ge](#)
- type(kim_species_name_type), public, protected [kim_species_name_as](#)
- type(kim_species_name_type), public, protected [kim_species_name_se](#)
- type(kim_species_name_type), public, protected [kim_species_name_br](#)
- type(kim_species_name_type), public, protected [kim_species_name_kr](#)
- type(kim_species_name_type), public, protected [kim_species_name_rb](#)
- type(kim_species_name_type), public, protected [kim_species_name_sr](#)
- type(kim_species_name_type), public, protected [kim_species_name_y](#)
- type(kim_species_name_type), public, protected [kim_species_name_zr](#)
- type(kim_species_name_type), public, protected [kim_species_name_nb](#)
- type(kim_species_name_type), public, protected [kim_species_name_mo](#)
- type(kim_species_name_type), public, protected [kim_species_name_tc](#)

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- `type(kim_species_name_type), public, protected` [kim_species_name_es](#)
- `type(kim_species_name_type), public, protected` [kim_species_name_fm](#)
- `type(kim_species_name_type), public, protected` [kim_species_name_md](#)
- `type(kim_species_name_type), public, protected` [kim_species_name_no](#)
- `type(kim_species_name_type), public, protected` [kim_species_name_lr](#)
- `type(kim_species_name_type), public, protected` [kim_species_name_rf](#)
- `type(kim_species_name_type), public, protected` [kim_species_name_db](#)
- `type(kim_species_name_type), public, protected` [kim_species_name_sg](#)
- `type(kim_species_name_type), public, protected` [kim_species_name_bh](#)
- `type(kim_species_name_type), public, protected` [kim_species_name_hs](#)
- `type(kim_species_name_type), public, protected` [kim_species_name_mt](#)
- `type(kim_species_name_type), public, protected` [kim_species_name_ds](#)
- `type(kim_species_name_type), public, protected` [kim_species_name_rg](#)
- `type(kim_species_name_type), public, protected` [kim_species_name_cn](#)
- `type(kim_species_name_type), public, protected` [kim_species_name_uut](#)
- `type(kim_species_name_type), public, protected` [kim_species_name_fl](#)
- `type(kim_species_name_type), public, protected` [kim_species_name_uup](#)
- `type(kim_species_name_type), public, protected` [kim_species_name_lv](#)
- `type(kim_species_name_type), public, protected` [kim_species_name_uus](#)
- `type(kim_species_name_type), public, protected` [kim_species_name_uuo](#)
- `type(kim_species_name_type), public, protected` [kim_species_name_user01](#)
- `type(kim_species_name_type), public, protected` [kim_species_name_user02](#)
- `type(kim_species_name_type), public, protected` [kim_species_name_user03](#)
- `type(kim_species_name_type), public, protected` [kim_species_name_user04](#)
- `type(kim_species_name_type), public, protected` [kim_species_name_user05](#)
- `type(kim_species_name_type), public, protected` [kim_species_name_user06](#)
- `type(kim_species_name_type), public, protected` [kim_species_name_user07](#)
- `type(kim_species_name_type), public, protected` [kim_species_name_user08](#)
- `type(kim_species_name_type), public, protected` [kim_species_name_user09](#)
- `type(kim_species_name_type), public, protected` [kim_species_name_user10](#)
- `type(kim_species_name_type), public, protected` [kim_species_name_user11](#)
- `type(kim_species_name_type), public, protected` [kim_species_name_user12](#)
- `type(kim_species_name_type), public, protected` [kim_species_name_user13](#)
- `type(kim_species_name_type), public, protected` [kim_species_name_user14](#)
- `type(kim_species_name_type), public, protected` [kim_species_name_user15](#)
- `type(kim_species_name_type), public, protected` [kim_species_name_user16](#)
- `type(kim_species_name_type), public, protected` [kim_species_name_user17](#)
- `type(kim_species_name_type), public, protected` [kim_species_name_user18](#)
- `type(kim_species_name_type), public, protected` [kim_species_name_user19](#)
- `type(kim_species_name_type), public, protected` [kim_species_name_user20](#)

10.43.1 Variable Documentation

10.43.1.1 `kim_species_name_ac`

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_ac
```

Definition at line 460 of file `kim_species_name_module.f90`.

10.43.1.2 kim_species_name_ag

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_ag
```

Definition at line 334 of file kim_species_name_module.f90.

10.43.1.3 kim_species_name_al

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_al
```

Definition at line 232 of file kim_species_name_module.f90.

10.43.1.4 kim_species_name_am

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_am
```

Definition at line 478 of file kim_species_name_module.f90.

10.43.1.5 kim_species_name_ar

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_ar
```

Definition at line 247 of file kim_species_name_module.f90.

10.43.1.6 kim_species_name_as

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_as
```

Definition at line 292 of file kim_species_name_module.f90.

10.43.1.7 kim_species_name_at

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_at
```

Definition at line 448 of file kim_species_name_module.f90.

10.43.1.8 kim_species_name_au

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_au
```

Definition at line 430 of file kim_species_name_module.f90.

10.43.1.9 kim_species_name_b

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_b
```

Definition at line 208 of file kim_species_name_module.f90.

10.43.1.10 kim_species_name_ba

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_ba
```

Definition at line 361 of file kim_species_name_module.f90.

10.43.1.11 kim_species_name_be

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_be
```

Definition at line 205 of file kim_species_name_module.f90.

10.43.1.12 kim_species_name_bh

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_bh
```

Definition at line 514 of file kim_species_name_module.f90.

10.43.1.13 kim_species_name_bi

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_bi
```

Definition at line 442 of file kim_species_name_module.f90.

10.43.1.14 kim_species_name_bk

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_bk
```

Definition at line 484 of file kim_species_name_module.f90.

10.43.1.15 kim_species_name_br

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_br
```

Definition at line 298 of file kim_species_name_module.f90.

10.43.1.16 kim_species_name_c

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_c
```

Definition at line 211 of file kim_species_name_module.f90.

10.43.1.17 kim_species_name_ca

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_ca
```

Definition at line 253 of file kim_species_name_module.f90.

10.43.1.18 kim_species_name_cd

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_cd
```

Definition at line 337 of file kim_species_name_module.f90.

10.43.1.19 kim_species_name_ce

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_ce
```

Definition at line 367 of file kim_species_name_module.f90.

10.43.1.20 kim_species_name_cf

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_cf
```

Definition at line 487 of file kim_species_name_module.f90.

10.43.1.21 kim_species_name_cl

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_cl
```

Definition at line 244 of file kim_species_name_module.f90.

10.43.1.22 kim_species_name_cm

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_cm
```

Definition at line 481 of file kim_species_name_module.f90.

10.43.1.23 kim_species_name_cn

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_cn
```

Definition at line 529 of file kim_species_name_module.f90.

10.43.1.24 kim_species_name_co

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_co
```

Definition at line 274 of file kim_species_name_module.f90.

10.43.1.25 kim_species_name_cr

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_cr
```

Definition at line 265 of file kim_species_name_module.f90.

10.43.1.26 kim_species_name_cs

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_cs
```

Definition at line 358 of file kim_species_name_module.f90.

10.43.1.27 kim_species_name_cu

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_cu
```

Definition at line 280 of file kim_species_name_module.f90.

10.43.1.28 kim_species_name_db

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_db
```

Definition at line 508 of file kim_species_name_module.f90.

10.43.1.29 kim_species_name_ds

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_ds
```

Definition at line 523 of file kim_species_name_module.f90.

10.43.1.30 kim_species_name_dy

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_dy
```

Definition at line 391 of file kim_species_name_module.f90.

10.43.1.31 kim_species_name_electron

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_electron
```

Definition at line 193 of file kim_species_name_module.f90.

10.43.1.32 kim_species_name_er

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_er
```

Definition at line 397 of file kim_species_name_module.f90.

10.43.1.33 kim_species_name_es

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_es
```

Definition at line 490 of file kim_species_name_module.f90.

10.43.1.34 kim_species_name_eu

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_eu
```

Definition at line 382 of file kim_species_name_module.f90.

10.43.1.35 kim_species_name_f

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_f
```

Definition at line 220 of file kim_species_name_module.f90.

10.43.1.36 kim_species_name_fe

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_fe
```

Definition at line 271 of file kim_species_name_module.f90.

10.43.1.37 kim_species_name_fl

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_fl
```

Definition at line 535 of file kim_species_name_module.f90.

10.43.1.38 kim_species_name_fm

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_fm
```

Definition at line 493 of file kim_species_name_module.f90.

10.43.1.39 kim_species_name_fr

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_fr
```

Definition at line 454 of file kim_species_name_module.f90.

10.43.1.40 kim_species_name_ga

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_ga
```

Definition at line 286 of file kim_species_name_module.f90.

10.43.1.41 kim_species_name_gd

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_gd
```

Definition at line 385 of file kim_species_name_module.f90.

10.43.1.42 kim_species_name_ge

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_ge
```

Definition at line 289 of file kim_species_name_module.f90.

10.43.1.43 kim_species_name_h

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_h
```

Definition at line 196 of file kim_species_name_module.f90.

10.43.1.44 kim_species_name_he

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_he
```

Definition at line 199 of file kim_species_name_module.f90.

10.43.1.45 kim_species_name_hf

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_hf
```

Definition at line 409 of file kim_species_name_module.f90.

10.43.1.46 kim_species_name_hg

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_hg
```

Definition at line 433 of file kim_species_name_module.f90.

10.43.1.47 kim_species_name_ho

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_ho
```

Definition at line 394 of file kim_species_name_module.f90.

10.43.1.48 kim_species_name_hs

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_hs
```

Definition at line 517 of file kim_species_name_module.f90.

10.43.1.49 kim_species_name_i

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_i
```

Definition at line 352 of file kim_species_name_module.f90.

10.43.1.50 kim_species_name_in

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_in
```

Definition at line 340 of file kim_species_name_module.f90.

10.43.1.51 kim_species_name_ir

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_ir
```

Definition at line 424 of file kim_species_name_module.f90.

10.43.1.52 kim_species_name_k

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_k
```

Definition at line 250 of file kim_species_name_module.f90.

10.43.1.53 kim_species_name_kr

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_kr
```

Definition at line 301 of file kim_species_name_module.f90.

10.43.1.54 kim_species_name_la

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_la
```

Definition at line 364 of file kim_species_name_module.f90.

10.43.1.55 kim_species_name_li

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_li
```

Definition at line 202 of file kim_species_name_module.f90.

10.43.1.56 kim_species_name_lr

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_lr
```

Definition at line 502 of file kim_species_name_module.f90.

10.43.1.57 kim_species_name_lu

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_lu
```

Definition at line 406 of file kim_species_name_module.f90.

10.43.1.58 kim_species_name_lv

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_lv
```

Definition at line 541 of file kim_species_name_module.f90.

10.43.1.59 kim_species_name_md

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_md
```

Definition at line 496 of file kim_species_name_module.f90.

10.43.1.60 kim_species_name_mg

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_mg
```

Definition at line 229 of file kim_species_name_module.f90.

10.43.1.61 kim_species_name_mn

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_mn
```

Definition at line 268 of file kim_species_name_module.f90.

10.43.1.62 kim_species_name_mo

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_mo
```

Definition at line 319 of file kim_species_name_module.f90.

10.43.1.63 kim_species_name_mt

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_mt
```

Definition at line 520 of file kim_species_name_module.f90.

10.43.1.64 kim_species_name_n

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_n
```

Definition at line 214 of file kim_species_name_module.f90.

10.43.1.65 kim_species_name_na

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_na
```

Definition at line 226 of file kim_species_name_module.f90.

10.43.1.66 kim_species_name_nb

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_nb
```

Definition at line 316 of file kim_species_name_module.f90.

10.43.1.67 kim_species_name_nd

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_nd
```

Definition at line 373 of file kim_species_name_module.f90.

10.43.1.68 kim_species_name_ne

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_ne
```

Definition at line 223 of file kim_species_name_module.f90.

10.43.1.69 kim_species_name_ni

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_ni
```

Definition at line 277 of file kim_species_name_module.f90.

10.43.1.70 kim_species_name_no

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_no
```

Definition at line 499 of file kim_species_name_module.f90.

10.43.1.71 kim_species_name_np

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_np
```

Definition at line 472 of file kim_species_name_module.f90.

10.43.1.72 kim_species_name_o

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_o
```

Definition at line 217 of file kim_species_name_module.f90.

10.43.1.73 kim_species_name_os

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_os
```

Definition at line 421 of file kim_species_name_module.f90.

10.43.1.74 kim_species_name_p

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_p
```

Definition at line 238 of file kim_species_name_module.f90.

10.43.1.75 kim_species_name_pa

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_pa
```

Definition at line 466 of file kim_species_name_module.f90.

10.43.1.76 kim_species_name_pb

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_pb
```

Definition at line 439 of file kim_species_name_module.f90.

10.43.1.77 kim_species_name_pd

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_pd
```

Definition at line 331 of file kim_species_name_module.f90.

10.43.1.78 kim_species_name_pm

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_pm
```

Definition at line 376 of file kim_species_name_module.f90.

10.43.1.79 kim_species_name_po

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_po
```

Definition at line 445 of file kim_species_name_module.f90.

10.43.1.80 kim_species_name_pr

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_pr
```

Definition at line 370 of file kim_species_name_module.f90.

10.43.1.81 kim_species_name_pt

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_pt
```

Definition at line 427 of file kim_species_name_module.f90.

10.43.1.82 kim_species_name_pu

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_pu
```

Definition at line 475 of file kim_species_name_module.f90.

10.43.1.83 kim_species_name_ra

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_ra
```

Definition at line 457 of file kim_species_name_module.f90.

10.43.1.84 kim_species_name_rb

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_rb
```

Definition at line 304 of file kim_species_name_module.f90.

10.43.1.85 kim_species_name_re

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_re
```

Definition at line 418 of file kim_species_name_module.f90.

10.43.1.86 kim_species_name_rf

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_rf
```

Definition at line 505 of file kim_species_name_module.f90.

10.43.1.87 kim_species_name_rg

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_rg
```

Definition at line 526 of file kim_species_name_module.f90.

10.43.1.88 kim_species_name_rh

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_rh
```

Definition at line 328 of file kim_species_name_module.f90.

10.43.1.89 kim_species_name_rn

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_rn
```

Definition at line 451 of file kim_species_name_module.f90.

10.43.1.90 kim_species_name_ru

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_ru
```

Definition at line 325 of file kim_species_name_module.f90.

10.43.1.91 kim_species_name_s

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_s
```

Definition at line 241 of file kim_species_name_module.f90.

10.43.1.92 kim_species_name_sb

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_sb
```

Definition at line 346 of file kim_species_name_module.f90.

10.43.1.93 kim_species_name_sc

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_sc
```

Definition at line 256 of file kim_species_name_module.f90.

10.43.1.94 kim_species_name_se

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_se
```

Definition at line 295 of file kim_species_name_module.f90.

10.43.1.95 kim_species_name_sg

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_sg
```

Definition at line 511 of file kim_species_name_module.f90.

10.43.1.96 kim_species_name_si

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_si
```

Definition at line 235 of file kim_species_name_module.f90.

10.43.1.97 kim_species_name_sm

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_sm
```

Definition at line 379 of file kim_species_name_module.f90.

10.43.1.98 kim_species_name_sn

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_sn
```

Definition at line 343 of file kim_species_name_module.f90.

10.43.1.99 kim_species_name_sr

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_sr
```

Definition at line 307 of file kim_species_name_module.f90.

10.43.1.100 kim_species_name_ta

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_ta
```

Definition at line 412 of file kim_species_name_module.f90.

10.43.1.101 kim_species_name_tb

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_tb
```

Definition at line 388 of file kim_species_name_module.f90.

10.43.1.102 kim_species_name_tc

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_tc
```

Definition at line 322 of file kim_species_name_module.f90.

10.43.1.103 kim_species_name_te

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_te
```

Definition at line 349 of file kim_species_name_module.f90.

10.43.1.104 kim_species_name_th

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_th
```

Definition at line 463 of file kim_species_name_module.f90.

10.43.1.105 kim_species_name_ti

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_ti
```

Definition at line 259 of file kim_species_name_module.f90.

10.43.1.106 kim_species_name_tl

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_tl
```

Definition at line 436 of file kim_species_name_module.f90.

10.43.1.107 kim_species_name_tm

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_tm
```

Definition at line 400 of file kim_species_name_module.f90.

10.43.1.108 kim_species_name_u

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_u
```

Definition at line 469 of file kim_species_name_module.f90.

10.43.1.109 kim_species_name_user01

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_↔  
user01
```

Definition at line 550 of file kim_species_name_module.f90.

10.43.1.110 kim_species_name_user02

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_↵  
user02
```

Definition at line 553 of file kim_species_name_module.f90.

10.43.1.111 kim_species_name_user03

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_↵  
user03
```

Definition at line 556 of file kim_species_name_module.f90.

10.43.1.112 kim_species_name_user04

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_↵  
user04
```

Definition at line 559 of file kim_species_name_module.f90.

10.43.1.113 kim_species_name_user05

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_↵  
user05
```

Definition at line 562 of file kim_species_name_module.f90.

10.43.1.114 kim_species_name_user06

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_↵  
user06
```

Definition at line 565 of file kim_species_name_module.f90.

10.43.1.115 kim_species_name_user07

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_↵  
user07
```

Definition at line 568 of file kim_species_name_module.f90.

10.43.1.116 kim_species_name_user08

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_↵  
user08
```

Definition at line 571 of file kim_species_name_module.f90.

10.43.1.117 kim_species_name_user09

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_↵  
user09
```

Definition at line 574 of file kim_species_name_module.f90.

10.43.1.118 kim_species_name_user10

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_↵  
user10
```

Definition at line 577 of file kim_species_name_module.f90.

10.43.1.119 kim_species_name_user11

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_↵  
user11
```

Definition at line 580 of file kim_species_name_module.f90.

10.43.1.120 kim_species_name_user12

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_↵  
user12
```

Definition at line 583 of file kim_species_name_module.f90.

10.43.1.121 kim_species_name_user13

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_↵  
user13
```

Definition at line 586 of file kim_species_name_module.f90.

10.43.1.122 kim_species_name_user14

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_↵  
user14
```

Definition at line 589 of file kim_species_name_module.f90.

10.43.1.123 kim_species_name_user15

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_↵  
user15
```

Definition at line 592 of file kim_species_name_module.f90.

10.43.1.124 kim_species_name_user16

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_↵  
user16
```

Definition at line 595 of file kim_species_name_module.f90.

10.43.1.125 kim_species_name_user17

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_↵  
user17
```

Definition at line 598 of file kim_species_name_module.f90.

10.43.1.126 kim_species_name_user18

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_↵  
user18
```

Definition at line 601 of file kim_species_name_module.f90.

10.43.1.127 kim_species_name_user19

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_↵  
user19
```

Definition at line 604 of file kim_species_name_module.f90.

10.43.1.128 kim_species_name_user20

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_↵  
user20
```

Definition at line 607 of file kim_species_name_module.f90.

10.43.1.129 kim_species_name_uuo

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_uuo
```

Definition at line 547 of file kim_species_name_module.f90.

10.43.1.130 kim_species_name_uup

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_uup
```

Definition at line 538 of file kim_species_name_module.f90.

10.43.1.131 kim_species_name_uus

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_uus
```

Definition at line 544 of file kim_species_name_module.f90.

10.43.1.132 kim_species_name_uut

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_uut
```

Definition at line 532 of file kim_species_name_module.f90.

10.43.1.133 kim_species_name_v

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_v
```

Definition at line 262 of file kim_species_name_module.f90.

10.43.1.134 kim_species_name_w

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_w
```

Definition at line 415 of file kim_species_name_module.f90.

10.43.1.135 kim_species_name_xe

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_xe
```

Definition at line 355 of file kim_species_name_module.f90.

10.43.1.136 kim_species_name_y

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_y
```

Definition at line 310 of file kim_species_name_module.f90.

10.43.1.137 kim_species_name_yb

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_yb
```

Definition at line 403 of file kim_species_name_module.f90.

10.43.1.138 kim_species_name_zn

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_zn
```

Definition at line 283 of file kim_species_name_module.f90.

10.43.1.139 kim_species_name_zr

```
type(kim_species_name_type), public, protected kim_species_name_module::kim_species_name_zr
```

Definition at line 313 of file kim_species_name_module.f90.

10.44 kim_support_status_module Module Reference

Variables

- type(kim_support_status_type), public, protected [kim_support_status_required_by_api](#)
- type(kim_support_status_type), public, protected [kim_support_status_not_supported](#)
- type(kim_support_status_type), public, protected [kim_support_status_required](#)
- type(kim_support_status_type), public, protected [kim_support_status_optional](#)

10.44.1 Variable Documentation

10.44.1.1 kim_support_status_not_supported

```
type(kim_support_status_type), public, protected kim_support_status_module::kim_support_↔  
status_not_supported
```

Definition at line 62 of file kim_support_status_module.f90.

10.44.1.2 kim_support_status_optional

```
type(kim_support_status_type), public, protected kim_support_status_module::kim_support_↔  
status_optional
```

Definition at line 68 of file kim_support_status_module.f90.

10.44.1.3 kim_support_status_required

```
type(kim_support_status_type), public, protected kim_support_status_module::kim_support_↔  
status_required
```

Definition at line 65 of file kim_support_status_module.f90.

10.44.1.4 kim_support_status_required_by_api

```
type(kim_support_status_type), public, protected kim_support_status_module::kim_support_↔  
status_required_by_api
```

Definition at line 59 of file kim_support_status_module.f90.

10.45 kim_temperature_unit_module Module Reference

Variables

- type(kim_temperature_unit_type), public, protected [kim_temperature_unit_unused](#)
- type(kim_temperature_unit_type), public, protected [kim_temperature_unit_k](#)

10.45.1 Variable Documentation

10.45.1.1 kim_temperature_unit_k

```
type(kim_temperature_unit_type), public, protected kim_temperature_unit_module::kim_temperature↔  
_unit_k
```

Definition at line 60 of file kim_temperature_unit_module.f90.

10.45.1.2 kim_temperature_unit_unused

```
type(kim_temperature_unit_type), public, protected kim_temperature_unit_module::kim_temperature↔  
_unit_unused
```

Definition at line 57 of file kim_temperature_unit_module.f90.

10.46 kim_time_unit_module Module Reference

Variables

- type(kim_time_unit_type), public, protected [kim_time_unit_unused](#)
- type(kim_time_unit_type), public, protected [kim_time_unit_fs](#)
- type(kim_time_unit_type), public, protected [kim_time_unit_ps](#)
- type(kim_time_unit_type), public, protected [kim_time_unit_ns](#)
- type(kim_time_unit_type), public, protected [kim_time_unit_s](#)

10.46.1 Variable Documentation

10.46.1.1 kim_time_unit_fs

```
type(kim_time_unit_type), public, protected kim_time_unit_module::kim_time_unit_fs
```

Definition at line 62 of file kim_time_unit_module.f90.

10.46.1.2 kim_time_unit_ns

```
type(kim_time_unit_type), public, protected kim_time_unit_module::kim_time_unit_ns
```

Definition at line 66 of file kim_time_unit_module.f90.

10.46.1.3 kim_time_unit_ps

```
type(kim_time_unit_type), public, protected kim_time_unit_module::kim_time_unit_ps
```

Definition at line 64 of file kim_time_unit_module.f90.

10.46.1.4 kim_time_unit_s

```
type(kim_time_unit_type), public, protected kim_time_unit_module::kim_time_unit_s
```

Definition at line 68 of file kim_time_unit_module.f90.

10.46.1.5 kim_time_unit_unused

```
type(kim_time_unit_type), public, protected kim_time_unit_module::kim_time_unit_unused
```

Definition at line 60 of file kim_time_unit_module.f90.

10.47 kim_unit_system_module Module Reference

10.48 mod_neighborlist Module Reference

Data Types

- type [neighobject_type](#)

Functions/Subroutines

- integer(c_int) function, public [get_neigh](#) (pkim, mode, request, part, numnei, pnei1part, pRij)
- subroutine, public [get_neigh](#) (data_object, number_of_cutoffs, cutoffs, neighbor_list_index, request, numnei, pnei1part, ierr)

10.48.1 Function/Subroutine Documentation

10.48.1.1 `get_neigh()` [1/2]

```
integer(c_int) function, public mod_neighborlist::get_neigh (
    type(c_ptr), intent(in) pkim,
    integer(c_int), intent(in) mode,
    integer(c_int), intent(in) request,
    integer(c_int), intent(out) part,
    integer(c_int), intent(out) numnei,
    type(c_ptr), intent(out) pneilpart,
    type(c_ptr), intent(out) pRij )
```

Definition at line 66 of file `ex_test_Ar_fcc_cluster_fortran.F90`.

10.48.1.2 `get_neigh()` [2/2]

```
subroutine public mod_neighborlist::get_neigh (
    type(c_ptr), intent(in), value data_object,
    integer(c_int), intent(in), value number_of_cutoffs,
    real(c_double), dimension(number_of_cutoffs), intent(in) cutoffs,
    integer(c_int), intent(in), value neighbor_list_index,
    integer(c_int), intent(in), value request,
    integer(c_int), intent(out) numnei,
    type(c_ptr), intent(out) pneilpart,
    integer(c_int), intent(out) ierr )
```

Definition at line 89 of file `ex_test_Ar_fcc_cluster_fortran.F90`.

10.49 mod_utilities Module Reference

Functions/Subroutines

- subroutine [check_model_compatibility](#) (*compute_arguments_handle*, *forces_optional*, *model_is_compatible*, *ierr*)
- subroutine [get_model_supported_species](#) (*model_handle*, *max_species*, *model_species*, *num_species*, *ier*)
- subroutine [update_neighborlist](#) (*DIM*, *N*, *coords*, *cutoff*, *cutpad*, *do_update_list*, *coordsave*, *neighObject*, *ierr*)
- subroutine [neigh_pure_cluster_neighborlist](#) (*half*, *numberOfParticles*, *coords*, *cutoff*, *neighObject*)
- subroutine [create_fcc_configuration](#) (*FCCspacing*, *nCellsPerSide*, *periodic*, *coords*, *MiddlePartId*)
- subroutine [compute_numer_deriv](#) (*partnum*, *dir*, *model_handle*, *compute_arguments_handle*, *DIM*, *N*, *coords*, *cutoff*, *cutpad*, *energy*, *do_update_list*, *coordsave*, *neighObject*, *deriv*, *deriv_err*, *ierr*)

10.49.1 Function/Subroutine Documentation

10.49.1.1 `check_model_compatibility()`

```
subroutine mod_utilities::check_model_compatibility (
    type(kim_compute_arguments_handle_type), intent(in) compute_arguments_handle,
    logical, intent(out) forces_optional,
    logical, intent(out) model_is_compatible,
    integer(c_int), intent(out) ierr )
```

Definition at line 174 of file `utility_forces_numer_deriv.F03`.

10.49.1.2 `compute_numer_deriv()`

```
subroutine mod_utilities::compute_numer_deriv (
    integer(c_int), intent(in) partnum,
    integer(c_int), intent(in) dir,
    type(kim_model_handle_type), intent(in) model_handle,
    type(kim_compute_arguments_handle_type), intent(in) compute_arguments_handle,
    integer(c_int), intent(in) DIM,
    integer(c_int), intent(in) N,
    real(c_double), dimension(dim,n), intent(inout) coords,
    real(c_double), intent(in) cutoff,
    real(c_double), intent(in) cutpad,
    real(c_double), intent(inout) energy,
    logical, intent(inout) do_update_list,
    real(c_double), dimension(dim,n), intent(inout) coordsave,
    type(neighobject_type), intent(inout) neighObject,
    real(c_double), intent(out) deriv,
    real(c_double), intent(out) deriv_err,
    integer(c_int), intent(out) ierr )
```

Definition at line 578 of file `utility_forces_numer_deriv.F03`.

10.49.1.3 `create_fcc_configuration()`

```
subroutine mod_utilities::create_fcc_configuration (
    real(c_double), intent(in) FCCspacing,
    integer(c_int), intent(in) nCellsPerSide,
    logical, intent(in) periodic,
    real(c_double), dimension(3,*), intent(out) coords,
    integer(c_int), intent(out) MiddlePartId )
```

Definition at line 477 of file `utility_forces_numer_deriv.F03`.

10.49.1.4 get_model_supported_species()

```

subroutine mod_utilities::get_model_supported_species (
    type(kim_model_handle_type), intent(in) model_handle,
    integer(c_int), intent(in) max_species,
    type(kim_species_name_type), dimension(max_species), intent(out) model_species,
    integer(c_int), intent(out) num_species,
    integer(c_int), intent(out) ier )

```

Definition at line 297 of file utility_forces_numer_deriv.F03.

10.49.1.5 neigh_pure_cluster_neighborlist()

```

subroutine mod_utilities::neigh_pure_cluster_neighborlist (
    logical, intent(in) half,
    integer(c_int), intent(in) numberOfParticles,
    real(c_double), dimension(3,numberOfParticles), intent(in) coords,
    real(c_double), intent(in) cutoff,
    type(neighobject_type), intent(inout) neighObject )

```

Definition at line 415 of file utility_forces_numer_deriv.F03.

10.49.1.6 update_neighborlist()

```

subroutine mod_utilities::update_neighborlist (
    integer(c_int), intent(in) DIM,
    integer(c_int), intent(in) N,
    real(c_double), dimension(dim,n), intent(in) coords,
    real(c_double), intent(in) cutoff,
    real(c_double), intent(in) cutpad,
    logical, intent(inout) do_update_list,
    real(c_double), dimension(dim,n), intent(inout) coordsave,
    type(neighobject_type), intent(inout) neighObject,
    integer(c_int), intent(out) ierr )

```

Definition at line 340 of file utility_forces_numer_deriv.F03.

10.50 mod_utility Module Reference

Functions/Subroutines

- subroutine [mi_opbc_cluster_neighborlist](#) (half, numberOfParticles, coords, rcut, boxSideLengths, neighObject)
- subroutine [neigh_pure_cluster_neighborlist](#) (half, numberOfParticles, coords, cutoff, neighObject)
- subroutine [neigh_rvec_cluster_neighborlist](#) (half, numberOfParticles, coords, cutoff, neighObject)
- subroutine [create_fcc_configuration](#) (FCCspacing, nCellsPerSide, periodic, coords, MiddlePartId)

10.50.1 Function/Subroutine Documentation

10.50.1.1 `create_fcc_configuration()`

```
subroutine mod_utility::create_fcc_configuration (
    real(c_double), intent(in) FCCspacing,
    integer(c_int), intent(in) nCellsPerSide,
    logical, intent(in) periodic,
    real(c_double), dimension(3,*), intent(out) coords,
    integer(c_int), intent(out) MiddlePartId )
```

Definition at line 349 of file `ex_test_Ar_fcc_cluster_fortran.F90`.

10.50.1.2 `mi_opbc_cluster_neighborlist()`

```
subroutine mod_utility::mi_opbc_cluster_neighborlist (
    logical, intent(in) half,
    integer(c_int), intent(in) numberOfParticles,
    real(c_double), dimension(3,numberOfparticles), intent(in) coords,
    real(c_double), intent(in) rcut,
    real(c_double), dimension(3), intent(in) boxSideLengths,
    type(neighobject_type), intent(inout) neighObject )
```

Definition at line 182 of file `ex_test_Ar_fcc_cluster_fortran.F90`.

10.50.1.3 `neigh_pure_cluster_neighborlist()`

```
subroutine mod_utility::neigh_pure_cluster_neighborlist (
    logical, intent(in) half,
    integer(c_int), intent(in) numberOfParticles,
    real(c_double), dimension(3,numberOfparticles), intent(in) coords,
    real(c_double), intent(in) cutoff,
    type(neighobject_type), intent(inout) neighObject )
```

Definition at line 238 of file `ex_test_Ar_fcc_cluster_fortran.F90`.

10.50.1.4 `neigh_rvec_cluster_neighborlist()`

```
subroutine mod_utility::neigh_rvec_cluster_neighborlist (
    logical, intent(in) half,
    integer(c_int), intent(in) numberOfParticles,
    real(c_double), dimension(3,numberOfparticles), intent(in) coords,
    real(c_double), intent(in) cutoff,
    type(neighobject_type), intent(inout) neighObject )
```

Definition at line 287 of file `ex_test_Ar_fcc_cluster_fortran.F90`.

Chapter 11

Class Documentation

11.1 KIM::ChargeUnit Class Reference

```
#include <KIM_ChargeUnit.hpp>
```

Public Member Functions

- [ChargeUnit](#) ()
- [ChargeUnit](#) (int const id)
- [ChargeUnit](#) (std::string const &str)
- bool [operator==](#) ([ChargeUnit](#) const &rhs) const
- bool [operator!=](#) ([ChargeUnit](#) const &rhs) const
- std::string const & [String](#) () const

Public Attributes

- int [chargeUnitID](#)

11.1.1 Detailed Description

Definition at line 42 of file KIM_ChargeUnit.hpp.

11.1.2 Constructor & Destructor Documentation

11.1.2.1 [ChargeUnit](#)() [1/3]

```
KIM::ChargeUnit::ChargeUnit ( )
```

11.1.2.2 ChargeUnit() [2/3]

```
KIM::ChargeUnit::ChargeUnit (
    int const id )
```

11.1.2.3 ChargeUnit() [3/3]

```
KIM::ChargeUnit::ChargeUnit (
    std::string const & str )
```

11.1.3 Member Function Documentation

11.1.3.1 operator!=(())

```
bool KIM::ChargeUnit::operator!= (
    ChargeUnit const & rhs ) const
```

11.1.3.2 operator==(())

```
bool KIM::ChargeUnit::operator== (
    ChargeUnit const & rhs ) const
```

11.1.3.3 String()

```
std::string const& KIM::ChargeUnit::String ( ) const
```

11.1.4 Member Data Documentation

11.1.4.1 chargeUnitID

```
int KIM::ChargeUnit::chargeUnitID
```

Definition at line 45 of file KIM_ChargeUnit.hpp.

The documentation for this class was generated from the following file:

- [kim-api-v2.0.0-beta.0/cpp/include/KIM_ChargeUnit.hpp](#)

11.2 KIM::COMPUTE_ARGUMENT_NAME::Comparator Struct Reference

```
#include <KIM_ComputeArgumentName.hpp>
```

Public Member Functions

- bool [operator\(\)](#) ([ComputeArgumentName](#) const &a, [ComputeArgumentName](#) const &b) const

11.2.1 Detailed Description

Definition at line 76 of file [KIM_ComputeArgumentName.hpp](#).

11.2.2 Member Function Documentation

11.2.2.1 [operator\(\)](#)

```
bool KIM::COMPUTE_ARGUMENT_NAME::Comparator::operator() (
    ComputeArgumentName const & a,
    ComputeArgumentName const & b ) const    [inline]
```

Definition at line 78 of file [KIM_ComputeArgumentName.hpp](#).

The documentation for this struct was generated from the following file:

- [kim-api-v2.0.0-beta.0/cpp/include/KIM_ComputeArgumentName.hpp](#)

11.3 KIM::NUMBERING::Comparator Struct Reference

```
#include <KIM_Numbering.hpp>
```

Public Member Functions

- bool [operator\(\)](#) ([Numbering](#) const &a, [Numbering](#) const &b) const

11.3.1 Detailed Description

Definition at line 63 of file [KIM_Numbering.hpp](#).

11.3.2 Member Function Documentation

11.3.2.1 operator()

```
bool KIM::NUMBERING::Comparator::operator() (
    Numbering const & a,
    Numbering const & b ) const [inline]
```

Definition at line 65 of file KIM_Numbering.hpp.

The documentation for this struct was generated from the following file:

- [kim-api-v2.0.0-beta.0/cpp/include/KIM_Numbering.hpp](#)

11.4 KIM::LANGUAGE_NAME::Comparator Struct Reference

```
#include <KIM_LanguageName.hpp>
```

Public Member Functions

- bool [operator\(\)](#) ([LanguageName](#) const &a, [LanguageName](#) const &b) const

11.4.1 Detailed Description

Definition at line 63 of file KIM_LanguageName.hpp.

11.4.2 Member Function Documentation

11.4.2.1 operator()

```
bool KIM::LANGUAGE_NAME::Comparator::operator() (
    LanguageName const & a,
    LanguageName const & b ) const [inline]
```

Definition at line 65 of file KIM_LanguageName.hpp.

The documentation for this struct was generated from the following file:

- [kim-api-v2.0.0-beta.0/cpp/include/KIM_LanguageName.hpp](#)

11.5 KIM::SPECIES_NAME::Comparator Struct Reference

```
#include <KIM_SpeciesName.hpp>
```

Public Member Functions

- bool [operator\(\)](#) ([SpeciesName](#) const &a, [SpeciesName](#) const &b) const

11.5.1 Detailed Description

Definition at line 200 of file KIM_SpeciesName.hpp.

11.5.2 Member Function Documentation

11.5.2.1 [operator\(\)](#)()

```
bool KIM::SPECIES_NAME::Comparator::operator() (
    SpeciesName const & a,
    SpeciesName const & b ) const    [inline]
```

Definition at line 202 of file KIM_SpeciesName.hpp.

The documentation for this struct was generated from the following file:

- [kim-api-v2.0.0-beta.0/cpp/include/KIM_SpeciesName.hpp](#)

11.6 KIM::LENGTH_UNIT::Comparator Struct Reference

```
#include <KIM_LengthUnit.hpp>
```

Public Member Functions

- bool [operator\(\)](#) ([LengthUnit](#) const &a, [LengthUnit](#) const &b) const

11.6.1 Detailed Description

Definition at line 67 of file KIM_LengthUnit.hpp.

11.6.2 Member Function Documentation

11.6.2.1 operator()

```
bool KIM::LENGTH_UNIT::Comparator::operator() (
    LengthUnit const & a,
    LengthUnit const & b ) const [inline]
```

Definition at line 69 of file KIM_LengthUnit.hpp.

The documentation for this struct was generated from the following file:

- [kim-api-v2.0.0-beta.0/cpp/include/KIM_LengthUnit.hpp](#)

11.7 KIM::SUPPORT_STATUS::Comparator Struct Reference

```
#include <KIM_SupportStatus.hpp>
```

Public Member Functions

- bool [operator\(\)](#) ([SupportStatus](#) const &a, [SupportStatus](#) const &b) const

11.7.1 Detailed Description

Definition at line 65 of file KIM_SupportStatus.hpp.

11.7.2 Member Function Documentation

11.7.2.1 operator()

```
bool KIM::SUPPORT_STATUS::Comparator::operator() (
    SupportStatus const & a,
    SupportStatus const & b ) const [inline]
```

Definition at line 67 of file KIM_SupportStatus.hpp.

The documentation for this struct was generated from the following file:

- [kim-api-v2.0.0-beta.0/cpp/include/KIM_SupportStatus.hpp](#)

11.8 KIM::TEMPERATURE_UNIT::Comparator Struct Reference

```
#include <KIM_TemperatureUnit.hpp>
```

Public Member Functions

- bool [operator\(\)](#) ([TemperatureUnit](#) const &a, [TemperatureUnit](#) const &b) const

11.8.1 Detailed Description

Definition at line 64 of file KIM_TemperatureUnit.hpp.

11.8.2 Member Function Documentation

11.8.2.1 [operator\(\)](#)()

```
bool KIM::TEMPERATURE_UNIT::Comparator::operator() (
    TemperatureUnit const & a,
    TemperatureUnit const & b ) const [inline]
```

Definition at line 66 of file KIM_TemperatureUnit.hpp.

The documentation for this struct was generated from the following file:

- [kim-api-v2.0.0-beta.0/cpp/include/KIM_TemperatureUnit.hpp](#)

11.9 KIM::TIME_UNIT::Comparator Struct Reference

```
#include <KIM_TimeUnit.hpp>
```

Public Member Functions

- bool [operator\(\)](#) ([TimeUnit](#) const &a, [TimeUnit](#) const &b) const

11.9.1 Detailed Description

Definition at line 66 of file KIM_TimeUnit.hpp.

11.9.2 Member Function Documentation

11.9.2.1 operator()

```
bool KIM::TIME_UNIT::Comparator::operator() (
    TimeUnit const & a,
    TimeUnit const & b ) const [inline]
```

Definition at line 68 of file KIM_TimeUnit.hpp.

The documentation for this struct was generated from the following file:

- [kim-api-v2.0.0-beta.0/cpp/include/KIM_TimeUnit.hpp](#)

11.10 KIM::COMPUTE_CALLBACK_NAME::Comparator Struct Reference

```
#include <KIM_ComputeCallbackName.hpp>
```

Public Member Functions

- bool [operator\(\)](#) ([ComputeCallbackName](#) const &a, [ComputeCallbackName](#) const &b) const

11.10.1 Detailed Description

Definition at line 65 of file KIM_ComputeCallbackName.hpp.

11.10.2 Member Function Documentation

11.10.2.1 operator()

```
bool KIM::COMPUTE_CALLBACK_NAME::Comparator::operator() (
    ComputeCallbackName const & a,
    ComputeCallbackName const & b ) const [inline]
```

Definition at line 67 of file KIM_ComputeCallbackName.hpp.

The documentation for this struct was generated from the following file:

- [kim-api-v2.0.0-beta.0/cpp/include/KIM_ComputeCallbackName.hpp](#)

11.11 KIM::LOG_VERBOSITY::Comparator Struct Reference

```
#include <KIM_LogVerbosity.hpp>
```


Public Member Functions

- bool [operator\(\)](#) ([LogVerbosity](#) const &a, [LogVerbosity](#) const &b) const

11.11.1 Detailed Description

Definition at line 75 of file KIM_LogVerbosity.hpp.

11.11.2 Member Function Documentation

11.11.2.1 operator()

```
bool KIM::LOG_VERBOSITY::Comparator::operator() (
    LogVerbosity const & a,
    LogVerbosity const & b ) const    [inline]
```

Definition at line 77 of file KIM_LogVerbosity.hpp.

The documentation for this struct was generated from the following file:

- kim-api-v2.0.0-beta.0/cpp/include/[KIM_LogVerbosity.hpp](#)

11.12 KIM::CHARGE_UNIT::Comparator Struct Reference

```
#include <KIM_ChargeUnit.hpp>
```

Public Member Functions

- bool [operator\(\)](#) ([ChargeUnit](#) const &a, [ChargeUnit](#) const &b) const

11.12.1 Detailed Description

Definition at line 65 of file KIM_ChargeUnit.hpp.

11.12.2 Member Function Documentation

11.12.2.1 operator()

```
bool KIM::CHARGE_UNIT::Comparator::operator() (
    ChargeUnit const & a,
    ChargeUnit const & b ) const [inline]
```

Definition at line 67 of file KIM_ChargeUnit.hpp.

The documentation for this struct was generated from the following file:

- [kim-api-v2.0.0-beta.0/cpp/include/KIM_ChargeUnit.hpp](#)

11.13 KIM::DATA_TYPE::Comparator Struct Reference

```
#include <KIM_DataType.hpp>
```

Public Member Functions

- bool [operator\(\)](#) ([DataType](#) const &a, [DataType](#) const &b) const

11.13.1 Detailed Description

Definition at line 63 of file KIM_DataType.hpp.

11.13.2 Member Function Documentation

11.13.2.1 operator()

```
bool KIM::DATA_TYPE::Comparator::operator() (
    DataType const & a,
    DataType const & b ) const [inline]
```

Definition at line 65 of file KIM_DataType.hpp.

The documentation for this struct was generated from the following file:

- [kim-api-v2.0.0-beta.0/cpp/include/KIM_DataType.hpp](#)

11.14 KIM::ENERGY_UNIT::Comparator Struct Reference

```
#include <KIM_EnergyUnit.hpp>
```

Public Member Functions

- bool [operator\(\)](#) ([EnergyUnit](#) const &a, [EnergyUnit](#) const &b) const

11.14.1 Detailed Description

Definition at line 68 of file KIM_EnergyUnit.hpp.

11.14.2 Member Function Documentation

11.14.2.1 [operator\(\)](#)

```
bool KIM::ENERGY_UNIT::Comparator::operator() (
    EnergyUnit const & a,
    EnergyUnit const & b ) const [inline]
```

Definition at line 70 of file KIM_EnergyUnit.hpp.

The documentation for this struct was generated from the following file:

- kim-api-v2.0.0-beta.0/cpp/include/[KIM_EnergyUnit.hpp](#)

11.15 KIM::ComputeArgumentName Class Reference

```
#include <KIM_ComputeArgumentName.hpp>
```

Public Member Functions

- [ComputeArgumentName](#) ()
- [ComputeArgumentName](#) (int const id)
- [ComputeArgumentName](#) (std::string const &str)
- bool [operator==](#) ([ComputeArgumentName](#) const &rhs) const
- bool [operator!=](#) ([ComputeArgumentName](#) const &rhs) const
- std::string const & [String](#) () const

Public Attributes

- int [computeArgumentNameID](#)

11.15.1 Detailed Description

Definition at line 44 of file KIM_ComputeArgumentName.hpp.

11.15.2 Constructor & Destructor Documentation

11.15.2.1 ComputeArgumentName() [1/3]

```
KIM::ComputeArgumentName::ComputeArgumentName ( )
```

11.15.2.2 ComputeArgumentName() [2/3]

```
KIM::ComputeArgumentName::ComputeArgumentName (
    int const id )
```

11.15.2.3 ComputeArgumentName() [3/3]

```
KIM::ComputeArgumentName::ComputeArgumentName (
    std::string const & str )
```

11.15.3 Member Function Documentation

11.15.3.1 operator!=()

```
bool KIM::ComputeArgumentName::operator!= (
    ComputeArgumentName const & rhs ) const
```

11.15.3.2 operator==()

```
bool KIM::ComputeArgumentName::operator== (
    ComputeArgumentName const & rhs ) const
```

11.15.3.3 String()

```
std::string const& KIM::ComputeArgumentName::String ( ) const
```

11.15.4 Member Data Documentation

11.15.4.1 computeArgumentNameID

int KIM::ComputeArgumentName::computeArgumentNameID

Definition at line 47 of file KIM_ComputeArgumentName.hpp.

The documentation for this class was generated from the following file:

- [kim-api-v2.0.0-beta.0/cpp/include/KIM_ComputeArgumentName.hpp](#)

11.16 KIM::ComputeArguments Class Reference

```
#include <KIM_ComputeArguments.hpp>
```

Public Member Functions

- int [GetArgumentSupportStatus](#) ([ComputeArgumentName](#) const computeArgumentName, [SupportStatus](#) *const supportStatus) const
- int [GetCallbackSupportStatus](#) ([ComputeCallbackName](#) const computeCallbackName, [SupportStatus](#) *const supportStatus) const
- int [SetArgumentPointer](#) ([ComputeArgumentName](#) const computeArgumentName, int const *const ptr)
- int [SetArgumentPointer](#) ([ComputeArgumentName](#) const computeArgumentName, double const *const ptr)
- int [SetCallbackPointer](#) ([ComputeCallbackName](#) const computeCallbackName, [LanguageName](#) const languageName, func *const fptr, void const *const dataObject)
- void [AreAllRequiredArgumentsAndCallbacksPresent](#) (int *const result) const
- void [SetSimulatorBufferPointer](#) (void *const ptr)
- void [GetSimulatorBufferPointer](#) (void **const ptr) const
- std::string const & [String](#) () const
- void [SetLogID](#) (std::string const &logID)
- void [PushLogVerbosity](#) ([LogVerbosity](#) const logVerbosity)
- void [PopLogVerbosity](#) ()

Friends

- class [ModelImplementation](#)

11.16.1 Detailed Description

Definition at line 55 of file KIM_ComputeArguments.hpp.

11.16.2 Member Function Documentation

11.16.2.1 AreAllRequiredArgumentsAndCallbacksPresent()

```
void KIM::ComputeArguments::AreAllRequiredArgumentsAndCallbacksPresent (
    int *const result ) const
```

11.16.2.2 GetArgumentSupportStatus()

```
int KIM::ComputeArguments::GetArgumentSupportStatus (
    ComputeArgumentName const computeArgumentName,
    SupportStatus *const supportStatus ) const
```

11.16.2.3 GetCallbackSupportStatus()

```
int KIM::ComputeArguments::GetCallbackSupportStatus (
    ComputeCallbackName const computeCallbackName,
    SupportStatus *const supportStatus ) const
```

11.16.2.4 GetSimulatorBufferPointer()

```
void KIM::ComputeArguments::GetSimulatorBufferPointer (
    void **const ptr ) const
```

11.16.2.5 PopLogVerbosity()

```
void KIM::ComputeArguments::PopLogVerbosity ( )
```

11.16.2.6 PushLogVerbosity()

```
void KIM::ComputeArguments::PushLogVerbosity (
    LogVerbosity const logVerbosity )
```

11.16.2.7 SetArgumentPointer() [1/2]

```
int KIM::ComputeArguments::SetArgumentPointer (
    ComputeArgumentName const computeArgumentName,
    int const *const ptr )
```

11.16.2.8 SetArgumentPointer() [2/2]

```
int KIM::ComputeArguments::SetArgumentPointer (
    ComputeArgumentName const computeArgumentName,
    double const *const ptr )
```

11.16.2.9 SetCallbackPointer()

```
int KIM::ComputeArguments::SetCallbackPointer (
    ComputeCallbackName const computeCallbackName,
    LanguageName const languageName,
    func *const fptr,
    void const *const dataObject )
```

11.16.2.10 SetLogID()

```
void KIM::ComputeArguments::SetLogID (
    std::string const & logID )
```

11.16.2.11 SetSimulatorBufferPointer()

```
void KIM::ComputeArguments::SetSimulatorBufferPointer (
    void *const ptr )
```

11.16.2.12 String()

```
std::string const& KIM::ComputeArguments::String ( ) const
```

11.16.3 Friends And Related Function Documentation

11.16.3.1 ModelImplementation

```
friend class ModelImplementation [friend]
```

Definition at line 85 of file KIM_ComputeArguments.hpp.

The documentation for this class was generated from the following file:

- [kim-api-v2.0.0-beta.0/cpp/include/KIM_ComputeArguments.hpp](#)

11.17 KIM::ComputeCallbackName Class Reference

```
#include <KIM_ComputeCallbackName.hpp>
```

Public Member Functions

- [ComputeCallbackName](#) ()
- [ComputeCallbackName](#) (int const id)
- [ComputeCallbackName](#) (std::string const &str)
- bool [operator==](#) ([ComputeCallbackName](#) const &rhs) const
- bool [operator!=](#) ([ComputeCallbackName](#) const &rhs) const
- std::string const & [String](#) () const

Public Attributes

- int [computeCallbackNameID](#)

11.17.1 Detailed Description

Definition at line 42 of file KIM_ComputeCallbackName.hpp.

11.17.2 Constructor & Destructor Documentation

11.17.2.1 [ComputeCallbackName\(\)](#) [1/3]

```
KIM::ComputeCallbackName::ComputeCallbackName ( )
```

11.17.2.2 [ComputeCallbackName\(\)](#) [2/3]

```
KIM::ComputeCallbackName::ComputeCallbackName (
    int const id )
```

11.17.2.3 [ComputeCallbackName\(\)](#) [3/3]

```
KIM::ComputeCallbackName::ComputeCallbackName (
    std::string const & str )
```


11.17.3 Member Function Documentation

11.17.3.1 operator!=(())

```
bool KIM::ComputeCallbackName::operator!= (
    ComputeCallbackName const & rhs ) const
```

11.17.3.2 operator==(())

```
bool KIM::ComputeCallbackName::operator== (
    ComputeCallbackName const & rhs ) const
```

11.17.3.3 String()

```
std::string const& KIM::ComputeCallbackName::String ( ) const
```

11.17.4 Member Data Documentation

11.17.4.1 computeCallbackNameID

```
int KIM::ComputeCallbackName::computeCallbackNameID
```

Definition at line 45 of file KIM_ComputeCallbackName.hpp.

The documentation for this class was generated from the following file:

- [kim-api-v2.0.0-beta.0/cpp/include/KIM_ComputeCallbackName.hpp](#)

11.18 KIM::DataType Class Reference

```
#include <KIM_DataType.hpp>
```

Public Member Functions

- [DataType](#) ()
- [DataType](#) (int const id)
- [DataType](#) (std::string const &str)
- bool [operator==](#) ([DataType](#) const &rhs) const
- bool [operator!=](#) ([DataType](#) const &rhs) const
- std::string const & [String](#) () const

Public Attributes

- int [dataTypeID](#)

11.18.1 Detailed Description

Definition at line 42 of file KIM_DataType.hpp.

11.18.2 Constructor & Destructor Documentation

11.18.2.1 [DataType\(\)](#) [1/3]

```
KIM::DataType::DataType ( )
```

11.18.2.2 [DataType\(\)](#) [2/3]

```
KIM::DataType::DataType (
    int const id )
```

11.18.2.3 [DataType\(\)](#) [3/3]

```
KIM::DataType::DataType (
    std::string const & str )
```

11.18.3 Member Function Documentation

11.18.3.1 operator!=()

```
bool KIM::DataType::operator!= (
    DataType const & rhs ) const
```

11.18.3.2 operator==()

```
bool KIM::DataType::operator== (
    DataType const & rhs ) const
```

11.18.3.3 String()

```
std::string const& KIM::DataType::String ( ) const
```

11.18.4 Member Data Documentation

11.18.4.1 dataTypeID

```
int KIM::DataType::dataTypeID
```

Definition at line 45 of file KIM_DataType.hpp.

The documentation for this class was generated from the following file:

- kim-api-v2.0.0-beta.0/cpp/include/[KIM_DataType.hpp](#)

11.19 KIM::EnergyUnit Class Reference

```
#include <KIM_EnergyUnit.hpp>
```

Public Member Functions

- [EnergyUnit](#) ()
- [EnergyUnit](#) (int const id)
- [EnergyUnit](#) (std::string const &str)
- bool [operator==](#) ([EnergyUnit](#) const &rhs) const
- bool [operator!=](#) ([EnergyUnit](#) const &rhs) const
- std::string const & [String](#) () const

Public Attributes

- int [energyUnitID](#)

11.19.1 Detailed Description

Definition at line 42 of file KIM_EnergyUnit.hpp.

11.19.2 Constructor & Destructor Documentation

11.19.2.1 EnergyUnit() [1/3]

```
KIM::EnergyUnit::EnergyUnit ( )
```

11.19.2.2 EnergyUnit() [2/3]

```
KIM::EnergyUnit::EnergyUnit (
    int const id )
```

11.19.2.3 EnergyUnit() [3/3]

```
KIM::EnergyUnit::EnergyUnit (
    std::string const & str )
```

11.19.3 Member Function Documentation

11.19.3.1 operator!=()

```
bool KIM::EnergyUnit::operator!= (
    EnergyUnit const & rhs ) const
```

11.19.3.2 operator==()

```
bool KIM::EnergyUnit::operator== (
    EnergyUnit const & rhs ) const
```

11.19.3.3 String()

```
std::string const& KIM::EnergyUnit::String ( ) const
```

11.19.4 Member Data Documentation

11.19.4.1 energyUnitID

```
int KIM::EnergyUnit::energyUnitID
```

Definition at line 45 of file KIM_EnergyUnit.hpp.

The documentation for this class was generated from the following file:

- [kim-api-v2.0.0-beta.0/cpp/include/KIM_EnergyUnit.hpp](#)

11.20 KIM_ChargeUnit Struct Reference

```
#include <KIM_ChargeUnit.h>
```

Public Attributes

- int [chargeUnitID](#)

11.20.1 Detailed Description

Definition at line 39 of file KIM_ChargeUnit.h.

11.20.2 Member Data Documentation

11.20.2.1 `chargeUnitID`

```
int KIM_ChargeUnit::chargeUnitID
```

Definition at line 41 of file `KIM_ChargeUnit.h`.

The documentation for this struct was generated from the following file:

- [kim-api-v2.0.0-beta.0/c/include/KIM_ChargeUnit.h](#)

11.21 `kim_compute_arguments_module::kim_compute_arguments_are_all_required_` `present` Interface Reference

11.21.1 Detailed Description

Definition at line 228 of file `kim_compute_arguments_module.f90`.

The documentation for this interface was generated from the following file:

- [kim-api-v2.0.0-beta.0/fortran/include/kim_compute_arguments_module.f90](#)

11.22 `kim_compute_arguments_module::kim_compute_arguments_get_argument_` `support_status` Interface Reference

11.22.1 Detailed Description

Definition at line 177 of file `kim_compute_arguments_module.f90`.

The documentation for this interface was generated from the following file:

- [kim-api-v2.0.0-beta.0/fortran/include/kim_compute_arguments_module.f90](#)

11.23 `kim_compute_arguments_module::kim_compute_arguments_get_callback_` `support_status` Interface Reference

11.23.1 Detailed Description

Definition at line 193 of file `kim_compute_arguments_module.f90`.

The documentation for this interface was generated from the following file:

- [kim-api-v2.0.0-beta.0/fortran/include/kim_compute_arguments_module.f90](#)

11.24 kim_compute_arguments_module::kim_compute_arguments_pop_log_verbosity Interface Reference

11.24.1 Detailed Description

Definition at line 291 of file kim_compute_arguments_module.f90.

The documentation for this interface was generated from the following file:

- kim-api-v2.0.0-beta.0/fortran/include/[kim_compute_arguments_module.f90](#)

11.25 kim_compute_arguments_module::kim_compute_arguments_set_callback_↔ pointer Interface Reference

11.25.1 Detailed Description

Definition at line 209 of file kim_compute_arguments_module.f90.

The documentation for this interface was generated from the following file:

- kim-api-v2.0.0-beta.0/fortran/include/[kim_compute_arguments_module.f90](#)

11.26 KIM_ComputeArgumentName Struct Reference

```
#include <KIM_ComputeArgumentName.h>
```

Public Attributes

- int [computeArgumentNameID](#)

11.26.1 Detailed Description

Definition at line 45 of file KIM_ComputeArgumentName.h.

11.26.2 Member Data Documentation

11.26.2.1 computeArgumentNameID

```
int KIM_ComputeArgumentName::computeArgumentNameID
```

Definition at line 47 of file KIM_ComputeArgumentName.h.

The documentation for this struct was generated from the following file:

- [kim-api-v2.0.0-beta.0/c/include/KIM_ComputeArgumentName.h](#)

11.27 KIM_ComputeCallbackName Struct Reference

```
#include <KIM_ComputeCallbackName.h>
```

Public Attributes

- int [computeCallbackNameID](#)

11.27.1 Detailed Description

Definition at line 39 of file KIM_ComputeCallbackName.h.

11.27.2 Member Data Documentation

11.27.2.1 computeCallbackNameID

```
int KIM_ComputeCallbackName::computeCallbackNameID
```

Definition at line 41 of file KIM_ComputeCallbackName.h.

The documentation for this struct was generated from the following file:

- [kim-api-v2.0.0-beta.0/c/include/KIM_ComputeCallbackName.h](#)

11.28 KIM_DataType Struct Reference

```
#include <KIM_DataType.h>
```

Public Attributes

- int [dataTypeID](#)

11.28.1 Detailed Description

Definition at line 39 of file KIM_DataType.h.

11.28.2 Member Data Documentation

11.28.2.1 dataTypeID

```
int KIM_DataType::dataTypeID
```

Definition at line 41 of file KIM_DataType.h.

The documentation for this struct was generated from the following file:

- kim-api-v2.0.0-beta.0/c/include/[KIM_DataType.h](#)

11.29 KIM_EnergyUnit Struct Reference

```
#include <KIM_EnergyUnit.h>
```

Public Attributes

- int [energyUnitID](#)

11.29.1 Detailed Description

Definition at line 39 of file KIM_EnergyUnit.h.

11.29.2 Member Data Documentation

11.29.2.1 energyUnitID

```
int KIM_EnergyUnit::energyUnitID
```

Definition at line 41 of file KIM_EnergyUnit.h.

The documentation for this struct was generated from the following file:

- kim-api-v2.0.0-beta.0/c/include/[KIM_EnergyUnit.h](#)

11.30 KIM_LanguageName Struct Reference

```
#include <KIM_LanguageName.h>
```

Public Attributes

- int [languageNameID](#)

11.30.1 Detailed Description

Definition at line 39 of file KIM_LanguageName.h.

11.30.2 Member Data Documentation

11.30.2.1 languageNameID

```
int KIM_LanguageName::languageNameID
```

Definition at line 41 of file KIM_LanguageName.h.

The documentation for this struct was generated from the following file:

- kim-api-v2.0.0-beta.0/c/include/[KIM_LanguageName.h](#)

11.31 KIM_LengthUnit Struct Reference

```
#include <KIM_LengthUnit.h>
```

Public Attributes

- int [lengthUnitID](#)

11.31.1 Detailed Description

Definition at line 39 of file KIM_LengthUnit.h.

11.31.2 Member Data Documentation

11.31.2.1 lengthUnitID

```
int KIM_LengthUnit::lengthUnitID
```

Definition at line 41 of file KIM_LengthUnit.h.

The documentation for this struct was generated from the following file:

- [kim-api-v2.0.0-beta.0/c/include/KIM_LengthUnit.h](#)

11.32 kim_log_module::kim_log_pop_verbosity Interface Reference

11.32.1 Detailed Description

Definition at line 120 of file kim_log_module.f90.

The documentation for this interface was generated from the following file:

- [kim-api-v2.0.0-beta.0/fortran/include/kim_log_module.f90](#)

11.33 KIM_LogVerbosity Struct Reference

```
#include <KIM_LogVerbosity.h>
```

Public Attributes

- int [logVerbosityID](#)

11.33.1 Detailed Description

Definition at line 42 of file KIM_LogVerbosity.h.

11.33.2 Member Data Documentation

11.33.2.1 logVerbosityID

```
int KIM_LogVerbosity::logVerbosityID
```

Definition at line 44 of file KIM_LogVerbosity.h.

The documentation for this struct was generated from the following file:

- [kim-api-v2.0.0-beta.0/c/include/KIM_LogVerbosity.h](#)

11.34 kim_model_module::kim_model_clear_influence_dist_and_cutoffs_then_refresh↔ _model Interface Reference

11.34.1 Detailed Description

Definition at line 257 of file kim_model_module.f90.

The documentation for this interface was generated from the following file:

- kim-api-v2.0.0-beta.0/fortran/include/[kim_model_module.f90](#)

11.35 kim_model_module::kim_model_compute Interface Reference

11.35.1 Detailed Description

Definition at line 246 of file kim_model_module.f90.

The documentation for this interface was generated from the following file:

- kim-api-v2.0.0-beta.0/fortran/include/[kim_model_module.f90](#)

11.36 kim_model_module::kim_model_compute_arguments_create Interface Reference

11.36.1 Detailed Description

Definition at line 220 of file kim_model_module.f90.

The documentation for this interface was generated from the following file:

- kim-api-v2.0.0-beta.0/fortran/include/[kim_model_module.f90](#)

11.37 kim_model_compute_arguments_create_module::kim_model_compute_arguments↔ _create_set_callback_support_status Interface Reference

11.37.1 Detailed Description

Definition at line 97 of file kim_model_compute_arguments_create_module.f90.

The documentation for this interface was generated from the following file:

- kim-api-v2.0.0-beta.0/fortran/include/[kim_model_compute_arguments_create_module.f90](#)

11.38 kim_model_compute_arguments_create_module::kim_model_compute_arguments_create_set_model_buffer_pointer Interface

Reference

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11.38 kim_model_compute_arguments_create_module::kim_model_compute_arguments_create_set_model_buffer_pointer Interface Reference

11.38.1 Detailed Description

Definition at line 114 of file kim_model_compute_arguments_create_module.f90.

The documentation for this interface was generated from the following file:

- kim-api-v2.0.0-beta.0/fortran/include/[kim_model_compute_arguments_create_module.f90](#)

11.39 kim_model_compute_arguments_create_module::kim_model_compute_arguments_create_string Interface Reference

11.39.1 Detailed Description

Definition at line 138 of file kim_model_compute_arguments_create_module.f90.

The documentation for this interface was generated from the following file:

- kim-api-v2.0.0-beta.0/fortran/include/[kim_model_compute_arguments_create_module.f90](#)

11.40 kim_model_module::kim_model_compute_arguments_destroy Interface Reference

11.40.1 Detailed Description

Definition at line 233 of file kim_model_module.f90.

The documentation for this interface was generated from the following file:

- kim-api-v2.0.0-beta.0/fortran/include/[kim_model_module.f90](#)

11.41 kim_model_compute_arguments_destroy_module::kim_model_compute_arguments_destroy_string Interface Reference

11.41.1 Detailed Description

Definition at line 102 of file kim_model_compute_arguments_destroy_module.f90.

The documentation for this interface was generated from the following file:

- kim-api-v2.0.0-beta.0/fortran/include/[kim_model_compute_arguments_destroy_module.f90](#)

11.42 kim_model_compute_arguments_module::kim_model_compute_arguments_get↔ _neighbor_list Interface Reference

11.42.1 Detailed Description

Definition at line 184 of file kim_model_compute_arguments_module.f90.

The documentation for this interface was generated from the following file:

- [kim-api-v2.0.0-beta.0/fortran/include/kim_model_compute_arguments_module.f90](#)

11.43 kim_model_compute_arguments_module::kim_model_compute_arguments_set↔ _model_buffer_pointer Interface Reference

11.43.1 Detailed Description

Definition at line 244 of file kim_model_compute_arguments_module.f90.

The documentation for this interface was generated from the following file:

- [kim-api-v2.0.0-beta.0/fortran/include/kim_model_compute_arguments_module.f90](#)

11.44 kim_model_compute_arguments_module::kim_model_compute_arguments_↔ string Interface Reference

11.44.1 Detailed Description

Definition at line 279 of file kim_model_compute_arguments_module.f90.

The documentation for this interface was generated from the following file:

- [kim-api-v2.0.0-beta.0/fortran/include/kim_model_compute_arguments_module.f90](#)

11.45 kim_model_compute_module::kim_model_compute_string Interface Reference

11.45.1 Detailed Description

Definition at line 98 of file kim_model_compute_module.f90.

The documentation for this interface was generated from the following file:

- [kim-api-v2.0.0-beta.0/fortran/include/kim_model_compute_module.f90](#)

11.46 kim_model_create_module::kim_model_create_convert_unit Interface Reference

11.46.1 Detailed Description

Definition at line 243 of file kim_model_create_module.f90.

The documentation for this interface was generated from the following file:

- kim-api-v2.0.0-beta.0/fortran/include/[kim_model_create_module.f90](#)

11.47 kim_model_create_module::kim_model_create_log_entry Interface Reference

11.47.1 Detailed Description

Definition at line 279 of file kim_model_create_module.f90.

The documentation for this interface was generated from the following file:

- kim-api-v2.0.0-beta.0/fortran/include/[kim_model_create_module.f90](#)

11.48 kim_model_create_module::kim_model_create_set_compute_arguments_create↵ _pointer Interface Reference

11.48.1 Detailed Description

Definition at line 166 of file kim_model_create_module.f90.

The documentation for this interface was generated from the following file:

- kim-api-v2.0.0-beta.0/fortran/include/[kim_model_create_module.f90](#)

11.49 kim_model_create_module::kim_model_create_set_compute_arguments_destroy↵ _pointer Interface Reference

11.49.1 Detailed Description

Definition at line 178 of file kim_model_create_module.f90.

The documentation for this interface was generated from the following file:

- kim-api-v2.0.0-beta.0/fortran/include/[kim_model_create_module.f90](#)

11.50 kim_model_create_module::kim_model_create_set_compute_pointer Interface Reference

11.50.1 Detailed Description

Definition at line 190 of file kim_model_create_module.f90.

The documentation for this interface was generated from the following file:

- kim-api-v2.0.0-beta.0/fortran/include/[kim_model_create_module.f90](#)

11.51 kim_model_create_module::kim_model_create_set_destroy_pointer Interface Reference

11.51.1 Detailed Description

Definition at line 154 of file kim_model_create_module.f90.

The documentation for this interface was generated from the following file:

- kim-api-v2.0.0-beta.0/fortran/include/[kim_model_create_module.f90](#)

11.52 kim_model_create_module::kim_model_create_set_influence_distance_pointer Interface Reference

11.52.1 Detailed Description

Definition at line 123 of file kim_model_create_module.f90.

The documentation for this interface was generated from the following file:

- kim-api-v2.0.0-beta.0/fortran/include/[kim_model_create_module.f90](#)

11.53 kim_model_create_module::kim_model_create_set_model_buffer_pointer Interface Reference

11.53.1 Detailed Description

Definition at line 214 of file kim_model_create_module.f90.

The documentation for this interface was generated from the following file:

- kim-api-v2.0.0-beta.0/fortran/include/[kim_model_create_module.f90](#)

11.54 kim_model_create_module::kim_model_create_set_species_code Interface Reference

11.54.1 Detailed Description

Definition at line 202 of file kim_model_create_module.f90.

The documentation for this interface was generated from the following file:

- [kim-api-v2.0.0-beta.0/fortran/include/kim_model_create_module.f90](#)

11.55 kim_model_create_module::kim_model_create_string Interface Reference

11.55.1 Detailed Description

Definition at line 292 of file kim_model_create_module.f90.

The documentation for this interface was generated from the following file:

- [kim-api-v2.0.0-beta.0/fortran/include/kim_model_create_module.f90](#)

11.56 kim_model_module::kim_model_destroy Interface Reference

11.56.1 Detailed Description

Definition at line 171 of file kim_model_module.f90.

The documentation for this interface was generated from the following file:

- [kim-api-v2.0.0-beta.0/fortran/include/kim_model_module.f90](#)

11.57 kim_model_destroy_module::kim_model_destroy_string Interface Reference

11.57.1 Detailed Description

Definition at line 98 of file kim_model_destroy_module.f90.

The documentation for this interface was generated from the following file:

- [kim-api-v2.0.0-beta.0/fortran/include/kim_model_destroy_module.f90](#)

11.58 kim_model_driver_create_module::kim_model_driver_create_convert_unit Interface Reference

11.58.1 Detailed Description

Definition at line 281 of file kim_model_driver_create_module.f90.

The documentation for this interface was generated from the following file:

- kim-api-v2.0.0-beta.0/fortran/include/[kim_model_driver_create_module.f90](#)

11.59 kim_model_driver_create_module::kim_model_driver_create_log_entry Interface Reference

11.59.1 Detailed Description

Definition at line 318 of file kim_model_driver_create_module.f90.

The documentation for this interface was generated from the following file:

- kim-api-v2.0.0-beta.0/fortran/include/[kim_model_driver_create_module.f90](#)

11.60 kim_model_driver_create_module::kim_model_driver_create_set_compute_↔arguments_create_pointer Interface Reference

11.60.1 Detailed Description

Definition at line 197 of file kim_model_driver_create_module.f90.

The documentation for this interface was generated from the following file:

- kim-api-v2.0.0-beta.0/fortran/include/[kim_model_driver_create_module.f90](#)

11.61 kim_model_driver_create_module::kim_model_driver_create_set_compute_↔arguments_destroy_pointer Interface Reference

11.61.1 Detailed Description

Definition at line 210 of file kim_model_driver_create_module.f90.

The documentation for this interface was generated from the following file:

- kim-api-v2.0.0-beta.0/fortran/include/[kim_model_driver_create_module.f90](#)

11.62 kim_model_driver_create_module::kim_model_driver_create_set_compute_pointer Interface Reference

11.62.1 Detailed Description

Definition at line 223 of file kim_model_driver_create_module.f90.

The documentation for this interface was generated from the following file:

- kim-api-v2.0.0-beta.0/fortran/include/[kim_model_driver_create_module.f90](#)

11.63 kim_model_driver_create_module::kim_model_driver_create_set_destroy_pointer Interface Reference

11.63.1 Detailed Description

Definition at line 184 of file kim_model_driver_create_module.f90.

The documentation for this interface was generated from the following file:

- kim-api-v2.0.0-beta.0/fortran/include/[kim_model_driver_create_module.f90](#)

11.64 kim_model_driver_create_module::kim_model_driver_create_set_influence_distance_pointer Interface Reference

11.64.1 Detailed Description

Definition at line 150 of file kim_model_driver_create_module.f90.

The documentation for this interface was generated from the following file:

- kim-api-v2.0.0-beta.0/fortran/include/[kim_model_driver_create_module.f90](#)

11.65 kim_model_driver_create_module::kim_model_driver_create_set_model_buffer_pointer Interface Reference

11.65.1 Detailed Description

Definition at line 249 of file kim_model_driver_create_module.f90.

The documentation for this interface was generated from the following file:

- kim-api-v2.0.0-beta.0/fortran/include/[kim_model_driver_create_module.f90](#)

11.66 kim_model_driver_create_module::kim_model_driver_create_set_species_code Interface Reference

11.66.1 Detailed Description

Definition at line 236 of file kim_model_driver_create_module.f90.

The documentation for this interface was generated from the following file:

- kim-api-v2.0.0-beta.0/fortran/include/[kim_model_driver_create_module.f90](#)

11.67 kim_model_driver_create_module::kim_model_driver_create_string Interface Reference

11.67.1 Detailed Description

Definition at line 333 of file kim_model_driver_create_module.f90.

The documentation for this interface was generated from the following file:

- kim-api-v2.0.0-beta.0/fortran/include/[kim_model_driver_create_module.f90](#)

11.68 kim_model_module::kim_model_get_number_of_parameters Interface Reference

11.68.1 Detailed Description

Definition at line 279 of file kim_model_module.f90.

The documentation for this interface was generated from the following file:

- kim-api-v2.0.0-beta.0/fortran/include/[kim_model_module.f90](#)

11.69 kim_model_module::kim_model_pop_log_verbosity Interface Reference

11.69.1 Detailed Description

Definition at line 343 of file kim_model_module.f90.

The documentation for this interface was generated from the following file:

- kim-api-v2.0.0-beta.0/fortran/include/[kim_model_module.f90](#)

11.70 kim_model_refresh_module::kim_model_refresh_string Interface Reference

11.70.1 Detailed Description

Definition at line 123 of file kim_model_refresh_module.f90.

The documentation for this interface was generated from the following file:

- kim-api-v2.0.0-beta.0/fortran/include/[kim_model_refresh_module.f90](#)

11.71 kim_model_module::kim_model_set_simulator_buffer_pointer Interface Reference

11.71.1 Detailed Description

Definition at line 302 of file kim_model_module.f90.

The documentation for this interface was generated from the following file:

- kim-api-v2.0.0-beta.0/fortran/include/[kim_model_module.f90](#)

11.72 KIM_Numbering Struct Reference

```
#include <KIM_Numbering.h>
```

Public Attributes

- int [numberingID](#)

11.72.1 Detailed Description

Definition at line 39 of file KIM_Numbering.h.

11.72.2 Member Data Documentation

11.72.2.1 numberingID

```
int KIM_Numbering::numberingID
```

Definition at line 41 of file KIM_Numbering.h.

The documentation for this struct was generated from the following file:

- kim-api-v2.0.0-beta.0/c/include/[KIM_Numbering.h](#)

11.73 KIM_SpeciesName Struct Reference

```
#include <KIM_SpeciesName.h>
```

Public Attributes

- int [speciesNameID](#)

11.73.1 Detailed Description

Definition at line 39 of file KIM_SpeciesName.h.

11.73.2 Member Data Documentation

11.73.2.1 [speciesNameID](#)

```
int KIM_SpeciesName::speciesNameID
```

Definition at line 41 of file KIM_SpeciesName.h.

The documentation for this struct was generated from the following file:

- kim-api-v2.0.0-beta.0/c/include/[KIM_SpeciesName.h](#)

11.74 KIM_SupportStatus Struct Reference

```
#include <KIM_SupportStatus.h>
```

Public Attributes

- int [supportStatusID](#)

11.74.1 Detailed Description

Definition at line 39 of file KIM_SupportStatus.h.

11.74.2 Member Data Documentation

11.74.2.1 supportStatusID

```
int KIM_SupportStatus::supportStatusID
```

Definition at line 41 of file KIM_SupportStatus.h.

The documentation for this struct was generated from the following file:

- [kim-api-v2.0.0-beta.0/c/include/KIM_SupportStatus.h](#)

11.75 KIM_TemperatureUnit Struct Reference

```
#include <KIM_TemperatureUnit.h>
```

Public Attributes

- int [temperatureUnitID](#)

11.75.1 Detailed Description

Definition at line 39 of file KIM_TemperatureUnit.h.

11.75.2 Member Data Documentation

11.75.2.1 temperatureUnitID

```
int KIM_TemperatureUnit::temperatureUnitID
```

Definition at line 41 of file KIM_TemperatureUnit.h.

The documentation for this struct was generated from the following file:

- [kim-api-v2.0.0-beta.0/c/include/KIM_TemperatureUnit.h](#)

11.76 KIM_TimeUnit Struct Reference

```
#include <KIM_TimeUnit.h>
```

Public Attributes

- int [timeUnitID](#)

11.76.1 Detailed Description

Definition at line 39 of file KIM_TimeUnit.h.

11.76.2 Member Data Documentation

11.76.2.1 timeUnitID

```
int KIM_TimeUnit::timeUnitID
```

Definition at line 41 of file KIM_TimeUnit.h.

The documentation for this struct was generated from the following file:

- kim-api-v2.0.0-beta.0/c/include/[KIM_TimeUnit.h](#)

11.77 KIM::LanguageName Class Reference

```
#include <KIM_LanguageName.hpp>
```

Public Member Functions

- [LanguageName](#) ()
- [LanguageName](#) (int const id)
- [LanguageName](#) (std::string const str)
- bool [operator==](#) ([LanguageName](#) const &rhs) const
- bool [operator!=](#) ([LanguageName](#) const &rhs) const
- std::string const & [String](#) () const

Public Attributes

- int [languageNameID](#)

11.77.1 Detailed Description

Definition at line 41 of file KIM_LanguageName.hpp.

11.77.2 Constructor & Destructor Documentation

11.77.2.1 LanguageName() [1/3]

```
KIM::LanguageName::LanguageName ( )
```

11.77.2.2 LanguageName() [2/3]

```
KIM::LanguageName::LanguageName (
    int const id )
```

11.77.2.3 LanguageName() [3/3]

```
KIM::LanguageName::LanguageName (
    std::string const str )
```

11.77.3 Member Function Documentation

11.77.3.1 operator!=(())

```
bool KIM::LanguageName::operator!= (
    LanguageName const & rhs ) const
```

11.77.3.2 operator==(())

```
bool KIM::LanguageName::operator== (
    LanguageName const & rhs ) const
```

11.77.3.3 String()

```
std::string const& KIM::LanguageName::String ( ) const
```

11.77.4 Member Data Documentation

11.77.4.1 languageNameID

```
int KIM::LanguageName::languageNameID
```

Definition at line 44 of file KIM_LanguageName.hpp.

The documentation for this class was generated from the following file:

- [kim-api-v2.0.0-beta.0/cpp/include/KIM_LanguageName.hpp](#)

11.78 KIM::LengthUnit Class Reference

```
#include <KIM_LengthUnit.hpp>
```

Public Member Functions

- [LengthUnit](#) ()
- [LengthUnit](#) (int const id)
- [LengthUnit](#) (std::string const &str)
- bool [operator==](#) ([LengthUnit](#) const &rhs) const
- bool [operator!=](#) ([LengthUnit](#) const &rhs) const
- std::string const & [String](#) () const

Public Attributes

- int [lengthUnitID](#)

11.78.1 Detailed Description

Definition at line 42 of file KIM_LengthUnit.hpp.

11.78.2 Constructor & Destructor Documentation

11.78.2.1 LengthUnit() [1/3]

```
KIM::LengthUnit::LengthUnit ( )
```

11.78.2.2 LengthUnit() [2/3]

```
KIM::LengthUnit::LengthUnit (
    int const id )
```

11.78.2.3 LengthUnit() [3/3]

```
KIM::LengthUnit::LengthUnit (
    std::string const & str )
```

11.78.3 Member Function Documentation

11.78.3.1 operator!=(())

```
bool KIM::LengthUnit::operator!= (
    LengthUnit const & rhs ) const
```

11.78.3.2 operator==(())

```
bool KIM::LengthUnit::operator== (
    LengthUnit const & rhs ) const
```

11.78.3.3 String()

```
std::string const& KIM::LengthUnit::String ( ) const
```

11.78.4 Member Data Documentation

11.78.4.1 lengthUnitID

```
int KIM::LengthUnit::lengthUnitID
```

Definition at line 45 of file KIM_LengthUnit.hpp.

The documentation for this class was generated from the following file:

- [kim-api-v2.0.0-beta.0/cpp/include/KIM_LengthUnit.hpp](#)

11.79 LennardJones612 Class Reference

```
#include <LennardJones612.hpp>
```

Public Member Functions

- [LennardJones612](#) ([KIM::ModelDriverCreate](#) *const modelDriverCreate, [KIM::LengthUnit](#) const requestedLengthUnit, [KIM::EnergyUnit](#) const requestedEnergyUnit, [KIM::ChargeUnit](#) const requestedChargeUnit, [KIM::TemperatureUnit](#) const requestedTemperatureUnit, [KIM::TimeUnit](#) const requestedTimeUnit, int *const ier)
- [~LennardJones612](#) ()

Static Public Member Functions

- static int [Destroy](#) ([KIM::ModelDestroy](#) *const modelDestroy)
- static int [Refresh](#) ([KIM::ModelRefresh](#) *const modelRefresh)
- static int [Compute](#) ([KIM::ModelCompute](#) const *const modelCompute, [KIM::ModelComputeArguments](#) const *const modelComputeArguments)
- static int [ComputeArgumentsCreate](#) ([KIM::ModelCompute](#) const *const modelCompute, [KIM::ModelComputeArgumentsCreate](#) *const modelComputeArgumentsCreate)
- static int [ComputeArgumentsDestroy](#) ([KIM::ModelCompute](#) const *const modelCompute, [KIM::ModelComputeArgumentsDestroy](#) *const modelComputeArgumentsDestroy)

11.79.1 Detailed Description

Definition at line 49 of file LennardJones612.hpp.

11.79.2 Constructor & Destructor Documentation

11.79.2.1 LennardJones612()

```
LennardJones612::LennardJones612 (
    KIM::ModelDriverCreate *const modelDriverCreate,
    KIM::LengthUnit const requestedLengthUnit,
    KIM::EnergyUnit const requestedEnergyUnit,
    KIM::ChargeUnit const requestedChargeUnit,
    KIM::TemperatureUnit const requestedTemperatureUnit,
    KIM::TimeUnit const requestedTimeUnit,
    int *const ier )
```

Definition at line 93 of file LennardJones612.cpp.

11.79.2.2 `~LennardJones612()`

```
LennardJones612::~~LennardJones612 ( )
```

Definition at line 113 of file LennardJones612.cpp.

11.79.3 Member Function Documentation

11.79.3.1 `Compute()`

```
int LennardJones612::Compute (
    KIM::ModelCompute const *const modelCompute,
    KIM::ModelComputeArguments const *const modelComputeArguments ) [static]
```

Definition at line 149 of file LennardJones612.cpp.

11.79.3.2 `ComputeArgumentsCreate()`

```
int LennardJones612::ComputeArgumentsCreate (
    KIM::ModelCompute const *const modelCompute,
    KIM::ModelComputeArgumentsCreate *const modelComputeArgumentsCreate ) [static]
```

Definition at line 162 of file LennardJones612.cpp.

11.79.3.3 `ComputeArgumentsDestroy()`

```
int LennardJones612::ComputeArgumentsDestroy (
    KIM::ModelCompute const *const modelCompute,
    KIM::ModelComputeArgumentsDestroy *const modelComputeArgumentsDestroy ) [static]
```

Definition at line 175 of file LennardJones612.cpp.

11.79.3.4 `Destroy()`

```
int LennardJones612::Destroy (
    KIM::ModelDestroy *const modelDestroy ) [static]
```

Definition at line 120 of file LennardJones612.cpp.

11.79.3.5 Refresh()

```
int LennardJones612::Refresh (
    KIM::ModelRefresh *const modelRefresh ) [static]
```

Definition at line 137 of file LennardJones612.cpp.

The documentation for this class was generated from the following files:

- [kim-api-v2.0.0-beta.0/examples/model_drivers/LennardJones612__MD_414112407348_003/LennardJones612.hpp](#)
- [kim-api-v2.0.0-beta.0/examples/model_drivers/LennardJones612__MD_414112407348_003/LennardJones612.cpp](#)

11.80 LennardJones612Implementation Class Reference

```
#include <LennardJones612Implementation.hpp>
```

Public Member Functions

- [LennardJones612Implementation](#) ([KIM::ModelDriverCreate](#) *const modelDriverCreate, [KIM::LengthUnit](#) const requestedLengthUnit, [KIM::EnergyUnit](#) const requestedEnergyUnit, [KIM::ChargeUnit](#) const requestedChargeUnit, [KIM::TemperatureUnit](#) const requestedTemperatureUnit, [KIM::TimeUnit](#) const requestedTimeUnit, int *const ier)
- [~LennardJones612Implementation](#) ()
- int [Refresh](#) ([KIM::ModelRefresh](#) *const modelRefresh)
- int [Compute](#) ([KIM::ModelCompute](#) const *const modelCompute, [KIM::ModelComputeArguments](#) const *const modelComputeArguments)
- int [ComputeArgumentsCreate](#) ([KIM::ModelComputeArgumentsCreate](#) *const modelComputeArguments↵ Create) const
- int [ComputeArgumentsDestroy](#) ([KIM::ModelComputeArgumentsDestroy](#) *const modelComputeArguments↵ Destroy) const

11.80.1 Detailed Description

Definition at line 76 of file LennardJones612Implementation.hpp.

11.80.2 Constructor & Destructor Documentation

11.80.2.1 LennardJones612Implementation()

```
LennardJones612Implementation::LennardJones612Implementation (
    KIM::ModelDriverCreate *const modelDriverCreate,
    KIM::LengthUnit const requestedLengthUnit,
    KIM::EnergyUnit const requestedEnergyUnit,
    KIM::ChargeUnit const requestedChargeUnit,
    KIM::TemperatureUnit const requestedTemperatureUnit,
    KIM::TimeUnit const requestedTimeUnit,
    int *const ier )
```

Definition at line 54 of file LennardJones612Implementation.cpp.

11.80.2.2 `~LennardJones612Implementation()`

```
LennardJones612Implementation::~LennardJones612Implementation ( )
```

Definition at line 119 of file LennardJones612Implementation.cpp.

11.80.3 Member Function Documentation

11.80.3.1 `Compute()`

```
int LennardJones612Implementation::Compute (
    KIM::ModelCompute const *const modelCompute,
    KIM::ModelComputeArguments const *const modelComputeArguments )
```

Definition at line 154 of file LennardJones612Implementation.cpp.

11.80.3.2 `ComputeArgumentsCreate()`

```
int LennardJones612Implementation::ComputeArgumentsCreate (
    KIM::ModelComputeArgumentsCreate *const modelComputeArgumentsCreate ) const
```

Definition at line 204 of file LennardJones612Implementation.cpp.

11.80.3.3 `ComputeArgumentsDestroy()`

```
int LennardJones612Implementation::ComputeArgumentsDestroy (
    KIM::ModelComputeArgumentsDestroy *const modelComputeArgumentsDestroy ) const
```

Definition at line 220 of file LennardJones612Implementation.cpp.

11.80.3.4 `Refresh()`

```
int LennardJones612Implementation::Refresh (
    KIM::ModelRefresh *const modelRefresh )
```

Definition at line 138 of file LennardJones612Implementation.cpp.

The documentation for this class was generated from the following files:

- kim-api-v2.0.0-beta.0/examples/model_drivers/LennardJones612__MD_414112407348_003/LennardJones612Implementation
- kim-api-v2.0.0-beta.0/examples/model_drivers/LennardJones612__MD_414112407348_003/LennardJones612Implementation

11.81 KIM::Log Class Reference

```
#include <KIM_Log.hpp>
```

Public Member Functions

- `std::string const & GetID () const`
- `void SetID (std::string const &id)`
- `void PushVerbosity (LogVerbosity const logVerbosity)`
- `void PopVerbosity ()`
- `void LogEntry (LogVerbosity const logVerbosity, std::string const &message, int const lineNumber, std::string const &fileName) const`
- `void LogEntry (LogVerbosity const logVerbosity, std::stringstream const &message, int const lineNumber, std::string const &fileName) const`

Static Public Member Functions

- `static int Create (Log **const log)`
- `static void Destroy (Log **const log)`

11.81.1 Detailed Description

Definition at line 46 of file KIM_Log.hpp.

11.81.2 Member Function Documentation

11.81.2.1 Create()

```
static int KIM::Log::Create (  
    Log **const log ) [static]
```

11.81.2.2 Destroy()

```
static void KIM::Log::Destroy (  
    Log **const log ) [static]
```

11.81.2.3 GetID()

```
std::string const& KIM::Log::GetID ( ) const
```


11.81.2.4 LogEntry() [1/2]

```
void KIM::Log::LogEntry (
    LogVerbosity const logVerbosity,
    std::string const & message,
    int const lineNumber,
    std::string const & fileName ) const
```

11.81.2.5 LogEntry() [2/2]

```
void KIM::Log::LogEntry (
    LogVerbosity const logVerbosity,
    std::stringstream const & message,
    int const lineNumber,
    std::string const & fileName ) const
```

11.81.2.6 PopVerbosity()

```
void KIM::Log::PopVerbosity ( )
```

11.81.2.7 PushVerbosity()

```
void KIM::Log::PushVerbosity (
    LogVerbosity const logVerbosity )
```

11.81.2.8 SetID()

```
void KIM::Log::SetID (
    std::string const & id )
```

The documentation for this class was generated from the following file:

- [kim-api-v2.0.0-beta.0/cpp/include/KIM_Log.hpp](#)

11.82 KIM::LogVerbosity Class Reference

```
#include <KIM_LogVerbosity.hpp>
```

Public Member Functions

- [LogVerbosity](#) ()
- [LogVerbosity](#) (int const id)
- [LogVerbosity](#) (std::string const &str)
- bool [operator<](#) ([LogVerbosity](#) const &rhs) const
- bool [operator>](#) ([LogVerbosity](#) const &rhs) const
- bool [operator<=](#) ([LogVerbosity](#) const &rhs) const
- bool [operator>=](#) ([LogVerbosity](#) const &rhs) const
- bool [operator==](#) ([LogVerbosity](#) const &rhs) const
- bool [operator!=](#) ([LogVerbosity](#) const &rhs) const
- std::string const & [String](#) () const

Public Attributes

- int [logVerbosityID](#)

11.82.1 Detailed Description

Definition at line 46 of file KIM_LogVerbosity.hpp.

11.82.2 Constructor & Destructor Documentation

11.82.2.1 [LogVerbosity\(\)](#) [1/3]

```
KIM::LogVerbosity::LogVerbosity ( )
```

11.82.2.2 [LogVerbosity\(\)](#) [2/3]

```
KIM::LogVerbosity::LogVerbosity (
    int const id )
```

11.82.2.3 [LogVerbosity\(\)](#) [3/3]

```
KIM::LogVerbosity::LogVerbosity (
    std::string const & str )
```

11.82.3 Member Function Documentation

11.82.3.1 operator!=(())

```
bool KIM::LogVerbosity::operator!= (
    LogVerbosity const & rhs ) const
```

11.82.3.2 operator<()

```
bool KIM::LogVerbosity::operator< (
    LogVerbosity const & rhs ) const
```

11.82.3.3 operator<=()

```
bool KIM::LogVerbosity::operator<= (
    LogVerbosity const & rhs ) const
```

11.82.3.4 operator==(())

```
bool KIM::LogVerbosity::operator==(
    LogVerbosity const & rhs ) const
```

11.82.3.5 operator>()

```
bool KIM::LogVerbosity::operator> (
    LogVerbosity const & rhs ) const
```

11.82.3.6 operator>=()

```
bool KIM::LogVerbosity::operator>= (
    LogVerbosity const & rhs ) const
```

11.82.3.7 String()

```
std::string const& KIM::LogVerbosity::String ( ) const
```

11.82.4 Member Data Documentation

11.82.4.1 logVerbosityID

```
int KIM::LogVerbosity::logVerbosityID
```

Definition at line 49 of file KIM_LogVerbosity.hpp.

The documentation for this class was generated from the following file:

- kim-api-v2.0.0-beta.0/cpp/include/KIM_LogVerbosity.hpp

11.83 KIM::Model Class Reference

```
#include <KIM_Model.hpp>
```

Public Member Functions

- void [GetInfluenceDistance](#) (double *const influenceDistance) const
- void [GetNeighborListCutoffsPointer](#) (int *const numberOfCutoffs, double const **const cutoffs) const
- void [GetUnits](#) ([LengthUnit](#) *const lengthUnit, [EnergyUnit](#) *const energyUnit, [ChargeUnit](#) *const chargeUnit, [TemperatureUnit](#) *const temperatureUnit, [TimeUnit](#) *const timeUnit) const
- int [ComputeArgumentsCreate](#) ([ComputeArguments](#) **const computeArguments) const
- int [ComputeArgumentsDestroy](#) ([ComputeArguments](#) **const computeArguments) const
- int [Compute](#) ([ComputeArguments](#) const *const computeArguments) const
- int [ClearInfluenceDistanceAndCutoffsThenRefreshModel](#) ()
- int [GetSpeciesSupportAndCode](#) ([SpeciesName](#) const speciesName, int *const speciesIsSupported, int *const code) const
- void [GetNumberOfParameters](#) (int *const numberOfParameters) const
- int [GetParameterDataTypeExtentAndDescription](#) (int const index, [DataType](#) *const dataType, int *extent, std::string const **const description) const
- int [GetParameter](#) (int const parameterIndex, int const arrayIndex, int *const parameterValue) const
- int [GetParameter](#) (int const parameterIndex, int const arrayIndex, double *const parameterValue) const
- int [SetParameter](#) (int const parameterIndex, int const arrayIndex, int const parameterValue)
- int [SetParameter](#) (int const parameterIndex, int const arrayIndex, double const parameterValue)
- void [SetSimulatorBufferPointer](#) (void *const ptr)
- void [GetSimulatorBufferPointer](#) (void **const ptr) const
- std::string const & [String](#) () const
- void [SetLogID](#) (std::string const &logID)
- void [PushLogVerbosity](#) ([LogVerbosity](#) const logVerbosity)
- void [PopLogVerbosity](#) ()

Static Public Member Functions

- static int [Create](#) ([Numbering](#) const numbering, [LengthUnit](#) const requestedLengthUnit, [EnergyUnit](#) const requestedEnergyUnit, [ChargeUnit](#) const requestedChargeUnit, [TemperatureUnit](#) const requestedTemperatureUnit, [TimeUnit](#) const requestedTimeUnit, std::string const &modelName, int *const requestedUnitsAccepted, [Model](#) **const model)
- static void [Destroy](#) ([Model](#) **const model)

11.83.1 Detailed Description

Definition at line 60 of file KIM_Model.hpp.

11.83.2 Member Function Documentation

11.83.2.1 ClearInfluenceDistanceAndCutoffsThenRefreshModel()

```
int KIM::Model::ClearInfluenceDistanceAndCutoffsThenRefreshModel ( )
```

11.83.2.2 Compute()

```
int KIM::Model::Compute (
    ComputeArguments const *const computeArguments ) const
```

11.83.2.3 ComputeArgumentsCreate()

```
int KIM::Model::ComputeArgumentsCreate (
    ComputeArguments **const computeArguments ) const
```

11.83.2.4 ComputeArgumentsDestroy()

```
int KIM::Model::ComputeArgumentsDestroy (
    ComputeArguments **const computeArguments ) const
```

11.83.2.5 Create()

```
static int KIM::Model::Create (
    Numbering const numbering,
    LengthUnit const requestedLengthUnit,
    EnergyUnit const requestedEnergyUnit,
    ChargeUnit const requestedChargeUnit,
    TemperatureUnit const requestedTemperatureUnit,
    TimeUnit const requestedTimeUnit,
    std::string const & modelName,
    int *const requestedUnitsAccepted,
    Model **const model ) [static]
```

11.83.2.6 Destroy()

```
static void KIM::Model::Destroy (
    Model **const model ) [static]
```

11.83.2.7 GetInfluenceDistance()

```
void KIM::Model::GetInfluenceDistance (
    double *const influenceDistance ) const
```

11.83.2.8 GetNeighborListCutoffsPointer()

```
void KIM::Model::GetNeighborListCutoffsPointer (
    int *const numberOfCutoffs,
    double const **const cutoffs ) const
```

11.83.2.9 GetNumberOfParameters()

```
void KIM::Model::GetNumberOfParameters (
    int *const numberOfParameters ) const
```

11.83.2.10 GetParameter() [1/2]

```
int KIM::Model::GetParameter (
    int const parameterIndex,
    int const arrayIndex,
    int *const parameterValue ) const
```

11.83.2.11 GetParameter() [2/2]

```
int KIM::Model::GetParameter (
    int const parameterIndex,
    int const arrayIndex,
    double *const parameterValue ) const
```

11.83.2.12 GetParameterDataTypeExtentAndDescription()

```
int KIM::Model::GetParameterDataTypeExtentAndDescription (
    int const index,
    DataType *const dataType,
    int * extent,
    std::string const **const description ) const
```

11.83.2.13 GetSimulatorBufferPointer()

```
void KIM::Model::GetSimulatorBufferPointer (
    void **const ptr ) const
```

11.83.2.14 GetSpeciesSupportAndCode()

```
int KIM::Model::GetSpeciesSupportAndCode (
    SpeciesName const speciesName,
    int *const speciesIsSupported,
    int *const code ) const
```

11.83.2.15 GetUnits()

```
void KIM::Model::GetUnits (
    LengthUnit *const lengthUnit,
    EnergyUnit *const energyUnit,
    ChargeUnit *const chargeUnit,
    TemperatureUnit *const temperatureUnit,
    TimeUnit *const timeUnit ) const
```

11.83.2.16 PopLogVerbosity()

```
void KIM::Model::PopLogVerbosity ( )
```

11.83.2.17 PushLogVerbosity()

```
void KIM::Model::PushLogVerbosity (
    LogVerbosity const logVerbosity )
```

11.83.2.18 SetLogID()

```
void KIM::Model::SetLogID (
    std::string const & logID )
```

11.83.2.19 SetParameter() [1/2]

```
int KIM::Model::SetParameter (
    int const parameterIndex,
    int const arrayIndex,
    int const parameterValue )
```

11.83.2.20 SetParameter() [2/2]

```
int KIM::Model::SetParameter (
    int const parameterIndex,
    int const arrayIndex,
    double const parameterValue )
```

11.83.2.21 SetSimulatorBufferPointer()

```
void KIM::Model::SetSimulatorBufferPointer (
    void *const ptr )
```

11.83.2.22 String()

```
std::string const& KIM::Model::String ( ) const
```

The documentation for this class was generated from the following file:

- [kim-api-v2.0.0-beta.0/cpp/include/KIM_Model.hpp](#)

11.84 KIM::ModelCompute Class Reference

```
#include <KIM_ModelCompute.hpp>
```


Public Member Functions

- void [GetModelBufferPointer](#) (void **const ptr) const
- void [LogEntry](#) ([LogVerbosity](#) const logVerbosity, std::string const &message, int const lineNumber, std::string const &fileName) const
- void [LogEntry](#) ([LogVerbosity](#) const logVerbosity, std::stringstream const &message, int const lineNumber, std::string const &fileName) const
- std::string const & [String](#) () const

11.84.1 Detailed Description

Definition at line 47 of file KIM_ModelCompute.hpp.

11.84.2 Member Function Documentation

11.84.2.1 GetModelBufferPointer()

```
void KIM::ModelCompute::GetModelBufferPointer (
    void **const ptr ) const
```

11.84.2.2 LogEntry() [1/2]

```
void KIM::ModelCompute::LogEntry (
    LogVerbosity const logVerbosity,
    std::string const & message,
    int const lineNumber,
    std::string const & fileName ) const
```

11.84.2.3 LogEntry() [2/2]

```
void KIM::ModelCompute::LogEntry (
    LogVerbosity const logVerbosity,
    std::stringstream const & message,
    int const lineNumber,
    std::string const & fileName ) const
```

11.84.2.4 String()

```
std::string const& KIM::ModelCompute::String ( ) const
```

The documentation for this class was generated from the following file:

- [kim-api-v2.0.0-beta.0/cpp/include/KIM_ModelCompute.hpp](#)

11.85 KIM::ModelComputeArguments Class Reference

```
#include <KIM_ModelComputeArguments.hpp>
```

Public Member Functions

- int [GetNeighborList](#) (int const neighborListIndex, int const particleNumber, int *const numberOfNeighbors, int const **const neighborsOfParticle) const
- int [ProcessDEDrTerm](#) (double const de, double const r, double const *const dx, int const i, int const j) const
- int [ProcessD2EDr2Term](#) (double const de, double const *const r, double const *const dx, int const *const i, int const *const j) const
- int [GetArgumentPointer](#) ([ComputeArgumentName](#) const computeArgumentName, int const **const ptr) const
- int [GetArgumentPointer](#) ([ComputeArgumentName](#) const computeArgumentName, int **const ptr) const
- int [GetArgumentPointer](#) ([ComputeArgumentName](#) const computeArgumentName, double const **const ptr) const
- int [GetArgumentPointer](#) ([ComputeArgumentName](#) const computeArgumentName, double **const ptr) const
- int [IsCallbackPresent](#) ([ComputeCallbackName](#) const computeCallbackName, int *const present) const
- void [SetModelBufferPointer](#) (void *const ptr)
- void [GetModelBufferPointer](#) (void **const ptr) const
- void [LogEntry](#) ([LogVerbosity](#) const logVerbosity, std::string const &message, int const lineNumber, std::string const &fileName) const
- void [LogEntry](#) ([LogVerbosity](#) const logVerbosity, std::stringstream const &message, int const lineNumber, std::string const &fileName) const
- std::string const & [String](#) () const

11.85.1 Detailed Description

Definition at line 49 of file [KIM_ModelComputeArguments.hpp](#).

11.85.2 Member Function Documentation

11.85.2.1 GetArgumentPointer() [1/4]

```
int KIM::ModelComputeArguments::GetArgumentPointer (
    ComputeArgumentName const computeArgumentName,
    int const **const ptr ) const
```

11.85.2.2 GetArgumentPointer() [2/4]

```
int KIM::ModelComputeArguments::GetArgumentPointer (
    ComputeArgumentName const computeArgumentName,
    int **const ptr ) const
```

11.85.2.3 GetArgumentPointer() [3/4]

```
int KIM::ModelComputeArguments::GetArgumentPointer (
    ComputeArgumentName const computeArgumentName,
    double const **const ptr ) const
```

11.85.2.4 GetArgumentPointer() [4/4]

```
int KIM::ModelComputeArguments::GetArgumentPointer (
    ComputeArgumentName const computeArgumentName,
    double **const ptr ) const
```

11.85.2.5 GetModelBufferPointer()

```
void KIM::ModelComputeArguments::GetModelBufferPointer (
    void **const ptr ) const
```

11.85.2.6 GetNeighborList()

```
int KIM::ModelComputeArguments::GetNeighborList (
    int const neighborListIndex,
    int const particleNumber,
    int *const numberOfNeighbors,
    int const **const neighborsOfParticle ) const
```

11.85.2.7 IsCallbackPresent()

```
int KIM::ModelComputeArguments::IsCallbackPresent (
    ComputeCallbackName const computeCallbackName,
    int *const present ) const
```

11.85.2.8 LogEntry() [1/2]

```
void KIM::ModelComputeArguments::LogEntry (
    LogVerbosity const logVerbosity,
    std::string const & message,
    int const lineNumber,
    std::string const & fileName ) const
```

11.85.2.9 LogEntry() [2/2]

```
void KIM::ModelComputeArguments::LogEntry (
    LogVerbosity const logVerbosity,
    std::stringstream const & message,
    int const lineNumber,
    std::string const & fileName ) const
```

11.85.2.10 ProcessD2EDr2Term()

```
int KIM::ModelComputeArguments::ProcessD2EDr2Term (
    double const de,
    double const *const r,
    double const *const dx,
    int const *const i,
    int const *const j ) const
```

11.85.2.11 ProcessDEDrTerm()

```
int KIM::ModelComputeArguments::ProcessDEDrTerm (
    double const de,
    double const r,
    double const *const dx,
    int const i,
    int const j ) const
```

11.85.2.12 SetModelBufferPointer()

```
void KIM::ModelComputeArguments::SetModelBufferPointer (
    void *const ptr )
```

11.85.2.13 String()

```
std::string const& KIM::ModelComputeArguments::String ( ) const
```

The documentation for this class was generated from the following file:

- [kim-api-v2.0.0-beta.0/cpp/include/KIM_ModelComputeArguments.hpp](#)

11.86 KIM::ModelComputeArgumentsCreate Class Reference

```
#include <KIM_ModelComputeArgumentsCreate.hpp>
```

Public Member Functions

- int [SetArgumentSupportStatus](#) ([ComputeArgumentName](#) const clomputeArgumentName, [SupportStatus](#) const supportStatus)
- int [SetCallbackSupportStatus](#) ([ComputeCallbackName](#) const computeCallbackName, [SupportStatus](#) const supportStatus)
- void [SetModelBufferPointer](#) (void *const ptr)
- void [LogEntry](#) ([LogVerbosity](#) const logVerbosity, std::string const &message, int const lineNumber, std::string const &fileName) const
- void [LogEntry](#) ([LogVerbosity](#) const logVerbosity, std::stringstream const &message, int const lineNumber, std::string const &fileName) const
- std::string const & [String](#) () const

11.86.1 Detailed Description

Definition at line 55 of file [KIM_ModelComputeArgumentsCreate.hpp](#).

11.86.2 Member Function Documentation

11.86.2.1 LogEntry() [1/2]

```
void KIM::ModelComputeArgumentsCreate::LogEntry (
    LogVerbosity const logVerbosity,
    std::string const & message,
    int const lineNumber,
    std::string const & fileName ) const
```

11.86.2.2 LogEntry() [2/2]

```
void KIM::ModelComputeArgumentsCreate::LogEntry (
    LogVerbosity const logVerbosity,
    std::stringstream const & message,
    int const lineNumber,
    std::string const & fileName ) const
```

11.86.2.3 SetArgumentSupportStatus()

```
int KIM::ModelComputeArgumentsCreate::SetArgumentSupportStatus (
    ComputeArgumentName const ccomputeArgumentName,
    SupportStatus const supportStatus )
```

11.86.2.4 SetCallbackSupportStatus()

```
int KIM::ModelComputeArgumentsCreate::SetCallbackSupportStatus (
    ComputeCallbackName const computeCallbackName,
    SupportStatus const supportStatus )
```

11.86.2.5 SetModelBufferPointer()

```
void KIM::ModelComputeArgumentsCreate::SetModelBufferPointer (
    void *const ptr )
```

11.86.2.6 String()

```
std::string const& KIM::ModelComputeArgumentsCreate::String ( ) const
```

The documentation for this class was generated from the following file:

- [kim-api-v2.0.0-beta.0/cpp/include/KIM_ModelComputeArgumentsCreate.hpp](#)

11.87 KIM::ModelComputeArgumentsDestroy Class Reference

```
#include <KIM_ModelComputeArgumentsDestroy.hpp>
```

Public Member Functions

- void [GetModelBufferPointer](#) (void **const ptr) const
- void [LogEntry](#) ([LogVerbosity](#) const logVerbosity, std::string const &message, int const lineNumber, std::string const &fileName) const
- void [LogEntry](#) ([LogVerbosity](#) const logVerbosity, std::stringstream const &message, int const lineNumber, std::string const &fileName) const
- std::string const & [String](#) () const

11.87.1 Detailed Description

Definition at line 47 of file KIM_ModelComputeArgumentsDestroy.hpp.

11.87.2 Member Function Documentation

11.87.2.1 [GetModelBufferPointer\(\)](#)

```
void KIM::ModelComputeArgumentsDestroy::GetModelBufferPointer (  
    void **const ptr ) const
```

11.87.2.2 [LogEntry\(\)](#) [1/2]

```
void KIM::ModelComputeArgumentsDestroy::LogEntry (  
    LogVerbosity const logVerbosity,  
    std::string const & message,  
    int const lineNumber,  
    std::string const & fileName ) const
```

11.87.2.3 [LogEntry\(\)](#) [2/2]

```
void KIM::ModelComputeArgumentsDestroy::LogEntry (  
    LogVerbosity const logVerbosity,  
    std::stringstream const & message,  
    int const lineNumber,  
    std::string const & fileName ) const
```

11.87.2.4 String()

```
std::string const& KIM::ModelComputeArgumentsDestroy::String ( ) const
```

The documentation for this class was generated from the following file:

- [kim-api-v2.0.0-beta.0/cpp/include/KIM_ModelComputeArgumentsDestroy.hpp](#)

11.88 KIM::ModelCreate Class Reference

```
#include <KIM_ModelCreate.hpp>
```

Public Member Functions

- int [SetModelNumbering](#) ([Numbering](#) const numbering)
- void [SetInfluenceDistancePointer](#) (double const *const influenceDistance)
- void [SetNeighborListCutoffsPointer](#) (int const numberOfCutoffs, double const *const cutoffs)
- int [SetRefreshPointer](#) ([LanguageName](#) const languageName, [func](#) *const fptr)
- int [SetDestroyPointer](#) ([LanguageName](#) const languageName, [func](#) *const fptr)
- int [SetComputeArgumentsCreatePointer](#) ([LanguageName](#) const languageName, [func](#) *const fptr)
- int [SetComputeArgumentsDestroyPointer](#) ([LanguageName](#) const languageName, [func](#) *const fptr)
- int [SetComputePointer](#) ([LanguageName](#) const languageName, [func](#) *const fptr)
- int [SetSpeciesCode](#) ([SpeciesName](#) const speciesName, int const code)
- int [SetParameterPointer](#) (int const extent, int *const ptr, std::string const &description)
- int [SetParameterPointer](#) (int const extent, double *const ptr, std::string const &description)
- void [SetModelBufferPointer](#) (void *const ptr)
- int [SetUnits](#) ([LengthUnit](#) const lengthUnit, [EnergyUnit](#) const energyUnit, [ChargeUnit](#) const chargeUnit, [TemperatureUnit](#) const temperatureUnit, [TimeUnit](#) const timeUnit)
- int [ConvertUnit](#) ([LengthUnit](#) const fromLengthUnit, [EnergyUnit](#) const fromEnergyUnit, [ChargeUnit](#) const fromChargeUnit, [TemperatureUnit](#) const fromTemperatureUnit, [TimeUnit](#) const fromTimeUnit, [LengthUnit](#) const toLengthUnit, [EnergyUnit](#) const toEnergyUnit, [ChargeUnit](#) const toChargeUnit, [TemperatureUnit](#) const toTemperatureUnit, [TimeUnit](#) const toTimeUnit, double const lengthExponent, double const energyExponent, double const chargeExponent, double const temperatureExponent, double const timeExponent, double *const conversionFactor) const
- void [LogEntry](#) ([LogVerbosity](#) const logVerbosity, std::string const &message, int const lineNumber, std::string const &fileName) const
- void [LogEntry](#) ([LogVerbosity](#) const logVerbosity, std::stringstream const &message, int const lineNumber, std::string const &fileName) const
- std::string const & [String](#) () const

11.88.1 Detailed Description

Definition at line 61 of file [KIM_ModelCreate.hpp](#).

11.88.2 Member Function Documentation

11.88.2.1 ConvertUnit()

```
int KIM::ModelCreate::ConvertUnit (
    LengthUnit const fromLengthUnit,
    EnergyUnit const fromEnergyUnit,
    ChargeUnit const fromChargeUnit,
    TemperatureUnit const fromTemperatureUnit,
    TimeUnit const fromTimeUnit,
    LengthUnit const toLengthUnit,
    EnergyUnit const toEnergyUnit,
    ChargeUnit const toChargeUnit,
    TemperatureUnit const toTemperatureUnit,
    TimeUnit const toTimeUnit,
    double const lengthExponent,
    double const energyExponent,
    double const chargeExponent,
    double const temperatureExponent,
    double const timeExponent,
    double *const conversionFactor ) const
```

11.88.2.2 LogEntry() [1/2]

```
void KIM::ModelCreate::LogEntry (
    LogVerbosity const logVerbosity,
    std::string const & message,
    int const lineNumber,
    std::string const & fileName ) const
```

11.88.2.3 LogEntry() [2/2]

```
void KIM::ModelCreate::LogEntry (
    LogVerbosity const logVerbosity,
    std::stringstream const & message,
    int const lineNumber,
    std::string const & fileName ) const
```

11.88.2.4 SetComputeArgumentsCreatePointer()

```
int KIM::ModelCreate::SetComputeArgumentsCreatePointer (
    LanguageName const languageName,
    func *const fptr )
```

11.88.2.5 SetComputeArgumentsDestroyPointer()

```
int KIM::ModelCreate::SetComputeArgumentsDestroyPointer (
    LanguageName const languageName,
    func *const fptr )
```

11.88.2.6 SetComputePointer()

```
int KIM::ModelCreate::SetComputePointer (
    LanguageName const languageName,
    func *const fptr )
```

11.88.2.7 SetDestroyPointer()

```
int KIM::ModelCreate::SetDestroyPointer (
    LanguageName const languageName,
    func *const fptr )
```

11.88.2.8 SetInfluenceDistancePointer()

```
void KIM::ModelCreate::SetInfluenceDistancePointer (
    double const *const influenceDistance )
```

11.88.2.9 SetModelBufferPointer()

```
void KIM::ModelCreate::SetModelBufferPointer (
    void *const ptr )
```

11.88.2.10 SetModelNumbering()

```
int KIM::ModelCreate::SetModelNumbering (
    Numbering const numbering )
```

11.88.2.11 SetNeighborListCutoffsPointer()

```
void KIM::ModelCreate::SetNeighborListCutoffsPointer (
    int const numberOfCutoffs,
    double const *const cutoffs )
```

11.88.2.12 SetParameterPointer() [1/2]

```
int KIM::ModelCreate::SetParameterPointer (
    int const extent,
    int *const ptr,
    std::string const & description )
```

11.88.2.13 SetParameterPointer() [2/2]

```
int KIM::ModelCreate::SetParameterPointer (
    int const extent,
    double *const ptr,
    std::string const & description )
```

11.88.2.14 SetRefreshPointer()

```
int KIM::ModelCreate::SetRefreshPointer (
    LanguageName const languageName,
    func *const fptr )
```

11.88.2.15 SetSpeciesCode()

```
int KIM::ModelCreate::SetSpeciesCode (
    SpeciesName const speciesName,
    int const code )
```

11.88.2.16 SetUnits()

```
int KIM::ModelCreate::SetUnits (
    LengthUnit const lengthUnit,
    EnergyUnit const energyUnit,
    ChargeUnit const chargeUnit,
    TemperatureUnit const temperatureUnit,
    TimeUnit const timeUnit )
```

11.88.2.17 String()

```
std::string const& KIM::ModelCreate::String ( ) const
```

The documentation for this class was generated from the following file:

- [kim-api-v2.0.0-beta.0/cpp/include/KIM_ModelCreate.hpp](#)

11.89 KIM::ModelDestroy Class Reference

```
#include <KIM_ModelDestroy.hpp>
```

Public Member Functions

- void [GetModelBufferPointer](#) (void **const ptr) const
- void [LogEntry](#) ([LogVerbosity](#) const logVerbosity, std::string const &message, int const lineNumber, std::string const &fileName) const
- void [LogEntry](#) ([LogVerbosity](#) const logVerbosity, std::stringstream const &message, int const lineNumber, std::string const &fileName) const
- std::string const & [String](#) () const

11.89.1 Detailed Description

Definition at line 47 of file `KIM_ModelDestroy.hpp`.

11.89.2 Member Function Documentation

11.89.2.1 GetModelBufferPointer()

```
void KIM::ModelDestroy::GetModelBufferPointer (
    void **const ptr ) const
```

11.89.2.2 LogEntry() [1/2]

```
void KIM::ModelDestroy::LogEntry (
    LogVerbosity const logVerbosity,
    std::string const & message,
    int const lineNumber,
    std::string const & fileName ) const
```

11.89.2.3 LogEntry() [2/2]

```
void KIM::ModelDestroy::LogEntry (
    LogVerbosity const logVerbosity,
    std::stringstream const & message,
    int const lineNumber,
    std::string const & fileName ) const
```

11.89.2.4 String()

```
std::string const& KIM::ModelDestroy::String ( ) const
```

The documentation for this class was generated from the following file:

- [kim-api-v2.0.0-beta.0/cpp/include/KIM_ModelDestroy.hpp](#)

11.90 KIM::ModelDriverCreate Class Reference

```
#include <KIM_ModelDriverCreate.hpp>
```

Public Member Functions

- void [GetNumberOfParameterFiles](#) (int *const numberOfParameterFiles) const
- int [GetParameterFileName](#) (int const index, std::string const **const parameterFileName) const
- int [SetModelNumbering](#) (Numbering const numbering)
- void [SetInfluenceDistancePointer](#) (double const *const influenceDistance)
- void [SetNeighborListCutoffsPointer](#) (int const numberOfCutoffs, double const *const cutoffs)
- int [SetRefreshPointer](#) (LanguageName const languageName, func *const fptr)
- int [SetDestroyPointer](#) (LanguageName const languageName, func *const fptr)
- int [SetComputeArgumentsCreatePointer](#) (LanguageName const languageName, func *const fptr)
- int [SetComputeArgumentsDestroyPointer](#) (LanguageName const languageName, func *const fptr)
- int [SetComputePointer](#) (LanguageName const languageName, func *const fptr)
- int [SetSpeciesCode](#) (SpeciesName const speciesName, int const code)
- int [SetParameterPointer](#) (int const extent, int *const ptr, std::string const &description)
- int [SetParameterPointer](#) (int const extent, double *const ptr, std::string const &description)
- void [SetModelBufferPointer](#) (void *const ptr)
- int [SetUnits](#) (LengthUnit const lengthUnit, EnergyUnit const energyUnit, ChargeUnit const chargeUnit, TemperatureUnit const temperatureUnit, TimeUnit const timeUnit)
- int [ConvertUnit](#) (LengthUnit const fromLengthUnit, EnergyUnit const fromEnergyUnit, ChargeUnit const fromChargeUnit, TemperatureUnit const fromTemperatureUnit, TimeUnit const fromTimeUnit, LengthUnit const toLengthUnit, EnergyUnit const toEnergyUnit, ChargeUnit const toChargeUnit, TemperatureUnit const toTemperatureUnit, TimeUnit const toTimeUnit, double const lengthExponent, double const energyExponent, double const chargeExponent, double const temperatureExponent, double const timeExponent, double *const conversionFactor) const
- void [LogEntry](#) (LogVerbosity const logVerbosity, std::string const &message, int const lineNumber, std::string const &fileName) const
- void [LogEntry](#) (LogVerbosity const logVerbosity, std::stringstream const &message, int const lineNumber, std::string const &fileName) const
- std::string const & [String](#) () const

11.90.1 Detailed Description

Definition at line 61 of file KIM_ModelDriverCreate.hpp.

11.90.2 Member Function Documentation

11.90.2.1 ConvertUnit()

```
int KIM::ModelDriverCreate::ConvertUnit (
    LengthUnit const fromLengthUnit,
    EnergyUnit const fromEnergyUnit,
    ChargeUnit const fromChargeUnit,
    TemperatureUnit const fromTemperatureUnit,
    TimeUnit const fromTimeUnit,
    LengthUnit const toLengthUnit,
    EnergyUnit const toEnergyUnit,
    ChargeUnit const toChargeUnit,
    TemperatureUnit const toTemperatureUnit,
    TimeUnit const toTimeUnit,
    double const lengthExponent,
    double const energyExponent,
    double const chargeExponent,
    double const temperatureExponent,
    double const timeExponent,
    double *const conversionFactor ) const
```

11.90.2.2 GetNumberOfParameterFiles()

```
void KIM::ModelDriverCreate::GetNumberOfParameterFiles (
    int *const numberOfParameterFiles ) const
```

11.90.2.3 GetParameterFileName()

```
int KIM::ModelDriverCreate::GetParameterFileName (
    int const index,
    std::string const **const parameterFileName ) const
```

11.90.2.4 LogEntry() [1/2]

```
void KIM::ModelDriverCreate::LogEntry (
    LogVerbosity const logVerbosity,
    std::string const & message,
    int const lineNumber,
    std::string const & fileName ) const
```

11.90.2.5 LogEntry() [2/2]

```
void KIM::ModelDriverCreate::LogEntry (
    LogVerbosity const logVerbosity,
    std::stringstream const & message,
    int const lineNumber,
    std::string const & fileName ) const
```

11.90.2.6 SetComputeArgumentsCreatePointer()

```
int KIM::ModelDriverCreate::SetComputeArgumentsCreatePointer (
    LanguageName const languageName,
    func *const fptr )
```

11.90.2.7 SetComputeArgumentsDestroyPointer()

```
int KIM::ModelDriverCreate::SetComputeArgumentsDestroyPointer (
    LanguageName const languageName,
    func *const fptr )
```

11.90.2.8 SetComputePointer()

```
int KIM::ModelDriverCreate::SetComputePointer (
    LanguageName const languageName,
    func *const fptr )
```

11.90.2.9 SetDestroyPointer()

```
int KIM::ModelDriverCreate::SetDestroyPointer (
    LanguageName const languageName,
    func *const fptr )
```

11.90.2.10 SetInfluenceDistancePointer()

```
void KIM::ModelDriverCreate::SetInfluenceDistancePointer (
    double const *const influenceDistance )
```

11.90.2.11 SetModelBufferPointer()

```
void KIM::ModelDriverCreate::SetModelBufferPointer (
    void *const ptr )
```

11.90.2.12 SetModelNumbering()

```
int KIM::ModelDriverCreate::SetModelNumbering (
    Numbering const numbering )
```

11.90.2.13 SetNeighborListCutoffsPointer()

```
void KIM::ModelDriverCreate::SetNeighborListCutoffsPointer (
    int const numberOfCutoffs,
    double const *const cutoffs )
```

11.90.2.14 SetParameterPointer() [1/2]

```
int KIM::ModelDriverCreate::SetParameterPointer (
    int const extent,
    int *const ptr,
    std::string const & description )
```

11.90.2.15 SetParameterPointer() [2/2]

```
int KIM::ModelDriverCreate::SetParameterPointer (
    int const extent,
    double *const ptr,
    std::string const & description )
```


11.90.2.16 SetRefreshPointer()

```
int KIM::ModelDriverCreate::SetRefreshPointer (
    LanguageName const languageName,
    func *const fptr )
```

11.90.2.17 SetSpeciesCode()

```
int KIM::ModelDriverCreate::SetSpeciesCode (
    SpeciesName const speciesName,
    int const code )
```

11.90.2.18 SetUnits()

```
int KIM::ModelDriverCreate::SetUnits (
    LengthUnit const lengthUnit,
    EnergyUnit const energyUnit,
    ChargeUnit const chargeUnit,
    TemperatureUnit const temperatureUnit,
    TimeUnit const timeUnit )
```

11.90.2.19 String()

```
std::string const& KIM::ModelDriverCreate::String ( ) const
```

The documentation for this class was generated from the following file:

- [kim-api-v2.0.0-beta.0/cpp/include/KIM_ModelDriverCreate.hpp](#)

11.91 KIM::ModelRefresh Class Reference

```
#include <KIM_ModelRefresh.hpp>
```

Public Member Functions

- void [SetInfluenceDistancePointer](#) (double const *const influenceDistance)
- void [SetNeighborListCutoffsPointer](#) (int const numberOfCutoffs, double const *const cutoffs)
- void [GetModelBufferPointer](#) (void **const ptr) const
- void [LogEntry](#) ([LogVerbosity](#) const logVerbosity, std::string const &message, int const lineNumber, std::string const &fileName) const
- void [LogEntry](#) ([LogVerbosity](#) const logVerbosity, std::stringstream const &message, int const lineNumber, std::string const &fileName) const
- std::string const & [String](#) () const

11.91.1 Detailed Description

Definition at line 47 of file KIM_ModelRefresh.hpp.

11.91.2 Member Function Documentation

11.91.2.1 GetModelBufferPointer()

```
void KIM::ModelRefresh::GetModelBufferPointer (
    void **const ptr ) const
```

11.91.2.2 LogEntry() [1/2]

```
void KIM::ModelRefresh::LogEntry (
    LogVerbosity const logVerbosity,
    std::string const & message,
    int const lineNumber,
    std::string const & fileName ) const
```

11.91.2.3 LogEntry() [2/2]

```
void KIM::ModelRefresh::LogEntry (
    LogVerbosity const logVerbosity,
    std::stringstream const & message,
    int const lineNumber,
    std::string const & fileName ) const
```

11.91.2.4 SetInfluenceDistancePointer()

```
void KIM::ModelRefresh::SetInfluenceDistancePointer (
    double const *const influenceDistance )
```

11.91.2.5 SetNeighborListCutoffsPointer()

```
void KIM::ModelRefresh::SetNeighborListCutoffsPointer (
    int const numberOfCutoffs,
    double const *const cutoffs )
```

11.91.2.6 String()

```
std::string const& KIM::ModelRefresh::String ( ) const
```

The documentation for this class was generated from the following file:

- kim-api-v2.0.0-beta.0/cpp/include/[KIM_ModelRefresh.hpp](#)

11.92 mod_neighborlist::neighobject_type Type Reference

Public Attributes

- integer(c_int), dimension(:,:), pointer [neighborlist](#)
- real(c_double), dimension(:,:), pointer [rijlist](#)
- real(c_double) [cutoff](#)
- integer(c_int) [number_of_particles](#)

11.92.1 Detailed Description

Definition at line 51 of file ex_test_Ar_fcc_cluster_fortran.F90.

11.92.2 Member Data Documentation

11.92.2.1 cutoff

```
real(c_double) mod_neighborlist::neighobject_type::cutoff
```

Definition at line 74 of file ex_test_Ar_fcc_cluster_fortran.F90.

11.92.2.2 neighborlist

```
integer(c_int), dimension(:,:), pointer mod_neighborlist::neighobject_type::neighborlist
```

Definition at line 52 of file ex_test_Ar_fcc_cluster_fortran.F90.

11.92.2.3 number_of_particles

```
integer(c_int) mod_neighborlist::neighobject_type::number_of_particles
```

Definition at line 75 of file ex_test_Ar_fcc_cluster_fortran.F90.

11.92.2.4 rijlist

```
real(c_double), dimension(:,:,:), pointer mod_neighborlist::neighobject_type::rijlist
```

Definition at line 53 of file `ex_test_Ar_fcc_cluster_fortran.F90`.

The documentation for this type was generated from the following files:

- [kim-api-v2.0.0-beta.0/docs/porting-content-from-v1-to-v2-examples/simulators/step0/ex_test_Ar_fcc_cluster_fortran/ex_test_Ar_fcc_cluster_fortran.F90](#)
- [kim-api-v2.0.0-beta.0/examples/simulators/utility_forces_numer_deriv/utility_forces_numer_deriv.F03](#)

11.93 KIM::Numbering Class Reference

```
#include <KIM_Numbering.hpp>
```

Public Member Functions

- [Numbering](#) ()
- [Numbering](#) (int const id)
- [Numbering](#) (std::string const &str)
- bool [operator==](#) ([Numbering](#) const &rhs) const
- bool [operator!=](#) ([Numbering](#) const &rhs) const
- std::string const & [String](#) () const

Public Attributes

- int [numberingID](#)

11.93.1 Detailed Description

Definition at line 42 of file `KIM_Numbering.hpp`.

11.93.2 Constructor & Destructor Documentation

11.93.2.1 Numbering() [1/3]

```
KIM::Numbering::Numbering ( )
```

11.93.2.2 Numbering() [2/3]

```
KIM::Numbering::Numbering (
    int const id )
```

11.93.2.3 Numbering() [3/3]

```
KIM::Numbering::Numbering (
    std::string const & str )
```

11.93.3 Member Function Documentation

11.93.3.1 operator!=(())

```
bool KIM::Numbering::operator!= (
    Numbering const & rhs ) const
```

11.93.3.2 operator==(())

```
bool KIM::Numbering::operator== (
    Numbering const & rhs ) const
```

11.93.3.3 String()

```
std::string const& KIM::Numbering::String ( ) const
```

11.93.4 Member Data Documentation

11.93.4.1 numberingID

```
int KIM::Numbering::numberingID
```

Definition at line 45 of file [KIM_Numbering.hpp](#).

The documentation for this class was generated from the following file:

- [kim-api-v2.0.0-beta.0/cpp/include/KIM_Numbering.hpp](#)

11.94 KIM::SpeciesName Class Reference

```
#include <KIM_SpeciesName.hpp>
```

Public Member Functions

- [SpeciesName](#) ()
- [SpeciesName](#) (int const id)
- [SpeciesName](#) (std::string const &str)
- bool [operator==](#) ([SpeciesName](#) const &rhs) const
- bool [operator!=](#) ([SpeciesName](#) const &rhs) const
- std::string const & [String](#) () const

Public Attributes

- int [speciesNameID](#)

11.94.1 Detailed Description

Definition at line 42 of file KIM_SpeciesName.hpp.

11.94.2 Constructor & Destructor Documentation

11.94.2.1 [SpeciesName\(\)](#) [1/3]

```
KIM::SpeciesName::SpeciesName ( )
```

11.94.2.2 [SpeciesName\(\)](#) [2/3]

```
KIM::SpeciesName::SpeciesName (
    int const id )
```

11.94.2.3 [SpeciesName\(\)](#) [3/3]

```
KIM::SpeciesName::SpeciesName (
    std::string const & str )
```

11.94.3 Member Function Documentation

11.94.3.1 operator!=(())

```
bool KIM::SpeciesName::operator!= (
    SpeciesName const & rhs ) const
```

11.94.3.2 operator==(())

```
bool KIM::SpeciesName::operator== (
    SpeciesName const & rhs ) const
```

11.94.3.3 String()

```
std::string const& KIM::SpeciesName::String ( ) const
```

11.94.4 Member Data Documentation

11.94.4.1 speciesNameID

```
int KIM::SpeciesName::speciesNameID
```

Definition at line 45 of file KIM_SpeciesName.hpp.

The documentation for this class was generated from the following file:

- kim-api-v2.0.0-beta.0/cpp/include/[KIM_SpeciesName.hpp](#)

11.95 KIM::SupportStatus Class Reference

```
#include <KIM_SupportStatus.hpp>
```

Public Member Functions

- [SupportStatus](#) ()
- [SupportStatus](#) (int const id)
- [SupportStatus](#) (std::string const &str)
- bool [operator==](#) ([SupportStatus](#) const &rhs) const
- bool [operator!=](#) ([SupportStatus](#) const &rhs) const
- std::string const & [String](#) () const

Public Attributes

- int [supportStatusID](#)

11.95.1 Detailed Description

Definition at line 42 of file KIM_SupportStatus.hpp.

11.95.2 Constructor & Destructor Documentation

11.95.2.1 [SupportStatus\(\)](#) [1/3]

```
KIM::SupportStatus::SupportStatus ( )
```

11.95.2.2 [SupportStatus\(\)](#) [2/3]

```
KIM::SupportStatus::SupportStatus (
    int const id )
```

11.95.2.3 [SupportStatus\(\)](#) [3/3]

```
KIM::SupportStatus::SupportStatus (
    std::string const & str )
```

11.95.3 Member Function Documentation

11.95.3.1 operator!=()

```
bool KIM::SupportStatus::operator!= (
    SupportStatus const & rhs ) const
```

11.95.3.2 operator==()

```
bool KIM::SupportStatus::operator== (
    SupportStatus const & rhs ) const
```

11.95.3.3 String()

```
std::string const& KIM::SupportStatus::String ( ) const
```

11.95.4 Member Data Documentation

11.95.4.1 supportStatusID

```
int KIM::SupportStatus::supportStatusID
```

Definition at line 45 of file `KIM_SupportStatus.hpp`.

The documentation for this class was generated from the following file:

- `kim-api-v2.0.0-beta.0/cpp/include/KIM_SupportStatus.hpp`

11.96 KIM::TemperatureUnit Class Reference

```
#include <KIM_TemperatureUnit.hpp>
```

Public Member Functions

- [TemperatureUnit](#) ()
- [TemperatureUnit](#) (int const id)
- [TemperatureUnit](#) (std::string const &str)
- bool [operator==](#) ([TemperatureUnit](#) const &rhs) const
- bool [operator!=](#) ([TemperatureUnit](#) const &rhs) const
- std::string const & [String](#) () const

Public Attributes

- int [temperatureUnitID](#)

11.96.1 Detailed Description

Definition at line 42 of file `KIM_TemperatureUnit.hpp`.

11.96.2 Constructor & Destructor Documentation

11.96.2.1 `TemperatureUnit()` [1/3]

```
KIM::TemperatureUnit::TemperatureUnit ( )
```

11.96.2.2 `TemperatureUnit()` [2/3]

```
KIM::TemperatureUnit::TemperatureUnit (
    int const id )
```

11.96.2.3 `TemperatureUnit()` [3/3]

```
KIM::TemperatureUnit::TemperatureUnit (
    std::string const & str )
```

11.96.3 Member Function Documentation

11.96.3.1 `operator!=()`

```
bool KIM::TemperatureUnit::operator!= (
    TemperatureUnit const & rhs ) const
```

11.96.3.2 operator==()

```
bool KIM::TemperatureUnit::operator== (
    TemperatureUnit const & rhs ) const
```

11.96.3.3 String()

```
std::string const& KIM::TemperatureUnit::String ( ) const
```

11.96.4 Member Data Documentation

11.96.4.1 temperatureUnitID

```
int KIM::TemperatureUnit::temperatureUnitID
```

Definition at line 45 of file KIM_TemperatureUnit.hpp.

The documentation for this class was generated from the following file:

- [kim-api-v2.0.0-beta.0/cpp/include/KIM_TemperatureUnit.hpp](#)

11.97 KIM::TimeUnit Class Reference

```
#include <KIM_TimeUnit.hpp>
```

Public Member Functions

- [TimeUnit](#) ()
- [TimeUnit](#) (int const id)
- [TimeUnit](#) (std::string const &str)
- bool [operator==](#) ([TimeUnit](#) const &rhs) const
- bool [operator!=](#) ([TimeUnit](#) const &rhs) const
- std::string const & [String](#) () const

Public Attributes

- int [timeUnitID](#)

11.97.1 Detailed Description

Definition at line 42 of file KIM_TimeUnit.hpp.

11.97.2 Constructor & Destructor Documentation

11.97.2.1 TimeUnit() [1/3]

```
KIM::TimeUnit::TimeUnit ( )
```

11.97.2.2 TimeUnit() [2/3]

```
KIM::TimeUnit::TimeUnit (
    int const id )
```

11.97.2.3 TimeUnit() [3/3]

```
KIM::TimeUnit::TimeUnit (
    std::string const & str )
```

11.97.3 Member Function Documentation

11.97.3.1 operator!=(())

```
bool KIM::TimeUnit::operator!= (
    TimeUnit const & rhs ) const
```

11.97.3.2 operator==(())

```
bool KIM::TimeUnit::operator== (
    TimeUnit const & rhs ) const
```

11.97.3.3 String()

```
std::string const& KIM::TimeUnit::String ( ) const
```

11.97.4 Member Data Documentation

11.97.4.1 timeUnitID

```
int KIM::TimeUnit::timeUnitID
```

Definition at line 45 of file `KIM_TimeUnit.hpp`.

The documentation for this class was generated from the following file:

- `kim-api-v2.0.0-beta.0/cpp/include/KIM_TimeUnit.hpp`

Chapter 12

File Documentation

12.1 kim-api-v2.0.0-beta.0/c/include/KIM_ChargeUnit.h File Reference

Classes

- struct [KIM_ChargeUnit](#)

Macros

- `#define` [KIM_CHARGE_UNIT_DEFINED_](#)

Typedefs

- typedef struct [KIM_ChargeUnit](#) [KIM_ChargeUnit](#)

Functions

- [KIM_ChargeUnit](#) [KIM_ChargeUnit_FromString](#) (char const *const str)
- int [KIM_ChargeUnit_Equal](#) ([KIM_ChargeUnit](#) const left, [KIM_ChargeUnit](#) right)
- int [KIM_ChargeUnit_NotEqual](#) ([KIM_ChargeUnit](#) const left, [KIM_ChargeUnit](#) right)
- char const *const [KIM_ChargeUnit_String](#) ([KIM_ChargeUnit](#) const chargeUnit)
- void [KIM_CHARGE_UNIT_GetNumberOfChargeUnits](#) (int *const numberOfChargeUnits)
- int [KIM_CHARGE_UNIT_GetChargeUnit](#) (int const index, [KIM_ChargeUnit](#) *const chargeUnit)

Variables

- [KIM_ChargeUnit](#) const [KIM_CHARGE_UNIT_unused](#)
- [KIM_ChargeUnit](#) const [KIM_CHARGE_UNIT_C](#)
- [KIM_ChargeUnit](#) const [KIM_CHARGE_UNIT_e](#)
- [KIM_ChargeUnit](#) const [KIM_CHARGE_UNIT_statC](#)

12.1.1 Macro Definition Documentation

12.1.1.1 KIM_CHARGE_UNIT_DEFINED_

```
#define KIM_CHARGE_UNIT_DEFINED_
```

Definition at line 44 of file KIM_ChargeUnit.h.

12.1.2 Typedef Documentation

12.1.2.1 KIM_ChargeUnit

```
typedef struct KIM_ChargeUnit KIM_ChargeUnit
```

Definition at line 45 of file KIM_ChargeUnit.h.

12.1.3 Function Documentation

12.1.3.1 KIM_CHARGE_UNIT_GetChargeUnit()

```
int KIM_CHARGE_UNIT_GetChargeUnit (
    int const index,
    KIM_ChargeUnit *const chargeUnit )
```

12.1.3.2 KIM_CHARGE_UNIT_GetNumberOfChargeUnits()

```
void KIM_CHARGE_UNIT_GetNumberOfChargeUnits (
    int *const numberOfChargeUnits )
```

12.1.3.3 KIM_ChargeUnit_Equal()

```
int KIM_ChargeUnit_Equal (
    KIM_ChargeUnit const left,
    KIM_ChargeUnit right )
```

12.1.3.4 KIM_ChargeUnit_FromString()

```
KIM_ChargeUnit KIM_ChargeUnit_FromString (  
    char const *const str )
```

12.1.3.5 KIM_ChargeUnit_NotEqual()

```
int KIM_ChargeUnit_NotEqual (  
    KIM_ChargeUnit const left,  
    KIM_ChargeUnit right )
```

12.1.3.6 KIM_ChargeUnit_String()

```
char const* const KIM_ChargeUnit_String (  
    KIM_ChargeUnit const chargeUnit )
```

12.1.4 Variable Documentation

12.1.4.1 KIM_CHARGE_UNIT_C

```
KIM_ChargeUnit const KIM_CHARGE_UNIT_C
```

12.1.4.2 KIM_CHARGE_UNIT_e

```
KIM_ChargeUnit const KIM_CHARGE_UNIT_e
```

12.1.4.3 KIM_CHARGE_UNIT_statC

```
KIM_ChargeUnit const KIM_CHARGE_UNIT_statC
```

12.1.4.4 KIM_CHARGE_UNIT_unused

```
KIM_ChargeUnit const KIM_CHARGE_UNIT_unused
```

12.2 kim-api-v2.0.0-beta.0/c/include/KIM_ComputeArgumentName.h File Reference

Classes

- struct [KIM_ComputeArgumentName](#)

Macros

- `#define` [KIM_DATA_TYPE_DEFINED_](#)
- `#define` [KIM_COMPUTE_ARGUMENT_NAME_DEFINED_](#)

Typedefs

- typedef struct [KIM_DataType](#) [KIM_DataType](#)
- typedef struct [KIM_ComputeArgumentName](#) [KIM_ComputeArgumentName](#)

Functions

- [KIM_ComputeArgumentName](#) [KIM_ComputeArgumentName_FromString](#) (char const *const str)
- int [KIM_ComputeArgumentName_Equal](#) ([KIM_ComputeArgumentName](#) const left, [KIM_ComputeArgumentName](#) const right)
- int [KIM_ComputeArgumentName_NotEqual](#) ([KIM_ComputeArgumentName](#) const left, [KIM_ComputeArgumentName](#) const right)
- char const *const [KIM_ComputeArgumentName_String](#) ([KIM_ComputeArgumentName](#) const computeArgumentName)
- void [KIM_COMPUTE_ARGUMENT_NAME_GetNumberOfComputeArgumentNames](#) (int *const numberOfComputeArgumentNames)
- int [KIM_COMPUTE_ARGUMENT_NAME_GetComputeArgumentName](#) (int const index, [KIM_ComputeArgumentName](#) *const computeArgumentName)
- int [KIM_COMPUTE_ARGUMENT_NAME_GetComputeArgumentDataType](#) ([KIM_ComputeArgumentName](#) const computeArgumentName, [KIM_DataType](#) *const dataType)

Variables

- [KIM_ComputeArgumentName](#) const [KIM_COMPUTE_ARGUMENT_NAME_numberOfParticles](#)
- [KIM_ComputeArgumentName](#) const [KIM_COMPUTE_ARGUMENT_NAME_particleSpeciesCodes](#)
- [KIM_ComputeArgumentName](#) const [KIM_COMPUTE_ARGUMENT_NAME_particleContributing](#)
- [KIM_ComputeArgumentName](#) const [KIM_COMPUTE_ARGUMENT_NAME_coordinates](#)
- [KIM_ComputeArgumentName](#) const [KIM_COMPUTE_ARGUMENT_NAME_partialEnergy](#)
- [KIM_ComputeArgumentName](#) const [KIM_COMPUTE_ARGUMENT_NAME_partialForces](#)
- [KIM_ComputeArgumentName](#) const [KIM_COMPUTE_ARGUMENT_NAME_partialParticleEnergy](#)
- [KIM_ComputeArgumentName](#) const [KIM_COMPUTE_ARGUMENT_NAME_partialVirial](#)
- [KIM_ComputeArgumentName](#) const [KIM_COMPUTE_ARGUMENT_NAME_partialParticleVirial](#)

12.2.1 Macro Definition Documentation

12.2.1.1 KIM_COMPUTE_ARGUMENT_NAME_DEFINED_

```
#define KIM_COMPUTE_ARGUMENT_NAME_DEFINED_
```

Definition at line 50 of file KIM_ComputeArgumentName.h.

12.2.1.2 KIM_DATA_TYPE_DEFINED_

```
#define KIM_DATA_TYPE_DEFINED_
```

Definition at line 41 of file KIM_ComputeArgumentName.h.

12.2.2 Typedef Documentation

12.2.2.1 KIM_ComputeArgumentName

```
typedef struct KIM_ComputeArgumentName KIM_ComputeArgumentName
```

Definition at line 51 of file KIM_ComputeArgumentName.h.

12.2.2.2 KIM_DataType

```
typedef struct KIM_DataType KIM_DataType
```

Definition at line 42 of file KIM_ComputeArgumentName.h.

12.2.3 Function Documentation

12.2.3.1 KIM_COMPUTE_ARGUMENT_NAME_GetComputeArgumentDataType()

```
int KIM_COMPUTE_ARGUMENT_NAME_GetComputeArgumentDataType (
    KIM_ComputeArgumentName const computeArgumentName,
    KIM_DataType *const dataType )
```

12.2.3.2 KIM_COMPUTE_ARGUMENT_NAME_GetComputeArgumentName()

```
int KIM_COMPUTE_ARGUMENT_NAME_GetComputeArgumentName (
    int const index,
    KIM_ComputeArgumentName *const computeArgumentName )
```

12.2.3.3 KIM_COMPUTE_ARGUMENT_NAME_GetNumberOfComputeArgumentNames()

```
void KIM_COMPUTE_ARGUMENT_NAME_GetNumberOfComputeArgumentNames (
    int *const numberOfComputeArgumentNames )
```

12.2.3.4 KIM_ComputeArgumentName_Equal()

```
int KIM_ComputeArgumentName_Equal (
    KIM_ComputeArgumentName const left,
    KIM_ComputeArgumentName const right )
```

12.2.3.5 KIM_ComputeArgumentName_FromString()

```
KIM_ComputeArgumentName KIM_ComputeArgumentName_FromString (
    char const *const str )
```

12.2.3.6 KIM_ComputeArgumentName_NotEqual()

```
int KIM_ComputeArgumentName_NotEqual (
    KIM_ComputeArgumentName const left,
    KIM_ComputeArgumentName const right )
```

12.2.3.7 KIM_ComputeArgumentName_String()

```
char const* const KIM_ComputeArgumentName_String (
    KIM_ComputeArgumentName const computeArgumentName )
```

12.2.4 Variable Documentation

12.2.4.1 KIM_COMPUTE_ARGUMENT_NAME_coordinates

`KIM_ComputeArgumentName` const KIM_COMPUTE_ARGUMENT_NAME_coordinates

12.2.4.2 KIM_COMPUTE_ARGUMENT_NAME_numberOfParticles

`KIM_ComputeArgumentName` const KIM_COMPUTE_ARGUMENT_NAME_numberOfParticles

12.2.4.3 KIM_COMPUTE_ARGUMENT_NAME_partialEnergy

`KIM_ComputeArgumentName` const KIM_COMPUTE_ARGUMENT_NAME_partialEnergy

12.2.4.4 KIM_COMPUTE_ARGUMENT_NAME_partialForces

`KIM_ComputeArgumentName` const KIM_COMPUTE_ARGUMENT_NAME_partialForces

12.2.4.5 KIM_COMPUTE_ARGUMENT_NAME_partialParticleEnergy

`KIM_ComputeArgumentName` const KIM_COMPUTE_ARGUMENT_NAME_partialParticleEnergy

12.2.4.6 KIM_COMPUTE_ARGUMENT_NAME_partialParticleVirial

`KIM_ComputeArgumentName` const KIM_COMPUTE_ARGUMENT_NAME_partialParticleVirial

12.2.4.7 KIM_COMPUTE_ARGUMENT_NAME_partialVirial

`KIM_ComputeArgumentName` const KIM_COMPUTE_ARGUMENT_NAME_partialVirial

12.2.4.8 KIM_COMPUTE_ARGUMENT_NAME_particleContributing

`KIM_ComputeArgumentName` const KIM_COMPUTE_ARGUMENT_NAME_particleContributing

12.2.4.9 KIM_COMPUTE_ARGUMENT_NAME_particleSpeciesCodes

`KIM_ComputeArgumentName` const KIM_COMPUTE_ARGUMENT_NAME_particleSpeciesCodes

12.3 kim-api-v2.0.0-beta.0/c/include/KIM_ComputeArguments.h File Reference

```
#include "KIM_func.h"
```

Macros

- `#define KIM_LOG_VERBOSITY_DEFINED_`
- `#define KIM_LANGUAGE_NAME_DEFINED_`
- `#define KIM_COMPUTE_ARGUMENT_NAME_DEFINED_`
- `#define KIM_COMPUTE_CALLBACK_NAME_DEFINED_`
- `#define KIM_SUPPORT_STATUS_DEFINED_`
- `#define KIM_COMPUTE_ARGUMENTS_DEFINED_`

Typedefs

- `typedef struct KIM_LogVerbosity KIM_LogVerbosity`
- `typedef struct KIM_LanguageName KIM_LanguageName`
- `typedef struct KIM_ComputeArgumentName KIM_ComputeArgumentName`
- `typedef struct KIM_ComputeCallbackName KIM_ComputeCallbackName`
- `typedef struct KIM_SupportStatus KIM_SupportStatus`
- `typedef struct KIM_ComputeArguments KIM_ComputeArguments`

Functions

- `int KIM_ComputeArguments_GetArgumentSupportStatus (KIM_ComputeArguments const *const computeArguments, KIM_ComputeArgumentName const computeArgumentName, KIM_SupportStatus *const supportStatus)`
- `int KIM_ComputeArguments_GetCallbackSupportStatus (KIM_ComputeArguments const *const computeArguments, KIM_ComputeCallbackName const computeCallbackName, KIM_SupportStatus *const supportStatus)`
- `int KIM_ComputeArguments_SetArgumentPointerInteger (KIM_ComputeArguments *const computeArguments, KIM_ComputeArgumentName const computeArgumentName, int const *const ptr)`
- `int KIM_ComputeArguments_SetArgumentPointerDouble (KIM_ComputeArguments *const computeArguments, KIM_ComputeArgumentName const computeArgumentName, double const *const ptr)`
- `int KIM_ComputeArguments_SetCallbackPointer (KIM_ComputeArguments *const computeArguments, KIM_ComputeCallbackName const computeCallbackName, KIM_LanguageName const languageName, func *const fptr, void const *const dataObject)`
- `void KIM_ComputeArguments_AreAllRequiredArgumentsAndCallbacksPresent (KIM_ComputeArguments const *const computeArguments, int *const result)`
- `void KIM_ComputeArguments_SetSimulatorBufferPointer (KIM_ComputeArguments *const computeArguments, void *const ptr)`
- `void KIM_ComputeArguments_GetSimulatorBufferPointer (KIM_ComputeArguments const *const computeArguments, void **const ptr)`
- `char const *const KIM_ComputeArguments_String (KIM_ComputeArguments const *const computeArguments)`
- `void KIM_ComputeArguments_SetLogID (KIM_ComputeArguments *const computeArguments, char const *const logID)`
- `void KIM_ComputeArguments_PushLogVerbosity (KIM_ComputeArguments *const computeArguments, KIM_LogVerbosity const logVerbosity)`
- `void KIM_ComputeArguments_PopLogVerbosity (KIM_ComputeArguments *const computeArguments)`

12.3.1 Macro Definition Documentation

12.3.1.1 KIM_COMPUTE_ARGUMENT_NAME_DEFINED_

```
#define KIM_COMPUTE_ARGUMENT_NAME_DEFINED_
```

Definition at line 55 of file KIM_ComputeArguments.h.

12.3.1.2 KIM_COMPUTE_ARGUMENTS_DEFINED_

```
#define KIM_COMPUTE_ARGUMENTS_DEFINED_
```

Definition at line 73 of file KIM_ComputeArguments.h.

12.3.1.3 KIM_COMPUTE_CALLBACK_NAME_DEFINED_

```
#define KIM_COMPUTE_CALLBACK_NAME_DEFINED_
```

Definition at line 60 of file KIM_ComputeArguments.h.

12.3.1.4 KIM_LANGUAGE_NAME_DEFINED_

```
#define KIM_LANGUAGE_NAME_DEFINED_
```

Definition at line 50 of file KIM_ComputeArguments.h.

12.3.1.5 KIM_LOG_VERBOSITY_DEFINED_

```
#define KIM_LOG_VERBOSITY_DEFINED_
```

Definition at line 45 of file KIM_ComputeArguments.h.

12.3.1.6 KIM_SUPPORT_STATUS_DEFINED_

```
#define KIM_SUPPORT_STATUS_DEFINED_
```

Definition at line 65 of file KIM_ComputeArguments.h.

12.3.2 Typedef Documentation

12.3.2.1 KIM_ComputeArgumentName

```
typedef struct KIM_ComputeArgumentName KIM_ComputeArgumentName
```

Definition at line 56 of file KIM_ComputeArguments.h.

12.3.2.2 KIM_ComputeArguments

```
typedef struct KIM_ComputeArguments KIM_ComputeArguments
```

Definition at line 74 of file KIM_ComputeArguments.h.

12.3.2.3 KIM_ComputeCallbackName

```
typedef struct KIM_ComputeCallbackName KIM_ComputeCallbackName
```

Definition at line 61 of file KIM_ComputeArguments.h.

12.3.2.4 KIM_LanguageName

```
typedef struct KIM_LanguageName KIM_LanguageName
```

Definition at line 51 of file KIM_ComputeArguments.h.

12.3.2.5 KIM_LogVerbosity

```
typedef struct KIM_LogVerbosity KIM_LogVerbosity
```

Definition at line 46 of file KIM_ComputeArguments.h.

12.3.2.6 KIM_SupportStatus

```
typedef struct KIM_SupportStatus KIM_SupportStatus
```

Definition at line 66 of file KIM_ComputeArguments.h.

12.3.3 Function Documentation

12.3.3.1 KIM_ComputeArguments_AreAllRequiredArgumentsAndCallbacksPresent()

```
void KIM_ComputeArguments_AreAllRequiredArgumentsAndCallbacksPresent (
    KIM_ComputeArguments const *const computeArguments,
    int *const result )
```

12.3.3.2 KIM_ComputeArguments_GetArgumentSupportStatus()

```
int KIM_ComputeArguments_GetArgumentSupportStatus (
    KIM_ComputeArguments const *const computeArguments,
    KIM_ComputeArgumentName const computeArgumentName,
    KIM_SupportStatus *const supportStatus )
```

12.3.3.3 KIM_ComputeArguments_GetCallbackSupportStatus()

```
int KIM_ComputeArguments_GetCallbackSupportStatus (
    KIM_ComputeArguments const *const computeArguments,
    KIM_ComputeCallbackName const computeCallbackName,
    KIM_SupportStatus *const supportStatus )
```

12.3.3.4 KIM_ComputeArguments_GetSimulatorBufferPointer()

```
void KIM_ComputeArguments_GetSimulatorBufferPointer (
    KIM_ComputeArguments const *const computeArguments,
    void **const ptr )
```

12.3.3.5 KIM_ComputeArguments_PopLogVerbosity()

```
void KIM_ComputeArguments_PopLogVerbosity (
    KIM_ComputeArguments *const computeArguments )
```

12.3.3.6 KIM_ComputeArguments_PushLogVerbosity()

```
void KIM_ComputeArguments_PushLogVerbosity (
    KIM_ComputeArguments *const computeArguments,
    KIM_LogVerbosity const logVerbosity )
```

12.3.3.7 KIM_ComputeArguments_SetArgumentPointerDouble()

```
int KIM_ComputeArguments_SetArgumentPointerDouble (
    KIM_ComputeArguments *const computeArguments,
    KIM_ComputeArgumentName const computeArgumentName,
    double const *const ptr )
```

12.3.3.8 KIM_ComputeArguments_SetArgumentPointerInteger()

```
int KIM_ComputeArguments_SetArgumentPointerInteger (
    KIM_ComputeArguments *const computeArguments,
    KIM_ComputeArgumentName const computeArgumentName,
    int const *const ptr )
```

12.3.3.9 KIM_ComputeArguments_SetCallbackPointer()

```
int KIM_ComputeArguments_SetCallbackPointer (
    KIM_ComputeArguments *const computeArguments,
    KIM_ComputeCallbackName const computeCallbackName,
    KIM_LanguageName const languageName,
    func *const fptr,
    void const *const dataObject )
```

12.3.3.10 KIM_ComputeArguments_SetLogID()

```
void KIM_ComputeArguments_SetLogID (
    KIM_ComputeArguments *const computeArguments,
    char const *const logID )
```

12.3.3.11 KIM_ComputeArguments_SetSimulatorBufferPointer()

```
void KIM_ComputeArguments_SetSimulatorBufferPointer (
    KIM_ComputeArguments *const computeArguments,
    void *const ptr )
```


12.3.3.12 KIM_ComputeArguments_String()

```
char const* const KIM_ComputeArguments_String (
    KIM_ComputeArguments const *const computeArguments )
```

12.4 kim-api-v2.0.0-beta.0/c/include/KIM_ComputeCallbackName.h File Reference

Classes

- struct [KIM_ComputeCallbackName](#)

Macros

- `#define` [KIM_COMPUTE_CALLBACK_NAME_DEFINED_](#)

Typedefs

- typedef struct [KIM_ComputeCallbackName](#) [KIM_ComputeCallbackName](#)

Functions

- [KIM_ComputeCallbackName](#) [KIM_ComputeCallbackName_FromString](#) (char const *const str)
- int [KIM_ComputeCallbackName_Equal](#) ([KIM_ComputeCallbackName](#) const left, [KIM_ComputeCallbackName](#) const right)
- int [KIM_ComputeCallbackName_NotEqual](#) ([KIM_ComputeCallbackName](#) const left, [KIM_ComputeCallbackName](#) const right)
- char const *const [KIM_ComputeCallbackName_String](#) ([KIM_ComputeCallbackName](#) const compute↔CallbackName)
- void [KIM_COMPUTE_CALLBACK_NAME_GetNumberOfComputeCallbackNames](#) (int *const numberOf↔ComputeCallbackNames)
- int [KIM_COMPUTE_CALLBACK_NAME_GetComputeCallbackName](#) (int const index, [KIM_ComputeCallbackName](#) *const computeCallbackName)

Variables

- [KIM_ComputeCallbackName](#) const [KIM_COMPUTE_CALLBACK_NAME_GetNeighborList](#)
- [KIM_ComputeCallbackName](#) const [KIM_COMPUTE_CALLBACK_NAME_ProcessDEDrTerm](#)
- [KIM_ComputeCallbackName](#) const [KIM_COMPUTE_CALLBACK_NAME_ProcessD2EDr2Term](#)

12.4.1 Macro Definition Documentation

12.4.1.1 KIM_COMPUTE_CALLBACK_NAME_DEFINED_

```
#define KIM_COMPUTE_CALLBACK_NAME_DEFINED_
```

Definition at line 44 of file KIM_ComputeCallbackName.h.

12.4.2 Typedef Documentation

12.4.2.1 KIM_ComputeCallbackName

```
typedef struct KIM_ComputeCallbackName KIM_ComputeCallbackName
```

Definition at line 45 of file KIM_ComputeCallbackName.h.

12.4.3 Function Documentation

12.4.3.1 KIM_COMPUTE_CALLBACK_NAME_GetComputeCallbackName()

```
int KIM_COMPUTE_CALLBACK_NAME_GetComputeCallbackName (
    int const index,
    KIM_ComputeCallbackName *const computeCallbackName )
```

12.4.3.2 KIM_COMPUTE_CALLBACK_NAME_GetNumberOfComputeCallbackNames()

```
void KIM_COMPUTE_CALLBACK_NAME_GetNumberOfComputeCallbackNames (
    int *const numberOfComputeCallbackNames )
```

12.4.3.3 KIM_ComputeCallbackName_Equal()

```
int KIM_ComputeCallbackName_Equal (
    KIM_ComputeCallbackName const left,
    KIM_ComputeCallbackName const right )
```

12.4.3.4 KIM_ComputeCallbackName_FromString()

```
KIM_ComputeCallbackName KIM_ComputeCallbackName_FromString (
    char const *const str )
```

12.4.3.5 KIM_ComputeCallbackName_NotEqual()

```
int KIM_ComputeCallbackName_NotEqual (
    KIM_ComputeCallbackName const left,
    KIM_ComputeCallbackName const right )
```

12.4.3.6 KIM_ComputeCallbackName_String()

```
char const* const KIM_ComputeCallbackName_String (
    KIM_ComputeCallbackName const computeCallbackName )
```

12.4.4 Variable Documentation

12.4.4.1 KIM_COMPUTE_CALLBACK_NAME_GetNeighborList

```
KIM_ComputeCallbackName const KIM_COMPUTE_CALLBACK_NAME_GetNeighborList
```

12.4.4.2 KIM_COMPUTE_CALLBACK_NAME_ProcessD2EDr2Term

```
KIM_ComputeCallbackName const KIM_COMPUTE_CALLBACK_NAME_ProcessD2EDr2Term
```

12.4.4.3 KIM_COMPUTE_CALLBACK_NAME_ProcessDEDrTerm

```
KIM_ComputeCallbackName const KIM_COMPUTE_CALLBACK_NAME_ProcessDEDrTerm
```

12.5 kim-api-v2.0.0-beta.0/c/include/KIM_DataType.h File Reference

Classes

- struct [KIM_DataType](#)

Macros

- `#define KIM_DATA_TYPE_DEFINED_`

Typedefs

- `typedef struct KIM_DataType KIM_DataType`

Functions

- `KIM_DataType KIM_DataType_FromString` (char const *const str)
- `int KIM_DataType_Equal` (KIM_DataType const left, KIM_DataType const right)
- `int KIM_DataType_NotEqual` (KIM_DataType const left, KIM_DataType const right)
- `char const *const KIM_DataType_String` (KIM_DataType const dataType)
- `void KIM_DATA_TYPE_GetNumberOfDataTypes` (int *const numberOfDataTypes)
- `int KIM_DATA_TYPE_GetDataType` (int const index, KIM_DataType *const dataType)

Variables

- `KIM_DataType const KIM_DATA_TYPE_Integer`
- `KIM_DataType const KIM_DATA_TYPE_Double`

12.5.1 Macro Definition Documentation

12.5.1.1 KIM_DATA_TYPE_DEFINED_

```
#define KIM_DATA_TYPE_DEFINED_
```

Definition at line 44 of file KIM_DataType.h.

12.5.2 Typedef Documentation

12.5.2.1 KIM_DataType

```
typedef struct KIM_DataType KIM_DataType
```

Definition at line 45 of file KIM_DataType.h.

12.5.3 Function Documentation

12.5.3.1 KIM_DATA_TYPE_GetDataType()

```
int KIM_DATA_TYPE_GetDataType (
    int const index,
    KIM_DataType *const dataType )
```

12.5.3.2 KIM_DATA_TYPE_GetNumberOfDataTypes()

```
void KIM_DATA_TYPE_GetNumberOfDataTypes (
    int *const numberOfDataTypes )
```

12.5.3.3 KIM_DataType_Equal()

```
int KIM_DataType_Equal (
    KIM_DataType const left,
    KIM_DataType const right )
```

12.5.3.4 KIM_DataType_FromString()

```
KIM_DataType KIM_DataType_FromString (
    char const *const str )
```

12.5.3.5 KIM_DataType_NotEqual()

```
int KIM_DataType_NotEqual (
    KIM_DataType const left,
    KIM_DataType const right )
```

12.5.3.6 KIM_DataType_String()

```
char const* const KIM_DataType_String (
    KIM_DataType const dataType )
```

12.5.4 Variable Documentation

12.5.4.1 KIM_DATA_TYPE_Double

`KIM_DataType` const KIM_DATA_TYPE_Double

12.5.4.2 KIM_DATA_TYPE_Integer

`KIM_DataType` const KIM_DATA_TYPE_Integer

12.6 kim-api-v2.0.0-beta.0/c/include/KIM_EnergyUnit.h File Reference

Classes

- struct `KIM_EnergyUnit`

Macros

- `#define KIM_ENERGY_UNIT_DEFINED_`

Typedefs

- typedef struct `KIM_EnergyUnit` `KIM_EnergyUnit`

Functions

- `KIM_EnergyUnit` `KIM_EnergyUnit_FromString` (char const *const str)
- int `KIM_EnergyUnit_Equal` (`KIM_EnergyUnit` const left, `KIM_EnergyUnit` const right)
- int `KIM_EnergyUnit_NotEqual` (`KIM_EnergyUnit` const left, `KIM_EnergyUnit` const right)
- char const *const `KIM_EnergyUnit_String` (`KIM_EnergyUnit` const energyUnit)
- void `KIM_ENERGY_UNIT_GetNumberOfEnergyUnits` (int *const numberOfEnergyUnits)
- int `KIM_ENERGY_UNIT_GetEnergyUnit` (int const index, `KIM_EnergyUnit` *const energyUnit)

Variables

- `KIM_EnergyUnit` const `KIM_ENERGY_UNIT_unused`
- `KIM_EnergyUnit` const `KIM_ENERGY_UNIT_amu_A2_per_ps2`
- `KIM_EnergyUnit` const `KIM_ENERGY_UNIT_erg`
- `KIM_EnergyUnit` const `KIM_ENERGY_UNIT_eV`
- `KIM_EnergyUnit` const `KIM_ENERGY_UNIT_Hartree`
- `KIM_EnergyUnit` const `KIM_ENERGY_UNIT_J`
- `KIM_EnergyUnit` const `KIM_ENERGY_UNIT_kcal_mol`

12.6.1 Macro Definition Documentation

12.6.1.1 KIM_ENERGY_UNIT_DEFINED_

```
#define KIM_ENERGY_UNIT_DEFINED_
```

Definition at line 44 of file KIM_EnergyUnit.h.

12.6.2 Typedef Documentation

12.6.2.1 KIM_EnergyUnit

```
typedef struct KIM_EnergyUnit KIM_EnergyUnit
```

Definition at line 45 of file KIM_EnergyUnit.h.

12.6.3 Function Documentation

12.6.3.1 KIM_ENERGY_UNIT_GetEnergyUnit()

```
int KIM_ENERGY_UNIT_GetEnergyUnit (
    int const index,
    KIM_EnergyUnit *const energyUnit )
```

12.6.3.2 KIM_ENERGY_UNIT_GetNumberOfEnergyUnits()

```
void KIM_ENERGY_UNIT_GetNumberOfEnergyUnits (
    int *const numberOfEnergyUnits )
```

12.6.3.3 KIM_EnergyUnit_Equal()

```
int KIM_EnergyUnit_Equal (
    KIM_EnergyUnit const left,
    KIM_EnergyUnit const right )
```

12.6.3.4 KIM_EnergyUnit_FromString()

```
KIM_EnergyUnit KIM_EnergyUnit_FromString (
    char const *const str )
```

12.6.3.5 KIM_EnergyUnit_NotEqual()

```
int KIM_EnergyUnit_NotEqual (
    KIM_EnergyUnit const left,
    KIM_EnergyUnit const right )
```

12.6.3.6 KIM_EnergyUnit_String()

```
char const* const KIM_EnergyUnit_String (
    KIM_EnergyUnit const energyUnit )
```

12.6.4 Variable Documentation

12.6.4.1 KIM_ENERGY_UNIT_amu_A2_per_ps2

```
KIM_EnergyUnit const KIM_ENERGY_UNIT_amu_A2_per_ps2
```

12.6.4.2 KIM_ENERGY_UNIT_erg

```
KIM_EnergyUnit const KIM_ENERGY_UNIT_erg
```

12.6.4.3 KIM_ENERGY_UNIT_eV

```
KIM_EnergyUnit const KIM_ENERGY_UNIT_eV
```

12.6.4.4 KIM_ENERGY_UNIT_Hartree

```
KIM_EnergyUnit const KIM_ENERGY_UNIT_Hartree
```


12.6.4.5 KIM_ENERGY_UNIT_J

`KIM_EnergyUnit` const KIM_ENERGY_UNIT_J

12.6.4.6 KIM_ENERGY_UNIT_kcal_mol

`KIM_EnergyUnit` const KIM_ENERGY_UNIT_kcal_mol

12.6.4.7 KIM_ENERGY_UNIT_unused

`KIM_EnergyUnit` const KIM_ENERGY_UNIT_unused

12.7 kim-api-v2.0.0-beta.0/c/include/KIM_func.h File Reference

Typedefs

- typedef void() `func()`

12.7.1 Typedef Documentation

12.7.1.1 func

```
typedef void() func()
```

Definition at line 39 of file KIM_func.h.

12.8 kim-api-v2.0.0-beta.0/c/include/KIM_LanguageName.h File Reference

Classes

- struct `KIM_LanguageName`

Macros

- #define `KIM_LANGUAGE_NAME_DEFINED_`

Typedefs

- typedef struct [KIM_LanguageName](#) [KIM_LanguageName](#)

Functions

- [KIM_LanguageName](#) [KIM_LanguageName_FromString](#) (char const *const str)
- int [KIM_LanguageName_Equal](#) ([KIM_LanguageName](#) const left, [KIM_LanguageName](#) const right)
- int [KIM_LanguageName_NotEqual](#) ([KIM_LanguageName](#) const left, [KIM_LanguageName](#) const right)
- char const *const [KIM_LanguageName_String](#) ([KIM_LanguageName](#) const languageName)
- void [KIM_LANGUAGE_NAME_GetNumberOfLanguageNames](#) (int *const numberOfLanguageNames)
- int [KIM_LANGUAGE_NAME_GetLanguageName](#) (int const index, [KIM_LanguageName](#) *const languageName)

Variables

- [KIM_LanguageName](#) const [KIM_LANGUAGE_NAME_cpp](#)
- [KIM_LanguageName](#) const [KIM_LANGUAGE_NAME_c](#)
- [KIM_LanguageName](#) const [KIM_LANGUAGE_NAME_fortran](#)

12.8.1 Macro Definition Documentation

12.8.1.1 KIM_LANGUAGE_NAME_DEFINED_

```
#define KIM_LANGUAGE_NAME_DEFINED_
```

Definition at line 44 of file [KIM_LanguageName.h](#).

12.8.2 Typedef Documentation

12.8.2.1 KIM_LanguageName

```
typedef struct KIM\_LanguageName KIM\_LanguageName
```

Definition at line 45 of file [KIM_LanguageName.h](#).

12.8.3 Function Documentation

12.8.3.1 KIM_LANGUAGE_NAME_GetLanguageName()

```
int KIM_LANGUAGE_NAME_GetLanguageName (
    int const index,
    KIM_LanguageName *const languageName )
```

12.8.3.2 KIM_LANGUAGE_NAME_GetNumberOfLanguageNames()

```
void KIM_LANGUAGE_NAME_GetNumberOfLanguageNames (
    int *const numberOfLanguageNames )
```

12.8.3.3 KIM_LanguageName_Equal()

```
int KIM_LanguageName_Equal (
    KIM_LanguageName const left,
    KIM_LanguageName const right )
```

12.8.3.4 KIM_LanguageName_FromString()

```
KIM_LanguageName KIM_LanguageName_FromString (
    char const *const str )
```

12.8.3.5 KIM_LanguageName_NotEqual()

```
int KIM_LanguageName_NotEqual (
    KIM_LanguageName const left,
    KIM_LanguageName const right )
```

12.8.3.6 KIM_LanguageName_String()

```
char const* const KIM_LanguageName_String (
    KIM_LanguageName const languageName )
```

12.8.4 Variable Documentation

12.8.4.1 KIM_LANGUAGE_NAME_c

`KIM_LanguageName` const KIM_LANGUAGE_NAME_c

12.8.4.2 KIM_LANGUAGE_NAME_cpp

`KIM_LanguageName` const KIM_LANGUAGE_NAME_cpp

12.8.4.3 KIM_LANGUAGE_NAME_fortran

`KIM_LanguageName` const KIM_LANGUAGE_NAME_fortran

12.9 kim-api-v2.0.0-beta.0/c/include/KIM_LengthUnit.h File Reference

Classes

- struct `KIM_LengthUnit`

Macros

- `#define KIM_LENGTH_UNIT_DEFINED_`

Typedefs

- typedef struct `KIM_LengthUnit` `KIM_LengthUnit`

Functions

- `KIM_LengthUnit KIM_LengthUnit_FromString` (char const *const str)
- int `KIM_LengthUnit_Equal` (KIM_LengthUnit left, KIM_LengthUnit right)
- int `KIM_LengthUnit_NotEqual` (KIM_LengthUnit left, KIM_LengthUnit right)
- char const *const `KIM_LengthUnit_String` (KIM_LengthUnit const lengthUnit)
- void `KIM_LENGTH_UNIT_GetNumberOfLengthUnits` (int *const numberOfLengthUnits)
- int `KIM_LENGTH_UNIT_GetLengthUnit` (int const index, KIM_LengthUnit *const lengthUnit)

Variables

- `KIM_LengthUnit` const `KIM_LENGTH_UNIT_unused`
- `KIM_LengthUnit` const `KIM_LENGTH_UNIT_A`
- `KIM_LengthUnit` const `KIM_LENGTH_UNIT_Bohr`
- `KIM_LengthUnit` const `KIM_LENGTH_UNIT_cm`
- `KIM_LengthUnit` const `KIM_LENGTH_UNIT_m`
- `KIM_LengthUnit` const `KIM_LENGTH_UNIT_nm`

12.9.1 Macro Definition Documentation

12.9.1.1 KIM_LENGTH_UNIT_DEFINED_

```
#define KIM_LENGTH_UNIT_DEFINED_
```

Definition at line 44 of file KIM_LengthUnit.h.

12.9.2 Typedef Documentation

12.9.2.1 KIM_LengthUnit

```
typedef struct KIM_LengthUnit KIM_LengthUnit
```

Definition at line 45 of file KIM_LengthUnit.h.

12.9.3 Function Documentation

12.9.3.1 KIM_LENGTH_UNIT_GetLengthUnit()

```
int KIM_LENGTH_UNIT_GetLengthUnit (
    int const index,
    KIM_LengthUnit *const lengthUnit )
```

12.9.3.2 KIM_LENGTH_UNIT_GetNumberOfLengthUnits()

```
void KIM_LENGTH_UNIT_GetNumberOfLengthUnits (
    int *const numberOfLengthUnits )
```

12.9.3.3 KIM_LengthUnit_Equal()

```
int KIM_LengthUnit_Equal (
    KIM_LengthUnit left,
    KIM_LengthUnit right )
```

12.9.3.4 KIM_LengthUnit_FromString()

```
KIM_LengthUnit KIM_LengthUnit_FromString (
    char const *const str )
```

12.9.3.5 KIM_LengthUnit_NotEqual()

```
int KIM_LengthUnit_NotEqual (
    KIM_LengthUnit left,
    KIM_LengthUnit right )
```

12.9.3.6 KIM_LengthUnit_String()

```
char const* const KIM_LengthUnit_String (
    KIM_LengthUnit const lengthUnit )
```

12.9.4 Variable Documentation

12.9.4.1 KIM_LENGTH_UNIT_A

```
KIM_LengthUnit const KIM_LENGTH_UNIT_A
```

12.9.4.2 KIM_LENGTH_UNIT_Bohr

```
KIM_LengthUnit const KIM_LENGTH_UNIT_Bohr
```

12.9.4.3 KIM_LENGTH_UNIT_cm

```
KIM_LengthUnit const KIM_LENGTH_UNIT_cm
```

12.9.4.4 KIM_LENGTH_UNIT_m

```
KIM_LengthUnit const KIM_LENGTH_UNIT_m
```

12.9.4.5 KIM_LENGTH_UNIT_nm

```
KIM_LengthUnit const KIM_LENGTH_UNIT_nm
```

12.9.4.6 KIM_LENGTH_UNIT_unused

```
KIM_LengthUnit const KIM_LENGTH_UNIT_unused
```

12.10 kim-api-v2.0.0-beta.0/c/include/KIM_Log.h File Reference

Macros

- `#define KIM_LOG_VERBOSITY_DEFINED_`
- `#define KIM_LOG_DEFINED_`

Typedefs

- `typedef struct KIM_LogVerbosity KIM_LogVerbosity`
- `typedef struct KIM_Log KIM_Log`

Functions

- `int KIM_Log_Create (KIM_Log **const log)`
- `void KIM_Log_Destroy (KIM_Log **const log)`
- `char const *const KIM_Log_GetID (KIM_Log const *const log)`
- `void KIM_Log_SetID (KIM_Log *const log, char const *const id)`
- `void KIM_Log_PushVerbosity (KIM_Log *const log, KIM_LogVerbosity const logVerbosity)`
- `void KIM_Log_PopVerbosity (KIM_Log *const log)`
- `void KIM_Log_LogEntry (KIM_Log const *const log, KIM_LogVerbosity const logVerbosity, char const *const message, int const lineNumber, char const *const fileName)`

12.10.1 Macro Definition Documentation

12.10.1.1 KIM_LOG_DEFINED_

```
#define KIM_LOG_DEFINED_
```

Definition at line 48 of file KIM_Log.h.

12.10.1.2 KIM_LOG_VERBOSITY_DEFINED_

```
#define KIM_LOG_VERBOSITY_DEFINED_
```

Definition at line 41 of file KIM_Log.h.

12.10.2 Typedef Documentation

12.10.2.1 KIM_Log

```
typedef struct KIM_Log KIM_Log
```

Definition at line 49 of file KIM_Log.h.

12.10.2.2 KIM_LogVerbosity

```
typedef struct KIM_LogVerbosity KIM_LogVerbosity
```

Definition at line 42 of file KIM_Log.h.

12.10.3 Function Documentation

12.10.3.1 KIM_Log_Create()

```
int KIM_Log_Create (
    KIM_Log **const log )
```

12.10.3.2 KIM_Log_Destroy()

```
void KIM_Log_Destroy (
    KIM_Log **const log )
```


12.10.3.3 KIM_Log_GetID()

```
char const* const KIM_Log_GetID (
    KIM_Log const *const log )
```

12.10.3.4 KIM_Log_LogEntry()

```
void KIM_Log_LogEntry (
    KIM_Log const *const log,
    KIM_LogVerbosity const logVerbosity,
    char const *const message,
    int const lineNumber,
    char const *const fileName )
```

12.10.3.5 KIM_Log_PopVerbosity()

```
void KIM_Log_PopVerbosity (
    KIM_Log *const log )
```

12.10.3.6 KIM_Log_PushVerbosity()

```
void KIM_Log_PushVerbosity (
    KIM_Log *const log,
    KIM_LogVerbosity const logVerbosity )
```

12.10.3.7 KIM_Log_SetID()

```
void KIM_Log_SetID (
    KIM_Log *const log,
    char const *const id )
```

12.11 kim-api-v2.0.0-beta.0/c/include/KIM_LogVerbosity.h File Reference

```
#include "KIM_LOG_DEFINES.inc"
```

Classes

- struct [KIM_LogVerbosity](#)

Macros

- `#define KIM_LOG_VERBOSITY_DEFINED_`

Typedefs

- `typedef struct KIM_LogVerbosity KIM_LogVerbosity`

Functions

- `KIM_LogVerbosity KIM_LogVerbosity_FromString` (char const *const str)
- `int KIM_LogVerbosity_LessThan` (KIM_LogVerbosity const left, KIM_LogVerbosity const right)
- `int KIM_LogVerbosity_GreaterThan` (KIM_LogVerbosity const left, KIM_LogVerbosity const right)
- `int KIM_LogVerbosity_LessThanEqual` (KIM_LogVerbosity const left, KIM_LogVerbosity const right)
- `int KIM_LogVerbosity_GreaterThanEqual` (KIM_LogVerbosity const left, KIM_LogVerbosity const right)
- `int KIM_LogVerbosity_Equal` (KIM_LogVerbosity const left, KIM_LogVerbosity const right)
- `int KIM_LogVerbosity_NotEqual` (KIM_LogVerbosity const left, KIM_LogVerbosity const right)
- `char const *const KIM_LogVerbosity_String` (KIM_LogVerbosity const logVerbosity)
- `void KIM_LOG_VERBOSITY_GetNumberOfLogVerbosities` (int *const numberOfLogVerbosities)
- `int KIM_LOG_VERBOSITY_GetLogVerbosity` (int const index, KIM_LogVerbosity *const logVerbosity)

Variables

- `KIM_LogVerbosity const KIM_LOG_VERBOSITY_silent`
- `KIM_LogVerbosity const KIM_LOG_VERBOSITY_fatal`
- `KIM_LogVerbosity const KIM_LOG_VERBOSITY_error`
- `KIM_LogVerbosity const KIM_LOG_VERBOSITY_warning`
- `KIM_LogVerbosity const KIM_LOG_VERBOSITY_information`
- `KIM_LogVerbosity const KIM_LOG_VERBOSITY_debug`

12.11.1 Macro Definition Documentation

12.11.1.1 KIM_LOG_VERBOSITY_DEFINED_

```
#define KIM_LOG_VERBOSITY_DEFINED_
```

Definition at line 47 of file KIM_LogVerbosity.h.

12.11.2 Typedef Documentation

12.11.2.1 KIM_LogVerbosity

```
typedef struct KIM_LogVerbosity KIM_LogVerbosity
```

Definition at line 48 of file KIM_LogVerbosity.h.

12.11.3 Function Documentation

12.11.3.1 KIM_LOG_VERBOSITY_GetLogVerbosity()

```
int KIM_LOG_VERBOSITY_GetLogVerbosity (
    int const index,
    KIM_LogVerbosity *const logVerbosity )
```

12.11.3.2 KIM_LOG_VERBOSITY_GetNumberOfLogVerbosities()

```
void KIM_LOG_VERBOSITY_GetNumberOfLogVerbosities (
    int *const numberOfLogVerbosities )
```

12.11.3.3 KIM_LogVerbosity_Equal()

```
int KIM_LogVerbosity_Equal (
    KIM_LogVerbosity const left,
    KIM_LogVerbosity const right )
```

12.11.3.4 KIM_LogVerbosity_FromString()

```
KIM_LogVerbosity KIM_LogVerbosity_FromString (
    char const *const str )
```

12.11.3.5 KIM_LogVerbosity_GreaterThan()

```
int KIM_LogVerbosity_GreaterThan (
    KIM_LogVerbosity const left,
    KIM_LogVerbosity const right )
```

12.11.3.6 KIM_LogVerbosity_GreaterThanEqual()

```
int KIM_LogVerbosity_GreaterThanEqual (
    KIM_LogVerbosity const left,
    KIM_LogVerbosity const right )
```

12.11.3.7 KIM_LogVerbosity_LessThan()

```
int KIM_LogVerbosity_LessThan (
    KIM_LogVerbosity const left,
    KIM_LogVerbosity const right )
```

12.11.3.8 KIM_LogVerbosity_LessThanEqual()

```
int KIM_LogVerbosity_LessThanEqual (
    KIM_LogVerbosity const left,
    KIM_LogVerbosity const right )
```

12.11.3.9 KIM_LogVerbosity_NotEqual()

```
int KIM_LogVerbosity_NotEqual (
    KIM_LogVerbosity const left,
    KIM_LogVerbosity const right )
```

12.11.3.10 KIM_LogVerbosity_String()

```
char const* const KIM_LogVerbosity_String (
    KIM_LogVerbosity const logVerbosity )
```

12.11.4 Variable Documentation

12.11.4.1 KIM_LOG_VERBOSITY_debug

```
KIM_LogVerbosity const KIM_LOG_VERBOSITY_debug
```

12.11.4.2 KIM_LOG_VERBOSITY_error

`KIM_LogVerbosity` const KIM_LOG_VERBOSITY_error

12.11.4.3 KIM_LOG_VERBOSITY_fatal

`KIM_LogVerbosity` const KIM_LOG_VERBOSITY_fatal

12.11.4.4 KIM_LOG_VERBOSITY_information

`KIM_LogVerbosity` const KIM_LOG_VERBOSITY_information

12.11.4.5 KIM_LOG_VERBOSITY_silent

`KIM_LogVerbosity` const KIM_LOG_VERBOSITY_silent

12.11.4.6 KIM_LOG_VERBOSITY_warning

`KIM_LogVerbosity` const KIM_LOG_VERBOSITY_warning

12.12 kim-api-v2.0.0-beta.0/c/include/KIM_Model.h File Reference

```
#include "KIM_func.h"
```

Macros

- `#define KIM_LOG_VERBOSITY_DEFINED_`
- `#define KIM_SPECIES_NAME_DEFINED_`
- `#define KIM_LANGUAGE_NAME_DEFINED_`
- `#define KIM_NUMBERING_DEFINED_`
- `#define KIM_LENGTH_UNIT_DEFINED_`
- `#define KIM_DATA_TYPE_DEFINED_`
- `#define KIM_ENERGY_UNIT_DEFINED_`
- `#define KIM_CHARGE_UNIT_DEFINED_`
- `#define KIM_TEMPERATURE_UNIT_DEFINED_`
- `#define KIM_TIME_UNIT_DEFINED_`
- `#define KIM_COMPUTE_ARGUMENTS_DEFINED_`
- `#define KIM_MODEL_DEFINED_`

Typedefs

- typedef struct [KIM_LogVerbosity](#) [KIM_LogVerbosity](#)
- typedef struct [KIM_SpeciesName](#) [KIM_SpeciesName](#)
- typedef struct [KIM_LanguageName](#) [KIM_LanguageName](#)
- typedef struct [KIM_Numbering](#) [KIM_Numbering](#)
- typedef struct [KIM_LengthUnit](#) [KIM_LengthUnit](#)
- typedef struct [KIM_DataType](#) [KIM_DataType](#)
- typedef struct [KIM_EnergyUnit](#) [KIM_EnergyUnit](#)
- typedef struct [KIM_ChargeUnit](#) [KIM_ChargeUnit](#)
- typedef struct [KIM_TemperatureUnit](#) [KIM_TemperatureUnit](#)
- typedef struct [KIM_TimeUnit](#) [KIM_TimeUnit](#)
- typedef struct [KIM_ComputeArguments](#) [KIM_ComputeArguments](#)
- typedef struct [KIM_Model](#) [KIM_Model](#)

Functions

- int [KIM_Model_Create](#) ([KIM_Numbering](#) const numbering, [KIM_LengthUnit](#) const requestedLength↵Unit, [KIM_EnergyUnit](#) const requestedEnergyUnit, [KIM_ChargeUnit](#) const requestedChargeUnit, [KIM_TemperatureUnit](#) const requestedTemperatureUnit, [KIM_TimeUnit](#) const requestedTimeUnit, char const *const modelName, int *const requestedUnitsAccepted, [KIM_Model](#) **const model)
- void [KIM_Model_Destroy](#) ([KIM_Model](#) **const model)
- void [KIM_Model_GetInfluenceDistance](#) ([KIM_Model](#) const *const model, double *const influenceDistance)
- void [KIM_Model_GetNeighborListCutoffsPointer](#) ([KIM_Model](#) const *const model, int *const numberOf↵Cutoffs, double const **const cutoffs)
- void [KIM_Model_GetUnits](#) ([KIM_Model](#) const *const model, [KIM_LengthUnit](#) *const lengthUnit, [KIM_EnergyUnit](#) *const energyUnit, [KIM_ChargeUnit](#) *const chargeUnit, [KIM_TemperatureUnit](#) *const temperatureUnit, [KIM_TimeUnit](#) *const timeUnit)
- int [KIM_Model_ComputeArgumentsCreate](#) ([KIM_Model](#) const *const model, [KIM_ComputeArguments](#) **const computeArguments)
- int [KIM_Model_ComputeArgumentsDestroy](#) ([KIM_Model](#) const *const model, [KIM_ComputeArguments](#) **const computeArguments)
- int [KIM_Model_Compute](#) ([KIM_Model](#) const *const model, [KIM_ComputeArguments](#) const *const compute↵Arguments)
- int [KIM_Model_ClearInfluenceDistanceAndCutoffsThenRefreshModel](#) ([KIM_Model](#) *const model)
- int [KIM_Model_GetSpeciesSupportAndCode](#) ([KIM_Model](#) const *const model, [KIM_SpeciesName](#) const speciesName, int *const speciesIsSupported, int *const code)
- void [KIM_Model_GetNumberOfParameters](#) ([KIM_Model](#) const *const model, int *const numberOf↵Parameters)
- int [KIM_Model_GetParameterDataTypeExtentAndDescription](#) ([KIM_Model](#) const *const model, int const parameterIndex, [KIM_DataType](#) *const dataType, int *const extent, char const **const description)
- int [KIM_Model_GetParameterInteger](#) ([KIM_Model](#) const *const model, int const parameterIndex, int const arrayIndex, int *const parameterValue)
- int [KIM_Model_GetParameterDouble](#) ([KIM_Model](#) const *const model, int const parameterIndex, int const arrayIndex, double *const parameterValue)
- int [KIM_Model_SetParameterInteger](#) ([KIM_Model](#) *const model, int const parameterIndex, int const array↵Index, int const parameterValue)
- int [KIM_Model_SetParameterDouble](#) ([KIM_Model](#) *const model, int const parameterIndex, int const array↵Index, double const parameterValue)
- void [KIM_Model_SetSimulatorBufferPointer](#) ([KIM_Model](#) *const model, void *const ptr)
- void [KIM_Model_GetSimulatorBufferPointer](#) ([KIM_Model](#) const *const model, void **const ptr)
- char const *const [KIM_Model_String](#) ([KIM_Model](#) const *const model)
- void [KIM_Model_SetLogID](#) ([KIM_Model](#) *const model, char const *const logID)
- void [KIM_Model_PushLogVerbosity](#) ([KIM_Model](#) *const model, [KIM_LogVerbosity](#) const logVerbosity)
- void [KIM_Model_PopLogVerbosity](#) ([KIM_Model](#) *const model)

12.12.1 Macro Definition Documentation

12.12.1.1 KIM_CHARGE_UNIT_DEFINED_

```
#define KIM_CHARGE_UNIT_DEFINED_
```

Definition at line 80 of file KIM_Model.h.

12.12.1.2 KIM_COMPUTE_ARGUMENTS_DEFINED_

```
#define KIM_COMPUTE_ARGUMENTS_DEFINED_
```

Definition at line 95 of file KIM_Model.h.

12.12.1.3 KIM_DATA_TYPE_DEFINED_

```
#define KIM_DATA_TYPE_DEFINED_
```

Definition at line 70 of file KIM_Model.h.

12.12.1.4 KIM_ENERGY_UNIT_DEFINED_

```
#define KIM_ENERGY_UNIT_DEFINED_
```

Definition at line 75 of file KIM_Model.h.

12.12.1.5 KIM_LANGUAGE_NAME_DEFINED_

```
#define KIM_LANGUAGE_NAME_DEFINED_
```

Definition at line 55 of file KIM_Model.h.

12.12.1.6 KIM_LENGTH_UNIT_DEFINED_

```
#define KIM_LENGTH_UNIT_DEFINED_
```

Definition at line 65 of file KIM_Model.h.

12.12.1.7 KIM_LOG_VERBOSITY_DEFINED_

```
#define KIM_LOG_VERBOSITY_DEFINED_
```

Definition at line 45 of file KIM_Model.h.

12.12.1.8 KIM_MODEL_DEFINED_

```
#define KIM_MODEL_DEFINED_
```

Definition at line 103 of file KIM_Model.h.

12.12.1.9 KIM_NUMBERING_DEFINED_

```
#define KIM_NUMBERING_DEFINED_
```

Definition at line 60 of file KIM_Model.h.

12.12.1.10 KIM_SPECIES_NAME_DEFINED_

```
#define KIM_SPECIES_NAME_DEFINED_
```

Definition at line 50 of file KIM_Model.h.

12.12.1.11 KIM_TEMPERATURE_UNIT_DEFINED_

```
#define KIM_TEMPERATURE_UNIT_DEFINED_
```

Definition at line 85 of file KIM_Model.h.

12.12.1.12 KIM_TIME_UNIT_DEFINED_

```
#define KIM_TIME_UNIT_DEFINED_
```

Definition at line 90 of file KIM_Model.h.

12.12.2 Typedef Documentation

12.12.2.1 KIM_ChargeUnit

```
typedef struct KIM_ChargeUnit KIM_ChargeUnit
```

Definition at line 81 of file KIM_Model.h.

12.12.2.2 KIM_ComputeArguments

```
typedef struct KIM_ComputeArguments KIM_ComputeArguments
```

Definition at line 96 of file KIM_Model.h.

12.12.2.3 KIM_DataType

```
typedef struct KIM_DataType KIM_DataType
```

Definition at line 71 of file KIM_Model.h.

12.12.2.4 KIM_EnergyUnit

```
typedef struct KIM_EnergyUnit KIM_EnergyUnit
```

Definition at line 76 of file KIM_Model.h.

12.12.2.5 KIM_LanguageName

```
typedef struct KIM_LanguageName KIM_LanguageName
```

Definition at line 56 of file KIM_Model.h.

12.12.2.6 KIM_LengthUnit

```
typedef struct KIM_LengthUnit KIM_LengthUnit
```

Definition at line 66 of file KIM_Model.h.

12.12.2.7 KIM_LogVerbosity

```
typedef struct KIM_LogVerbosity KIM_LogVerbosity
```

Definition at line 46 of file KIM_Model.h.

12.12.2.8 KIM_Model

```
typedef struct KIM_Model KIM_Model
```

Definition at line 104 of file KIM_Model.h.

12.12.2.9 KIM_Numbering

```
typedef struct KIM_Numbering KIM_Numbering
```

Definition at line 61 of file KIM_Model.h.

12.12.2.10 KIM_SpeciesName

```
typedef struct KIM_SpeciesName KIM_SpeciesName
```

Definition at line 51 of file KIM_Model.h.

12.12.2.11 KIM_TemperatureUnit

```
typedef struct KIM_TemperatureUnit KIM_TemperatureUnit
```

Definition at line 86 of file KIM_Model.h.

12.12.2.12 KIM_TimeUnit

```
typedef struct KIM_TimeUnit KIM_TimeUnit
```

Definition at line 91 of file KIM_Model.h.

12.12.3 Function Documentation

12.12.3.1 KIM_Model_ClearInfluenceDistanceAndCutoffsThenRefreshModel()

```
int KIM_Model_ClearInfluenceDistanceAndCutoffsThenRefreshModel (
    KIM_Model *const model )
```

12.12.3.2 KIM_Model_Compute()

```
int KIM_Model_Compute (
    KIM_Model const *const model,
    KIM_ComputeArguments const *const computeArguments )
```

12.12.3.3 KIM_Model_ComputeArgumentsCreate()

```
int KIM_Model_ComputeArgumentsCreate (
    KIM_Model const *const model,
    KIM_ComputeArguments **const computeArguments )
```

12.12.3.4 KIM_Model_ComputeArgumentsDestroy()

```
int KIM_Model_ComputeArgumentsDestroy (
    KIM_Model const *const model,
    KIM_ComputeArguments **const computeArguments )
```

12.12.3.5 KIM_Model_Create()

```
int KIM_Model_Create (
    KIM_Numbering const numbering,
    KIM_LengthUnit const requestedLengthUnit,
    KIM_EnergyUnit const requestedEnergyUnit,
    KIM_ChargeUnit const requestedChargeUnit,
    KIM_TemperatureUnit const requestedTemperatureUnit,
    KIM_TimeUnit const requestedTimeUnit,
    char const *const modelName,
    int *const requestedUnitsAccepted,
    KIM_Model **const model )
```

12.12.3.6 KIM_Model_Destroy()

```
void KIM_Model_Destroy (
    KIM_Model **const model )
```

12.12.3.7 KIM_Model_GetInfluenceDistance()

```
void KIM_Model_GetInfluenceDistance (
    KIM_Model const *const model,
    double *const influenceDistance )
```

12.12.3.8 KIM_Model_GetNeighborListCutoffsPointer()

```
void KIM_Model_GetNeighborListCutoffsPointer (
    KIM_Model const *const model,
    int *const numberOfCutoffs,
    double const **const cutoffs )
```

12.12.3.9 KIM_Model_GetNumberOfParameters()

```
void KIM_Model_GetNumberOfParameters (
    KIM_Model const *const model,
    int *const numberOfParameters )
```

12.12.3.10 KIM_Model_GetParameterDataTypeExtentAndDescription()

```
int KIM_Model_GetParameterDataTypeExtentAndDescription (
    KIM_Model const *const model,
    int const parameterIndex,
    KIM_DataType *const dataType,
    int *const extent,
    char const **const description )
```

12.12.3.11 KIM_Model_GetParameterDouble()

```
int KIM_Model_GetParameterDouble (
    KIM_Model const *const model,
    int const parameterIndex,
    int const arrayIndex,
    double *const parameterValue )
```

12.12.3.12 KIM_Model_GetParameterInteger()

```
int KIM_Model_GetParameterInteger (
    KIM_Model const *const model,
    int const parameterIndex,
    int const arrayIndex,
    int *const parameterValue )
```

12.12.3.13 KIM_Model_GetSimulatorBufferPointer()

```
void KIM_Model_GetSimulatorBufferPointer (
    KIM_Model const *const model,
    void **const ptr )
```

12.12.3.14 KIM_Model_GetSpeciesSupportAndCode()

```
int KIM_Model_GetSpeciesSupportAndCode (
    KIM_Model const *const model,
    KIM_SpeciesName const speciesName,
    int *const speciesIsSupported,
    int *const code )
```

12.12.3.15 KIM_Model_GetUnits()

```
void KIM_Model_GetUnits (
    KIM_Model const *const model,
    KIM_LengthUnit *const lengthUnit,
    KIM_EnergyUnit *const energyUnit,
    KIM_ChargeUnit *const chargeUnit,
    KIM_TemperatureUnit *const temperatureUnit,
    KIM_TimeUnit *const timeUnit )
```

12.12.3.16 KIM_Model_PopLogVerbosity()

```
void KIM_Model_PopLogVerbosity (
    KIM_Model *const model )
```

12.12.3.17 KIM_Model_PushLogVerbosity()

```
void KIM_Model_PushLogVerbosity (
    KIM_Model *const model,
    KIM_LogVerbosity const logVerbosity )
```

12.12.3.18 KIM_Model_SetLogID()

```
void KIM_Model_SetLogID (
    KIM_Model *const model,
    char const *const logID )
```

12.12.3.19 KIM_Model_SetParameterDouble()

```
int KIM_Model_SetParameterDouble (
    KIM_Model *const model,
    int const parameterIndex,
    int const arrayIndex,
    double const parameterValue )
```

12.12.3.20 KIM_Model_SetParameterInteger()

```
int KIM_Model_SetParameterInteger (
    KIM_Model *const model,
    int const parameterIndex,
    int const arrayIndex,
    int const parameterValue )
```

12.12.3.21 KIM_Model_SetSimulatorBufferPointer()

```
void KIM_Model_SetSimulatorBufferPointer (
    KIM_Model *const model,
    void *const ptr )
```

12.12.3.22 KIM_Model_String()

```
char const* const KIM_Model_String (
    KIM_Model const *const model )
```

12.13 kim-api-v2.0.0-beta.0/c/include/KIM_ModelCompute.h File Reference**Macros**

- `#define KIM_LOG_VERBOSITY_DEFINED_`
- `#define KIM_MODEL_COMPUTE_DEFINED_`

Typedefs

- `typedef struct KIM_LogVerbosity KIM_LogVerbosity`
- `typedef struct KIM_ModelCompute KIM_ModelCompute`

Functions

- `void KIM_ModelCompute_GetModelBufferPointer (KIM_ModelCompute const *const modelCompute, void **const ptr)`
- `void KIM_ModelCompute_LogEntry (KIM_ModelCompute const *const modelCompute, KIM_LogVerbosity const logVerbosity, char const *const message, int const lineNumber, char const *const fileName)`
- `char const *const KIM_ModelCompute_String (KIM_ModelCompute const *const modelCompute)`

12.13.1 Macro Definition Documentation

12.13.1.1 KIM_LOG_VERBOSITY_DEFINED_

```
#define KIM_LOG_VERBOSITY_DEFINED_
```

Definition at line 41 of file KIM_ModelCompute.h.

12.13.1.2 KIM_MODEL_COMPUTE_DEFINED_

```
#define KIM_MODEL_COMPUTE_DEFINED_
```

Definition at line 49 of file KIM_ModelCompute.h.

12.13.2 Typedef Documentation

12.13.2.1 KIM_LogVerbosity

```
typedef struct KIM_LogVerbosity KIM_LogVerbosity
```

Definition at line 42 of file KIM_ModelCompute.h.

12.13.2.2 KIM_ModelCompute

```
typedef struct KIM_ModelCompute KIM_ModelCompute
```

Definition at line 50 of file KIM_ModelCompute.h.

12.13.3 Function Documentation

12.13.3.1 KIM_ModelCompute_GetModelBufferPointer()

```
void KIM_ModelCompute_GetModelBufferPointer (
    KIM_ModelCompute const *const modelCompute,
    void **const ptr )
```


12.13.3.2 KIM_ModelCompute_LogEntry()

```
void KIM_ModelCompute_LogEntry (
    KIM_ModelCompute const *const modelCompute,
    KIM_LogVerbosity const logVerbosity,
    char const *const message,
    int const lineNumber,
    char const *const fileName )
```

12.13.3.3 KIM_ModelCompute_String()

```
char const* const KIM_ModelCompute_String (
    KIM_ModelCompute const *const modelCompute )
```

12.14 kim-api-v2.0.0-beta.0/c/include/KIM_ModelComputeArguments.h File Reference

Macros

- `#define KIM_LOG_VERBOSITY_DEFINED_`
- `#define KIM_COMPUTE_ARGUMENT_NAME_DEFINED_`
- `#define KIM_COMPUTE_CALLBACK_NAME_DEFINED_`
- `#define KIM_MODEL_COMPUTE_ARGUMENTS_DEFINED_`

Typedefs

- `typedef struct KIM_LogVerbosity KIM_LogVerbosity`
- `typedef struct KIM_ComputeArgumentName KIM_ComputeArgumentName`
- `typedef struct KIM_ComputeCallbackName KIM_ComputeCallbackName`
- `typedef struct KIM_ModelComputeArguments KIM_ModelComputeArguments`

Functions

- `int KIM_ModelComputeArguments_GetNeighborList (KIM_ModelComputeArguments const *const modelComputeArguments, int const neighborListIndex, int const particleNumber, int *const numberOfNeighbors, int const **const neighborsOfParticle)`
- `int KIM_ModelComputeArguments_ProcessDEDrTerm (KIM_ModelComputeArguments const *const modelComputeArguments, double const de, double const r, double const *const dx, int const i, int const j)`
- `int KIM_ModelComputeArguments_ProcessD2EDr2Term (KIM_ModelComputeArguments const *const modelComputeArguments, double const de, double const *const r, double const *const dx, int const *const i, int const *const j)`
- `int KIM_ModelComputeArguments_GetArgumentPointerInteger (KIM_ModelComputeArguments const *const modelComputeArguments, KIM_ComputeArgumentName const computeArgumentName, int **const ptr)`
- `int KIM_ModelComputeArguments_GetArgumentPointerDouble (KIM_ModelComputeArguments const *const modelComputeArguments, KIM_ComputeArgumentName const computeArgumentName, double **const ptr)`
- `int KIM_ModelComputeArguments_IsCallbackPresent (KIM_ModelComputeArguments const *const modelComputeArguments, KIM_ComputeCallbackName const computeCallbackName, int *const present)`

- void [KIM_ModelComputeArguments_SetModelBufferPointer](#) ([KIM_ModelComputeArguments](#) *const modelComputeArguments, void *const ptr)
- void [KIM_ModelComputeArguments_GetModelBufferPointer](#) ([KIM_ModelComputeArguments](#) const *const modelComputeArguments, void **const ptr)
- void [KIM_ModelComputeArguments_LogEntry](#) ([KIM_ModelComputeArguments](#) const *const modelComputeArguments, [KIM_LogVerbosity](#) const logVerbosity, char const *const message, int const lineNumber, char const *const fileName)
- char const *const [KIM_ModelComputeArguments_String](#) ([KIM_ModelComputeArguments](#) const *const modelComputeArguments)

12.14.1 Macro Definition Documentation

12.14.1.1 KIM_COMPUTE_ARGUMENT_NAME_DEFINED_

```
#define KIM_COMPUTE_ARGUMENT_NAME_DEFINED_
```

Definition at line 46 of file [KIM_ModelComputeArguments.h](#).

12.14.1.2 KIM_COMPUTE_CALLBACK_NAME_DEFINED_

```
#define KIM_COMPUTE_CALLBACK_NAME_DEFINED_
```

Definition at line 51 of file [KIM_ModelComputeArguments.h](#).

12.14.1.3 KIM_LOG_VERBOSITY_DEFINED_

```
#define KIM_LOG_VERBOSITY_DEFINED_
```

Definition at line 41 of file [KIM_ModelComputeArguments.h](#).

12.14.1.4 KIM_MODEL_COMPUTE_ARGUMENTS_DEFINED_

```
#define KIM_MODEL_COMPUTE_ARGUMENTS_DEFINED_
```

Definition at line 59 of file [KIM_ModelComputeArguments.h](#).

12.14.2 Typedef Documentation

12.14.2.1 KIM_ComputeArgumentName

```
typedef struct KIM_ComputeArgumentName KIM_ComputeArgumentName
```

Definition at line 47 of file KIM_ModelComputeArguments.h.

12.14.2.2 KIM_ComputeCallbackName

```
typedef struct KIM_ComputeCallbackName KIM_ComputeCallbackName
```

Definition at line 52 of file KIM_ModelComputeArguments.h.

12.14.2.3 KIM_LogVerbosity

```
typedef struct KIM_LogVerbosity KIM_LogVerbosity
```

Definition at line 42 of file KIM_ModelComputeArguments.h.

12.14.2.4 KIM_ModelComputeArguments

```
typedef struct KIM_ModelComputeArguments KIM_ModelComputeArguments
```

Definition at line 60 of file KIM_ModelComputeArguments.h.

12.14.3 Function Documentation

12.14.3.1 KIM_ModelComputeArguments_GetArgumentPointerDouble()

```
int KIM_ModelComputeArguments_GetArgumentPointerDouble (
    KIM_ModelComputeArguments const *const modelComputeArguments,
    KIM_ComputeArgumentName const computeArgumentName,
    double **const ptr )
```

12.14.3.2 KIM_ModelComputeArguments_GetArgumentPointerInteger()

```
int KIM_ModelComputeArguments_GetArgumentPointerInteger (
    KIM_ModelComputeArguments const *const modelComputeArguments,
    KIM_ComputeArgumentName const computeArgumentName,
    int **const ptr )
```

12.14.3.3 KIM_ModelComputeArguments_GetModelBufferPointer()

```
void KIM_ModelComputeArguments_GetModelBufferPointer (
    KIM_ModelComputeArguments const *const modelComputeArguments,
    void **const ptr )
```

12.14.3.4 KIM_ModelComputeArguments_GetNeighborList()

```
int KIM_ModelComputeArguments_GetNeighborList (
    KIM_ModelComputeArguments const *const modelComputeArguments,
    int const neighborListIndex,
    int const particleNumber,
    int *const numberOfNeighbors,
    int const **const neighborsOfParticle )
```

12.14.3.5 KIM_ModelComputeArguments_IsCallbackPresent()

```
int KIM_ModelComputeArguments_IsCallbackPresent (
    KIM_ModelComputeArguments const *const modelComputeArguments,
    KIM_ComputeCallbackName const computeCallbackName,
    int *const present )
```

12.14.3.6 KIM_ModelComputeArguments_LogEntry()

```
void KIM_ModelComputeArguments_LogEntry (
    KIM_ModelComputeArguments const *const modelComputeArguments,
    KIM_LogVerbosity const logVerbosity,
    char const *const message,
    int const lineNumber,
    char const *const fileName )
```

12.14.3.7 KIM_ModelComputeArguments_ProcessD2EDr2Term()

```
int KIM_ModelComputeArguments_ProcessD2EDr2Term (
    KIM_ModelComputeArguments const *const modelComputeArguments,
    double const de,
    double const *const r,
    double const *const dx,
    int const *const i,
    int const *const j )
```

12.14.3.8 KIM_ModelComputeArguments_ProcessDEDrTerm()

```
int KIM_ModelComputeArguments_ProcessDEDrTerm (
    KIM_ModelComputeArguments const *const modelComputeArguments,
    double const de,
    double const r,
    double const *const dx,
    int const i,
    int const j )
```

12.14.3.9 KIM_ModelComputeArguments_SetModelBufferPointer()

```
void KIM_ModelComputeArguments_SetModelBufferPointer (
    KIM_ModelComputeArguments *const modelComputeArguments,
    void *const ptr )
```

12.14.3.10 KIM_ModelComputeArguments_String()

```
char const* const KIM_ModelComputeArguments_String (
    KIM_ModelComputeArguments const *const modelComputeArguments )
```

12.15 kim-api-v2.0.0-beta.0/c/include/KIM_ModelComputeArgumentsCreate.h File Reference

```
#include "KIM_func.h"
```

Macros

- `#define KIM_LOG_VERBOSITY_DEFINED_`
- `#define KIM_SUPPORT_STATUS_DEFINED_`
- `#define KIM_COMPUTE_ARGUMENT_NAME_DEFINED_`
- `#define KIM_COMPUTE_CALLBACK_NAME_DEFINED_`
- `#define KIM_MODEL_COMPUTE_ARGUMENTS_CREATE_DEFINED_`

Typedefs

- typedef struct [KIM_LogVerbosity](#) [KIM_LogVerbosity](#)
- typedef struct [KIM_SupportStatus](#) [KIM_SupportStatus](#)
- typedef struct [KIM_ComputeArgumentName](#) [KIM_ComputeArgumentName](#)
- typedef struct [KIM_ComputeCallbackName](#) [KIM_ComputeCallbackName](#)
- typedef struct [KIM_ModelComputeArgumentsCreate](#) [KIM_ModelComputeArgumentsCreate](#)

Functions

- int [KIM_ModelComputeArgumentsCreate_SetArgumentSupportStatus](#) ([KIM_ModelComputeArgumentsCreate](#) *const modelComputeArgumentsCreate, [KIM_ComputeArgumentName](#) const computeArgumentName, [KIM_SupportStatus](#) const supportStatus)
- int [KIM_ModelComputeArgumentsCreate_SetCallbackSupportStatus](#) ([KIM_ModelComputeArgumentsCreate](#) *const modelComputeArgumentsCreate, [KIM_ComputeCallbackName](#) const computeCallbackName, [KIM_SupportStatus](#) const supportStatus)
- void [KIM_ModelComputeArgumentsCreate_SetModelBufferPointer](#) ([KIM_ModelComputeArgumentsCreate](#) *const modelComputeArgumentsCreate, void *const ptr)
- void [KIM_ModelComputeArgumentsCreate_LogEntry](#) ([KIM_ModelComputeArgumentsCreate](#) const *const modelComputeArgumentsCreate, [KIM_LogVerbosity](#) const logVerbosity, char const *const message, int const lineNumber, char const *const fileName)
- char const *const [KIM_ModelComputeArgumentsCreate_String](#) ([KIM_ModelComputeArgumentsCreate](#) const *const modelComputeArgumentsCreate)

12.15.1 Macro Definition Documentation

12.15.1.1 KIM_COMPUTE_ARGUMENT_NAME_DEFINED_

```
#define KIM_COMPUTE_ARGUMENT_NAME_DEFINED_
```

Definition at line 55 of file [KIM_ModelComputeArgumentsCreate.h](#).

12.15.1.2 KIM_COMPUTE_CALLBACK_NAME_DEFINED_

```
#define KIM_COMPUTE_CALLBACK_NAME_DEFINED_
```

Definition at line 60 of file [KIM_ModelComputeArgumentsCreate.h](#).

12.15.1.3 KIM_LOG_VERBOSITY_DEFINED_

```
#define KIM_LOG_VERBOSITY_DEFINED_
```

Definition at line 45 of file [KIM_ModelComputeArgumentsCreate.h](#).

12.15.1.4 KIM_MODEL_COMPUTE_ARGUMENTS_CREATE_DEFINED_

```
#define KIM_MODEL_COMPUTE_ARGUMENTS_CREATE_DEFINED_
```

Definition at line 68 of file KIM_ModelComputeArgumentsCreate.h.

12.15.1.5 KIM_SUPPORT_STATUS_DEFINED_

```
#define KIM_SUPPORT_STATUS_DEFINED_
```

Definition at line 50 of file KIM_ModelComputeArgumentsCreate.h.

12.15.2 Typedef Documentation

12.15.2.1 KIM_ComputeArgumentName

```
typedef struct KIM_ComputeArgumentName KIM_ComputeArgumentName
```

Definition at line 56 of file KIM_ModelComputeArgumentsCreate.h.

12.15.2.2 KIM_ComputeCallbackName

```
typedef struct KIM_ComputeCallbackName KIM_ComputeCallbackName
```

Definition at line 61 of file KIM_ModelComputeArgumentsCreate.h.

12.15.2.3 KIM_LogVerbosity

```
typedef struct KIM_LogVerbosity KIM_LogVerbosity
```

Definition at line 46 of file KIM_ModelComputeArgumentsCreate.h.

12.15.2.4 KIM_ModelComputeArgumentsCreate

```
typedef struct KIM_ModelComputeArgumentsCreate KIM_ModelComputeArgumentsCreate
```

Definition at line 69 of file KIM_ModelComputeArgumentsCreate.h.

12.15.2.5 KIM_SupportStatus

```
typedef struct KIM_SupportStatus KIM_SupportStatus
```

Definition at line 51 of file KIM_ModelComputeArgumentsCreate.h.

12.15.3 Function Documentation

12.15.3.1 KIM_ModelComputeArgumentsCreate_LogEntry()

```
void KIM_ModelComputeArgumentsCreate_LogEntry (
    KIM_ModelComputeArgumentsCreate const *const modelComputeArgumentsCreate,
    KIM_LogVerbosity const logVerbosity,
    char const *const message,
    int const lineNumber,
    char const *const fileName )
```

12.15.3.2 KIM_ModelComputeArgumentsCreate_SetArgumentSupportStatus()

```
int KIM_ModelComputeArgumentsCreate_SetArgumentSupportStatus (
    KIM_ModelComputeArgumentsCreate *const modelComputeArgumentsCreate,
    KIM_ComputeArgumentName const computeArgumentName,
    KIM_SupportStatus const supportStatus )
```

12.15.3.3 KIM_ModelComputeArgumentsCreate_SetCallbackSupportStatus()

```
int KIM_ModelComputeArgumentsCreate_SetCallbackSupportStatus (
    KIM_ModelComputeArgumentsCreate *const modelComputeArgumentsCreate,
    KIM_ComputeCallbackName const computeCallbackName,
    KIM_SupportStatus const supportStatus )
```

12.15.3.4 KIM_ModelComputeArgumentsCreate_SetModelBufferPointer()

```
void KIM_ModelComputeArgumentsCreate_SetModelBufferPointer (
    KIM_ModelComputeArgumentsCreate *const modelComputeArgumentsCreate,
    void *const ptr )
```


12.15.3.5 KIM_ModelComputeArgumentsCreate_String()

```
char const* const KIM_ModelComputeArgumentsCreate_String (
    KIM_ModelComputeArgumentsCreate const *const modelComputeArgumentsCreate )
```

12.16 kim-api-v2.0.0-beta.0/c/include/KIM_ModelComputeArgumentsCreateLogMacros.h File Reference

Macros

- #define [FATAL_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_FATAL_)
- #define [LOG_FATAL](#)(message)
- #define [ERROR_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_ERROR_)
- #define [LOG_ERROR](#)(message)
- #define [WARNING_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_WARNING_↵
_)
- #define [LOG_WARNING](#)(message)
- #define [INFORMATION_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_INFO↵
RMATION_)
- #define [LOG_INFORMATION](#)(message)
- #define [DEBUG_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_DEBUG_)
- #define [LOG_DEBUG](#)(message)

12.16.1 Macro Definition Documentation

12.16.1.1 DEBUG_VERBOSITY

```
#define DEBUG_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_DEBUG_)
```

Definition at line 94 of file KIM_ModelComputeArgumentsCreateLogMacros.h.

12.16.1.2 ERROR_VERBOSITY

```
#define ERROR_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_ERROR_)
```

Definition at line 51 of file KIM_ModelComputeArgumentsCreateLogMacros.h.

12.16.1.3 FATAL_VERBOSITY

```
#define FATAL_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_FATAL_)
```

Definition at line 37 of file KIM_ModelComputeArgumentsCreateLogMacros.h.

12.16.1.4 INFORMATION_VERBOSITY

```
#define INFORMATION_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_INFORMATION_)
```

Definition at line 79 of file KIM_ModelComputeArgumentsCreateLogMacros.h.

12.16.1.5 LOG_DEBUG

```
#define LOG_DEBUG(  
    message )
```

Value:

```
KIM_ModelComputeArgumentsCreate_LogEntry(  
    modelComputeArgumentsCreate, \n                                KIM_LOG_VERBOSITY_debug, message, \n                                __LINE__, __FILE__)
```

Definition at line 99 of file KIM_ModelComputeArgumentsCreateLogMacros.h.

12.16.1.6 LOG_ERROR

```
#define LOG_ERROR(  
    message )
```

Value:

```
KIM_ModelComputeArgumentsCreate_LogEntry(  
    modelComputeArgumentsCreate, \n                                KIM_LOG_VERBOSITY_error, message, \n                                __LINE__, __FILE__)
```

Definition at line 56 of file KIM_ModelComputeArgumentsCreateLogMacros.h.

12.16.1.7 LOG_FATAL

```
#define LOG_FATAL(  
    message )
```

Value:

```
KIM_ModelComputeArgumentsCreate_LogEntry(  
    modelComputeArgumentsCreate, \n                                KIM_LOG_VERBOSITY_fatal, message, \n                                __LINE__, __FILE__)
```

Definition at line 42 of file KIM_ModelComputeArgumentsCreateLogMacros.h.

12.16.1.8 LOG_INFORMATION

```
#define LOG_INFORMATION(  
    message )
```

Value:

```
KIM_ModelComputeArgumentsCreate_LogEntry(  
    modelComputeArgumentsCreate, \
                                     KIM_LOG_VERBOSITY_information, \
    message, \
    __LINE__, __FILE__)
```

Definition at line 84 of file KIM_ModelComputeArgumentsCreateLogMacros.h.

12.16.1.9 LOG_WARNING

```
#define LOG_WARNING(  
    message )
```

Value:

```
KIM_ModelComputeArgumentsCreate_LogEntry(  
    modelComputeArgumentsCreate, \
                                     KIM_LOG_VERBOSITY_warning, message, \
    __LINE__, __FILE__)
```

Definition at line 70 of file KIM_ModelComputeArgumentsCreateLogMacros.h.

12.16.1.10 WARNING_VERBOSITY

```
#define WARNING_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_WARNING_)
```

Definition at line 65 of file KIM_ModelComputeArgumentsCreateLogMacros.h.

12.17 kim-api-v2.0.0-beta.0/c/include/KIM_ModelComputeArgumentsDestroy.h File Reference

Macros

- #define [KIM_LOG_VERBOSITY_DEFINED_](#)
- #define [KIM_MODEL_COMPUTE_ARGUMENTS_DESTROY_DEFINED_](#)

Typedefs

- typedef struct [KIM_LogVerbosity](#) KIM_LogVerbosity
- typedef struct [KIM_ModelComputeArgumentsDestroy](#) KIM_ModelComputeArgumentsDestroy

Functions

- void [KIM_ModelComputeArgumentsDestroy_GetModelBufferPointer](#) ([KIM_ModelComputeArgumentsDestroy](#) const *const modelComputeArgumentsDestroy, void **const ptr)
- void [KIM_ModelComputeArgumentsDestroy_LogEntry](#) ([KIM_ModelComputeArgumentsDestroy](#) const *const modelComputeArgumentsDestroy, [KIM_LogVerbosity](#) const logVerbosity, char const *const message, int const lineNumber, char const *const fileName)
- char const *const [KIM_ModelComputeArgumentsDestroy_String](#) ([KIM_ModelComputeArgumentsDestroy](#) const *const modelComputeArgumentsDestroy)

12.17.1 Macro Definition Documentation

12.17.1.1 KIM_LOG_VERBOSITY_DEFINED_

```
#define KIM_LOG_VERBOSITY_DEFINED_
```

Definition at line 41 of file [KIM_ModelComputeArgumentsDestroy.h](#).

12.17.1.2 KIM_MODEL_COMPUTE_ARGUMENTS_DESTROY_DEFINED_

```
#define KIM_MODEL_COMPUTE_ARGUMENTS_DESTROY_DEFINED_
```

Definition at line 49 of file [KIM_ModelComputeArgumentsDestroy.h](#).

12.17.2 Typedef Documentation

12.17.2.1 KIM_LogVerbosity

```
typedef struct KIM\_LogVerbosity KIM\_LogVerbosity
```

Definition at line 42 of file [KIM_ModelComputeArgumentsDestroy.h](#).

12.17.2.2 KIM_ModelComputeArgumentsDestroy

```
typedef struct KIM\_ModelComputeArgumentsDestroy KIM\_ModelComputeArgumentsDestroy
```

Definition at line 50 of file [KIM_ModelComputeArgumentsDestroy.h](#).

12.17.3 Function Documentation

12.17.3.1 KIM_ModelComputeArgumentsDestroy_GetModelBufferPointer()

```
void KIM_ModelComputeArgumentsDestroy_GetModelBufferPointer (
    KIM_ModelComputeArgumentsDestroy const *const modelComputeArgumentsDestroy,
    void **const ptr )
```

12.17.3.2 KIM_ModelComputeArgumentsDestroy_LogEntry()

```
void KIM_ModelComputeArgumentsDestroy_LogEntry (
    KIM_ModelComputeArgumentsDestroy const *const modelComputeArgumentsDestroy,
    KIM_LogVerbosity const logVerbosity,
    char const *const message,
    int const lineNumber,
    char const *const fileName )
```

12.17.3.3 KIM_ModelComputeArgumentsDestroy_String()

```
char const* const KIM_ModelComputeArgumentsDestroy_String (
    KIM_ModelComputeArgumentsDestroy const *const modelComputeArgumentsDestroy )
```

12.18 kim-api-v2.0.0-beta.0/c/include/KIM_ModelComputeArgumentsDestroyLogMacros.h File Reference

Macros

- #define [FATAL_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_FATAL_)
- #define [LOG_FATAL](#)(message)
- #define [ERROR_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_ERROR_)
- #define [LOG_ERROR](#)(message)
- #define [WARNING_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_WARNING_)
- #define [LOG_WARNING](#)(message)
- #define [INFORMATION_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_INFORMATION_)
- #define [LOG_INFORMATION](#)(message)
- #define [DEBUG_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_DEBUG_)
- #define [LOG_DEBUG](#)(message)

12.18.1 Macro Definition Documentation

12.18.1.1 DEBUG_VERBOSITY

```
#define DEBUG_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_DEBUG_)
```

Definition at line 95 of file KIM_ModelComputeArgumentsDestroyLogMacros.h.

12.18.1.2 ERROR_VERBOSITY

```
#define ERROR_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_ERROR_)
```

Definition at line 51 of file KIM_ModelComputeArgumentsDestroyLogMacros.h.

12.18.1.3 FATAL_VERBOSITY

```
#define FATAL_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_FATAL_)
```

Definition at line 37 of file KIM_ModelComputeArgumentsDestroyLogMacros.h.

12.18.1.4 INFORMATION_VERBOSITY

```
#define INFORMATION_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_INFORMATION_)
```

Definition at line 80 of file KIM_ModelComputeArgumentsDestroyLogMacros.h.

12.18.1.5 LOG_DEBUG

```
#define LOG_DEBUG(  
    message )
```

Value:

```
KIM_ModelComputeArgumentsDestroy_LogEntry(  
    modelComputeArgumentsDestroy, \n                                KIM_LOG_VERBOSITY_debug, message, \n                                __LINE__, __FILE__)
```

Definition at line 100 of file KIM_ModelComputeArgumentsDestroyLogMacros.h.

12.18.1.6 LOG_ERROR

```
#define LOG_ERROR(  
    message )
```

Value:

```
KIM_ModelComputeArgumentsDestroy_LogEntry(  
    modelComputeArgumentsDestroy, \n                                KIM_LOG_VERBOSITY_error, message, \n                                __LINE__, __FILE__)
```

Definition at line 56 of file KIM_ModelComputeArgumentsDestroyLogMacros.h.

12.18.1.7 LOG_FATAL

```
#define LOG_FATAL(  
    message )
```

Value:

```
KIM_ModelComputeArgumentsDestroy_LogEntry(  
    modelComputeArgumentsDestroy, \n                                KIM_LOG_VERBOSITY_fatal, message, \n                                __LINE__, __FILE__)
```

Definition at line 42 of file KIM_ModelComputeArgumentsDestroyLogMacros.h.

12.18.1.8 LOG_INFORMATION

```
#define LOG_INFORMATION(  
    message )
```

Value:

```
KIM_ModelComputeArgumentsDestroy_LogEntry(  
    modelComputeArgumentsDestroy, \n                                KIM_LOG_VERBOSITY_information, \n                                message, \n                                __LINE__, __FILE__)
```

Definition at line 85 of file KIM_ModelComputeArgumentsDestroyLogMacros.h.

12.18.1.9 LOG_WARNING

```
#define LOG_WARNING(  
    message )
```

Value:

```
KIM_ModelComputeArgumentsDestroy_LogEntry(  
    \                                \  
    modelComputeArgumentsDestroy,    \  
    KIM_LOG_VERBOSITY_warning, message, \  
    __LINE__, __FILE__)
```

Definition at line 70 of file KIM_ModelComputeArgumentsDestroyLogMacros.h.

12.18.1.10 WARNING_VERBOSITY

```
#define WARNING_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_WARNING_)
```

Definition at line 65 of file KIM_ModelComputeArgumentsDestroyLogMacros.h.

12.19 kim-api-v2.0.0-beta.0/c/include/KIM_ModelComputeArgumentsLogMacros.h File Reference

Macros

- #define [FATAL_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_FATAL_)
- #define [LOG_FATAL](#)(message)
- #define [ERROR_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_ERROR_)
- #define [LOG_ERROR](#)(message)
- #define [WARNING_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_WARNING_)
- #define [LOG_WARNING](#)(message)
- #define [INFORMATION_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_INFORMATION_)
- #define [LOG_INFORMATION](#)(message)
- #define [DEBUG_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_DEBUG_)
- #define [LOG_DEBUG](#)(message)

12.19.1 Macro Definition Documentation

12.19.1.1 DEBUG_VERBOSITY

```
#define DEBUG_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_DEBUG_)
```

Definition at line 93 of file KIM_ModelComputeArgumentsLogMacros.h.

12.19.1.2 ERROR_VERBOSITY

```
#define ERROR_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_ERROR_)
```

Definition at line 51 of file KIM_ModelComputeArgumentsLogMacros.h.

12.19.1.3 FATAL_VERBOSITY

```
#define FATAL_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_FATAL_)
```

Definition at line 37 of file KIM_ModelComputeArgumentsLogMacros.h.

12.19.1.4 INFORMATION_VERBOSITY

```
#define INFORMATION_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_INFORMATION_)
```

Definition at line 79 of file KIM_ModelComputeArgumentsLogMacros.h.

12.19.1.5 LOG_DEBUG

```
#define LOG_DEBUG(  
    message )
```

Value:

```
KIM_ModelComputeArguments_LogEntry(modelComputeArguments,  
    KIM_LOG_VERBOSITY_debug, message, \  
    __LINE__, __FILE__)
```

Definition at line 98 of file KIM_ModelComputeArgumentsLogMacros.h.

12.19.1.6 LOG_ERROR

```
#define LOG_ERROR(  
    message )
```

Value:

```
KIM_ModelComputeArguments_LogEntry(modelComputeArguments,  
    KIM_LOG_VERBOSITY_error, message, \  
    __LINE__, __FILE__)
```

Definition at line 56 of file KIM_ModelComputeArgumentsLogMacros.h.

12.19.1.7 LOG_FATAL

```
#define LOG_FATAL(  
    message )
```

Value:

```
KIM_ModelComputeArguments_LogEntry (modelComputeArguments,  
    KIM_LOG_VERBOSITY_fatal, message, \  
    __LINE__, __FILE__)
```

Definition at line 42 of file KIM_ModelComputeArgumentsLogMacros.h.

12.19.1.8 LOG_INFORMATION

```
#define LOG_INFORMATION(  
    message )
```

Value:

```
KIM_ModelComputeArguments_LogEntry (modelComputeArguments,  
    KIM_LOG_VERBOSITY_information, message, \  
    __LINE__, __FILE__)
```

Definition at line 84 of file KIM_ModelComputeArgumentsLogMacros.h.

12.19.1.9 LOG_WARNING

```
#define LOG_WARNING(  
    message )
```

Value:

```
KIM_ModelComputeArguments_LogEntry (modelComputeArguments,  
    KIM_LOG_VERBOSITY_warning, message, \  
    __LINE__, __FILE__)
```

Definition at line 70 of file KIM_ModelComputeArgumentsLogMacros.h.

12.19.1.10 WARNING_VERBOSITY

```
#define WARNING_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_WARNING_)
```

Definition at line 65 of file KIM_ModelComputeArgumentsLogMacros.h.

12.20 kim-api-v2.0.0-beta.0/c/include/KIM_ModelComputeLogMacros.h File Reference

Macros

- `#define FATAL_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_FATAL_)`
- `#define LOG_FATAL(message)`
- `#define ERROR_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_ERROR_)`
- `#define LOG_ERROR(message)`
- `#define WARNING_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_WARNING_)`
- `#define LOG_WARNING(message)`
- `#define INFORMATION_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_INFORMATION_)`
- `#define LOG_INFORMATION(message)`
- `#define DEBUG_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_DEBUG_)`
- `#define LOG_DEBUG(message)`

12.20.1 Macro Definition Documentation

12.20.1.1 DEBUG_VERBOSITY

```
#define DEBUG_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_DEBUG_)
```

Definition at line 93 of file KIM_ModelComputeLogMacros.h.

12.20.1.2 ERROR_VERBOSITY

```
#define ERROR_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_ERROR_)
```

Definition at line 51 of file KIM_ModelComputeLogMacros.h.

12.20.1.3 FATAL_VERBOSITY

```
#define FATAL_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_FATAL_)
```

Definition at line 37 of file KIM_ModelComputeLogMacros.h.

12.20.1.4 INFORMATION_VERBOSITY

```
#define INFORMATION_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_INFORMATION_)
```

Definition at line 79 of file KIM_ModelComputeLogMacros.h.

12.20.1.5 LOG_DEBUG

```
#define LOG_DEBUG(  
    message )
```

Value:

```
KIM_ModelCompute_LogEntry(modelCompute,  
    KIM_LOG_VERBOSITY_debug, message,  
    __LINE__, __FILE__)
```

Definition at line 98 of file KIM_ModelComputeLogMacros.h.

12.20.1.6 LOG_ERROR

```
#define LOG_ERROR(  
    message )
```

Value:

```
KIM_ModelCompute_LogEntry(modelCompute,  
    KIM_LOG_VERBOSITY_error, message,  
    __LINE__, __FILE__)
```

Definition at line 56 of file KIM_ModelComputeLogMacros.h.

12.20.1.7 LOG_FATAL

```
#define LOG_FATAL(  
    message )
```

Value:

```
KIM_ModelCompute_LogEntry(modelCompute,  
    KIM_LOG_VERBOSITY_fatal, message,  
    __LINE__, __FILE__)
```

Definition at line 42 of file KIM_ModelComputeLogMacros.h.

12.20.1.8 LOG_INFORMATION

```
#define LOG_INFORMATION(  
    message )
```

Value:

```
KIM_ModelCompute_LogEntry(modelCompute,  
    KIM_LOG_VERBOSITY_information, message,  
    __LINE__, __FILE__)
```

Definition at line 84 of file KIM_ModelComputeLogMacros.h.

12.20.1.9 LOG_WARNING

```
#define LOG_WARNING(  
    message )
```

Value:

```
KIM_ModelCompute_LogEntry(modelCompute,  
    KIM_LOG_VERBOSITY_warning, message,  
    __LINE__, __FILE__)
```

Definition at line 70 of file KIM_ModelComputeLogMacros.h.

12.20.1.10 WARNING_VERBOSITY

```
#define WARNING_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_WARNING_)
```

Definition at line 65 of file KIM_ModelComputeLogMacros.h.

12.21 kim-api-v2.0.0-beta.0/c/include/KIM_ModelCreate.h File Reference

```
#include "KIM_func.h"
```

Macros

- #define [KIM_LOG_VERBOSITY_DEFINED_](#)
- #define [KIM_LANGUAGE_NAME_DEFINED_](#)
- #define [KIM_NUMBERING_DEFINED_](#)
- #define [KIM_SPECIES_NAME_DEFINED_](#)
- #define [KIM_SUPPORT_STATUS_DEFINED_](#)
- #define [KIM_LENGTH_UNIT_DEFINED_](#)
- #define [KIM_ENERGY_UNIT_DEFINED_](#)
- #define [KIM_CHARGE_UNIT_DEFINED_](#)
- #define [KIM_TEMPERATURE_UNIT_DEFINED_](#)
- #define [KIM_TIME_UNIT_DEFINED_](#)
- #define [KIM_MODEL_CREATE_DEFINED_](#)

Typedefs

- typedef struct [KIM_LogVerbosity](#) [KIM_LogVerbosity](#)
- typedef struct [KIM_LanguageName](#) [KIM_LanguageName](#)
- typedef struct [KIM_Numbering](#) [KIM_Numbering](#)
- typedef struct [KIM_SpeciesName](#) [KIM_SpeciesName](#)
- typedef struct [KIM_SupportStatus](#) [KIM_SupportStatus](#)
- typedef struct [KIM_LengthUnit](#) [KIM_LengthUnit](#)
- typedef struct [KIM_EnergyUnit](#) [KIM_EnergyUnit](#)
- typedef struct [KIM_ChargeUnit](#) [KIM_ChargeUnit](#)
- typedef struct [KIM_TemperatureUnit](#) [KIM_TemperatureUnit](#)
- typedef struct [KIM_TimeUnit](#) [KIM_TimeUnit](#)
- typedef struct [KIM_ModelCreate](#) [KIM_ModelCreate](#)

Functions

- int [KIM_ModelCreate_SetModelNumbering](#) ([KIM_ModelCreate](#) *const modelCreate, [KIM_Numbering](#) const numbering)
- void [KIM_ModelCreate_SetInfluenceDistancePointer](#) ([KIM_ModelCreate](#) *const modelCreate, double *const influenceDistance)
- void [KIM_ModelCreate_SetNeighborListCutoffsPointer](#) ([KIM_ModelCreate](#) *const modelCreate, int const numberOfCutoffs, double const *const cutoffs)
- int [KIM_ModelCreate_SetRefreshPointer](#) ([KIM_ModelCreate](#) *const modelCreate, [KIM_LanguageName](#) const languageName, func *const fptr)
- int [KIM_ModelCreate_SetDestroyPointer](#) ([KIM_ModelCreate](#) *const modelCreate, [KIM_LanguageName](#) const languageName, func *const fptr)
- int [KIM_ModelCreate_SetComputeArgumentsCreatePointer](#) ([KIM_ModelCreate](#) *const modelCreate, [KIM_LanguageName](#) const languageName, func *const fptr)
- int [KIM_ModelCreate_SetComputeArgumentsDestroyPointer](#) ([KIM_ModelCreate](#) *const modelCreate, [KIM_LanguageName](#) const languageName, func *const fptr)
- int [KIM_ModelCreate_SetComputePointer](#) ([KIM_ModelCreate](#) *const modelCreate, [KIM_LanguageName](#) const languageName, func *const fptr)
- int [KIM_ModelCreate_SetSpeciesCode](#) ([KIM_ModelCreate](#) *const modelCreate, [KIM_SpeciesName](#) const speciesName, int const code)
- int [KIM_ModelCreate_SetParameterPointerInteger](#) ([KIM_ModelCreate](#) *const modelCreate, int const extent, int *const ptr, char const *const description)
- int [KIM_ModelCreate_SetParameterPointerDouble](#) ([KIM_ModelCreate](#) *const modelCreate, int const extent, double *const ptr, char const *const description)
- void [KIM_ModelCreate_SetModelBufferPointer](#) ([KIM_ModelCreate](#) *const modelCreate, void *const ptr)
- int [KIM_ModelCreate_SetUnits](#) ([KIM_ModelCreate](#) *const modelCreate, [KIM_LengthUnit](#) const lengthUnit, [KIM_EnergyUnit](#) const energyUnit, [KIM_ChargeUnit](#) const chargeUnit, [KIM_TemperatureUnit](#) const temperatureUnit, [KIM_TimeUnit](#) const timeUnit)
- int [KIM_ModelCreate_ConvertUnit](#) ([KIM_ModelCreate](#) const *const modelCreate, [KIM_LengthUnit](#) const fromLengthUnit, [KIM_EnergyUnit](#) const fromEnergyUnit, [KIM_ChargeUnit](#) const fromChargeUnit, [KIM_TemperatureUnit](#) const fromTemperatureUnit, [KIM_TimeUnit](#) const fromTimeUnit, [KIM_LengthUnit](#) const toLengthUnit, [KIM_EnergyUnit](#) const toEnergyUnit, [KIM_ChargeUnit](#) const toChargeUnit, [KIM_TemperatureUnit](#) const toTemperatureUnit, [KIM_TimeUnit](#) const toTimeUnit, double const lengthExponent, double const energyExponent, double const chargeExponent, double const temperatureExponent, double const timeExponent, double *const conversionFactor)
- void [KIM_ModelCreate_LogEntry](#) ([KIM_ModelCreate](#) const *const modelCreate, [KIM_LogVerbosity](#) const logVerbosity, char const *const message, int const lineNumber, char const *const fileName)
- char const *const [KIM_ModelCreate_String](#) ([KIM_ModelCreate](#) const *const modelCreate)

12.21.1 Macro Definition Documentation

12.21.1.1 KIM_CHARGE_UNIT_DEFINED_

```
#define KIM_CHARGE_UNIT_DEFINED_
```

Definition at line 80 of file KIM_ModelCreate.h.

12.21.1.2 KIM_ENERGY_UNIT_DEFINED_

```
#define KIM_ENERGY_UNIT_DEFINED_
```

Definition at line 75 of file KIM_ModelCreate.h.

12.21.1.3 KIM_LANGUAGE_NAME_DEFINED_

```
#define KIM_LANGUAGE_NAME_DEFINED_
```

Definition at line 50 of file KIM_ModelCreate.h.

12.21.1.4 KIM_LENGTH_UNIT_DEFINED_

```
#define KIM_LENGTH_UNIT_DEFINED_
```

Definition at line 70 of file KIM_ModelCreate.h.

12.21.1.5 KIM_LOG_VERBOSITY_DEFINED_

```
#define KIM_LOG_VERBOSITY_DEFINED_
```

Definition at line 45 of file KIM_ModelCreate.h.

12.21.1.6 KIM_MODEL_CREATE_DEFINED_

```
#define KIM_MODEL_CREATE_DEFINED_
```

Definition at line 98 of file KIM_ModelCreate.h.

12.21.1.7 KIM_NUMBERING_DEFINED_

```
#define KIM_NUMBERING_DEFINED_
```

Definition at line 55 of file KIM_ModelCreate.h.

12.21.1.8 KIM_SPECIES_NAME_DEFINED_

```
#define KIM_SPECIES_NAME_DEFINED_
```

Definition at line 60 of file KIM_ModelCreate.h.

12.21.1.9 KIM_SUPPORT_STATUS_DEFINED_

```
#define KIM_SUPPORT_STATUS_DEFINED_
```

Definition at line 65 of file KIM_ModelCreate.h.

12.21.1.10 KIM_TEMPERATURE_UNIT_DEFINED_

```
#define KIM_TEMPERATURE_UNIT_DEFINED_
```

Definition at line 85 of file KIM_ModelCreate.h.

12.21.1.11 KIM_TIME_UNIT_DEFINED_

```
#define KIM_TIME_UNIT_DEFINED_
```

Definition at line 90 of file KIM_ModelCreate.h.

12.21.2 Typedef Documentation

12.21.2.1 KIM_ChargeUnit

```
typedef struct KIM_ChargeUnit KIM_ChargeUnit
```

Definition at line 81 of file KIM_ModelCreate.h.

12.21.2.2 KIM_EnergyUnit

```
typedef struct KIM_EnergyUnit KIM_EnergyUnit
```

Definition at line 76 of file KIM_ModelCreate.h.

12.21.2.3 KIM_LanguageName

```
typedef struct KIM_LanguageName KIM_LanguageName
```

Definition at line 51 of file KIM_ModelCreate.h.

12.21.2.4 KIM_LengthUnit

```
typedef struct KIM_LengthUnit KIM_LengthUnit
```

Definition at line 71 of file KIM_ModelCreate.h.

12.21.2.5 KIM_LogVerbosity

```
typedef struct KIM_LogVerbosity KIM_LogVerbosity
```

Definition at line 46 of file KIM_ModelCreate.h.

12.21.2.6 KIM_ModelCreate

```
typedef struct KIM_ModelCreate KIM_ModelCreate
```

Definition at line 99 of file KIM_ModelCreate.h.

12.21.2.7 KIM_Numbering

```
typedef struct KIM_Numbering KIM_Numbering
```

Definition at line 56 of file KIM_ModelCreate.h.

12.21.2.8 KIM_SpeciesName

```
typedef struct KIM_SpeciesName KIM_SpeciesName
```

Definition at line 61 of file KIM_ModelCreate.h.

12.21.2.9 KIM_SupportStatus

```
typedef struct KIM_SupportStatus KIM_SupportStatus
```

Definition at line 66 of file KIM_ModelCreate.h.

12.21.2.10 KIM_TemperatureUnit

```
typedef struct KIM_TemperatureUnit KIM_TemperatureUnit
```

Definition at line 86 of file KIM_ModelCreate.h.

12.21.2.11 KIM_TimeUnit

```
typedef struct KIM_TimeUnit KIM_TimeUnit
```

Definition at line 91 of file KIM_ModelCreate.h.

12.21.3 Function Documentation

12.21.3.1 KIM_ModelCreate_ConvertUnit()

```
int KIM_ModelCreate_ConvertUnit (
    KIM_ModelCreate const *const modelCreate,
    KIM_LengthUnit const fromLengthUnit,
    KIM_EnergyUnit const fromEnergyUnit,
    KIM_ChargeUnit const fromChargeUnit,
    KIM_TemperatureUnit const fromTemperatureUnit,
    KIM_TimeUnit const fromTimeUnit,
    KIM_LengthUnit const toLengthUnit,
    KIM_EnergyUnit const toEnergyUnit,
    KIM_ChargeUnit const toChargeUnit,
    KIM_TemperatureUnit const toTemperatureUnit,
    KIM_TimeUnit const toTimeUnit,
    double const lengthExponent,
    double const energyExponent,
    double const chargeExponent,
    double const temperatureExponent,
    double const timeExponent,
    double *const conversionFactor )
```

12.21.3.2 KIM_ModelCreate_LogEntry()

```
void KIM_ModelCreate_LogEntry (
    KIM_ModelCreate const *const modelCreate,
    KIM_LogVerbosity const logVerbosity,
    char const *const message,
    int const lineNumber,
    char const *const fileName )
```

12.21.3.3 KIM_ModelCreate_SetComputeArgumentsCreatePointer()

```
int KIM_ModelCreate_SetComputeArgumentsCreatePointer (
    KIM_ModelCreate *const modelCreate,
    KIM_LanguageName const languageName,
    func *const fptr )
```

12.21.3.4 KIM_ModelCreate_SetComputeArgumentsDestroyPointer()

```
int KIM_ModelCreate_SetComputeArgumentsDestroyPointer (
    KIM_ModelCreate *const modelCreate,
    KIM_LanguageName const languageName,
    func *const fptr )
```

12.21.3.5 KIM_ModelCreate_SetComputePointer()

```
int KIM_ModelCreate_SetComputePointer (
    KIM_ModelCreate *const modelCreate,
    KIM_LanguageName const languageName,
    func *const fptr )
```

12.21.3.6 KIM_ModelCreate_SetDestroyPointer()

```
int KIM_ModelCreate_SetDestroyPointer (
    KIM_ModelCreate *const modelCreate,
    KIM_LanguageName const languageName,
    func *const fptr )
```

12.21.3.7 KIM_ModelCreate_SetInfluenceDistancePointer()

```
void KIM_ModelCreate_SetInfluenceDistancePointer (
    KIM_ModelCreate *const modelCreate,
    double *const influenceDistance )
```

12.21.3.8 KIM_ModelCreate_SetModelBufferPointer()

```
void KIM_ModelCreate_SetModelBufferPointer (
    KIM_ModelCreate *const modelCreate,
    void *const ptr )
```

12.21.3.9 KIM_ModelCreate_SetModelNumbering()

```
int KIM_ModelCreate_SetModelNumbering (
    KIM_ModelCreate *const modelCreate,
    KIM_Numbering const numbering )
```

12.21.3.10 KIM_ModelCreate_SetNeighborListCutoffsPointer()

```
void KIM_ModelCreate_SetNeighborListCutoffsPointer (
    KIM_ModelCreate *const modelCreate,
    int const numberOfCutoffs,
    double const *const cutoffs )
```

12.21.3.11 KIM_ModelCreate_SetParameterPointerDouble()

```
int KIM_ModelCreate_SetParameterPointerDouble (
    KIM_ModelCreate *const modelCreate,
    int const extent,
    double *const ptr,
    char const *const description )
```

12.21.3.12 KIM_ModelCreate_SetParameterPointerInteger()

```
int KIM_ModelCreate_SetParameterPointerInteger (
    KIM_ModelCreate *const modelCreate,
    int const extent,
    int *const ptr,
    char const *const description )
```

12.21.3.13 KIM_ModelCreate_SetRefreshPointer()

```
int KIM_ModelCreate_SetRefreshPointer (
    KIM_ModelCreate *const modelCreate,
    KIM_LanguageName const languageName,
    func *const fptr )
```

12.21.3.14 KIM_ModelCreate_SetSpeciesCode()

```
int KIM_ModelCreate_SetSpeciesCode (
    KIM_ModelCreate *const modelCreate,
    KIM_SpeciesName const speciesName,
    int const code )
```

12.21.3.15 KIM_ModelCreate_SetUnits()

```
int KIM_ModelCreate_SetUnits (
    KIM_ModelCreate *const modelCreate,
    KIM_LengthUnit const lengthUnit,
    KIM_EnergyUnit const energyUnit,
    KIM_ChargeUnit const chargeUnit,
    KIM_TemperatureUnit const temperatureUnit,
    KIM_TimeUnit const timeUnit )
```

12.21.3.16 KIM_ModelCreate_String()

```
char const* const KIM_ModelCreate_String (
    KIM_ModelCreate const *const modelCreate )
```

12.22 kim-api-v2.0.0-beta.0/c/include/KIM_ModelCreateLogMacros.h File Reference

Macros

- #define [FATAL_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_FATAL_)
- #define [LOG_FATAL](#)(message)
- #define [ERROR_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_ERROR_)
- #define [LOG_ERROR](#)(message)
- #define [WARNING_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_WARNING_)
- #define [LOG_WARNING](#)(message)
- #define [INFORMATION_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_INFORMATION_)
- #define [LOG_INFORMATION](#)(message)
- #define [DEBUG_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_DEBUG_)
- #define [LOG_DEBUG](#)(message)

12.22.1 Macro Definition Documentation

12.22.1.1 DEBUG_VERBOSITY

```
#define DEBUG_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_DEBUG_)
```

Definition at line 93 of file KIM_ModelCreateLogMacros.h.

12.22.1.2 ERROR_VERBOSITY

```
#define ERROR_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_ERROR_)
```

Definition at line 51 of file KIM_ModelCreateLogMacros.h.

12.22.1.3 FATAL_VERBOSITY

```
#define FATAL_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_FATAL_)
```

Definition at line 37 of file KIM_ModelCreateLogMacros.h.

12.22.1.4 INFORMATION_VERBOSITY

```
#define INFORMATION_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_INFORMATION_)
```

Definition at line 79 of file KIM_ModelCreateLogMacros.h.

12.22.1.5 LOG_DEBUG

```
#define LOG_DEBUG(  
    message )
```

Value:

```
KIM_ModelCreate_LogEntry(modelCreate,  
    KIM_LOG_VERBOSITY_debug, message,  
    __LINE__, __FILE__)
```

Definition at line 98 of file KIM_ModelCreateLogMacros.h.

12.22.1.6 LOG_ERROR

```
#define LOG_ERROR(  
    message )
```

Value:

```
KIM_ModelCreate_LogEntry(modelCreate,  
    KIM_LOG_VERBOSITY_error, message,  
    __LINE__, __FILE__)
```

Definition at line 56 of file KIM_ModelCreateLogMacros.h.

12.22.1.7 LOG_FATAL

```
#define LOG_FATAL(  
    message )
```

Value:

```
KIM_ModelCreate_LogEntry(modelCreate,  
    KIM_LOG_VERBOSITY_fatal, message,  
    __LINE__, __FILE__)
```

Definition at line 42 of file KIM_ModelCreateLogMacros.h.

12.22.1.8 LOG_INFORMATION

```
#define LOG_INFORMATION(  
    message )
```

Value:

```
KIM_ModelCreate_LogEntry(modelCreate,  
    KIM_LOG_VERBOSITY_information, message,  
    __LINE__, __FILE__)
```

Definition at line 84 of file KIM_ModelCreateLogMacros.h.

12.22.1.9 LOG_WARNING

```
#define LOG_WARNING(  
    message )
```

Value:

```
KIM_ModelCreate_LogEntry(modelCreate,  
    KIM_LOG_VERBOSITY_warning, message,  
    __LINE__, __FILE__)
```

Definition at line 70 of file KIM_ModelCreateLogMacros.h.

12.22.1.10 WARNING_VERBOSITY

```
#define WARNING_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_WARNING_)
```

Definition at line 65 of file KIM_ModelCreateLogMacros.h.

12.23 kim-api-v2.0.0-beta.0/c/include/KIM_ModelDestroy.h File Reference

Macros

- #define [KIM_LOG_VERBOSITY_DEFINED_](#)
- #define [KIM_MODEL_DESTROY_DEFINED_](#)

Typedefs

- typedef struct [KIM_LogVerbosity](#) KIM_LogVerbosity
- typedef struct [KIM_ModelDestroy](#) KIM_ModelDestroy

Functions

- void [KIM_ModelDestroy_GetModelBufferPointer](#) ([KIM_ModelDestroy](#) const *const modelDestroy, void **const ptr)
- void [KIM_ModelDestroy_LogEntry](#) ([KIM_ModelDestroy](#) const *const modelDestroy, [KIM_LogVerbosity](#) const logVerbosity, char const *const message, int const lineNumber, char const *const fileName)
- char const *const [KIM_ModelDestroy_String](#) ([KIM_ModelDestroy](#) const *const modelDestroy)

12.23.1 Macro Definition Documentation

12.23.1.1 KIM_LOG_VERBOSITY_DEFINED_

```
#define KIM_LOG_VERBOSITY_DEFINED_
```

Definition at line 41 of file [KIM_ModelDestroy.h](#).

12.23.1.2 KIM_MODEL_DESTROY_DEFINED_

```
#define KIM_MODEL_DESTROY_DEFINED_
```

Definition at line 49 of file [KIM_ModelDestroy.h](#).

12.23.2 Typedef Documentation

12.23.2.1 KIM_LogVerbosity

```
typedef struct KIM\_LogVerbosity KIM\_LogVerbosity
```

Definition at line 42 of file [KIM_ModelDestroy.h](#).

12.23.2.2 KIM_ModelDestroy

```
typedef struct KIM\_ModelDestroy KIM\_ModelDestroy
```

Definition at line 50 of file [KIM_ModelDestroy.h](#).

12.23.3 Function Documentation

12.23.3.1 KIM_ModelDestroy_GetModelBufferPointer()

```
void KIM_ModelDestroy_GetModelBufferPointer (
    KIM_ModelDestroy const *const modelDestroy,
    void **const ptr )
```

12.23.3.2 KIM_ModelDestroy_LogEntry()

```
void KIM_ModelDestroy_LogEntry (
    KIM_ModelDestroy const *const modelDestroy,
    KIM_LogVerbosity const logVerbosity,
    char const *const message,
    int const lineNumber,
    char const *const fileName )
```

12.23.3.3 KIM_ModelDestroy_String()

```
char const* const KIM_ModelDestroy_String (
    KIM_ModelDestroy const *const modelDestroy )
```

12.24 kim-api-v2.0.0-beta.0/c/include/KIM_ModelDestroyLogMacros.h File Reference

Macros

- #define [FATAL_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_FATAL_)
- #define [LOG_FATAL](#)(message)
- #define [ERROR_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_ERROR_)
- #define [LOG_ERROR](#)(message)
- #define [WARNING_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_WARNING_↵
_)
- #define [LOG_WARNING](#)(message)
- #define [INFORMATION_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_INFO↵
RMATION_)
- #define [LOG_INFORMATION](#)(message)
- #define [DEBUG_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_DEBUG_)
- #define [LOG_DEBUG](#)(message)

12.24.1 Macro Definition Documentation

12.24.1.1 DEBUG_VERBOSITY

```
#define DEBUG_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_DEBUG_)
```

Definition at line 93 of file KIM_ModelDestroyLogMacros.h.

12.24.1.2 ERROR_VERBOSITY

```
#define ERROR_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_ERROR_)
```

Definition at line 51 of file KIM_ModelDestroyLogMacros.h.

12.24.1.3 FATAL_VERBOSITY

```
#define FATAL_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_FATAL_)
```

Definition at line 37 of file KIM_ModelDestroyLogMacros.h.

12.24.1.4 INFORMATION_VERBOSITY

```
#define INFORMATION_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_INFORMATION_)
```

Definition at line 79 of file KIM_ModelDestroyLogMacros.h.

12.24.1.5 LOG_DEBUG

```
#define LOG_DEBUG(  
    message )
```

Value:

```
KIM_ModelDestroy_LogEntry(modelDestroy,  
    KIM_LOG_VERBOSITY_debug, message,  
    __LINE__, __FILE__)
```

Definition at line 98 of file KIM_ModelDestroyLogMacros.h.

12.24.1.6 LOG_ERROR

```
#define LOG_ERROR(  
    message )
```

Value:

```
KIM_ModelDestroy_LogEntry(modelDestroy,  
    KIM_LOG_VERBOSITY_error, message,  
    __LINE__, __FILE__)
```

Definition at line 56 of file KIM_ModelDestroyLogMacros.h.

12.24.1.7 LOG_FATAL

```
#define LOG_FATAL(  
    message )
```

Value:

```
KIM_ModelDestroy_LogEntry(modelDestroy,  
    KIM_LOG_VERBOSITY_fatal, message,  
    __LINE__, __FILE__)
```

Definition at line 42 of file KIM_ModelDestroyLogMacros.h.

12.24.1.8 LOG_INFORMATION

```
#define LOG_INFORMATION(  
    message )
```

Value:

```
KIM_ModelDestroy_LogEntry(modelDestroy,  
    KIM_LOG_VERBOSITY_information, message,  
    __LINE__, __FILE__)
```

Definition at line 84 of file KIM_ModelDestroyLogMacros.h.

12.24.1.9 LOG_WARNING

```
#define LOG_WARNING(  
    message )
```

Value:

```
KIM_ModelDestroy_LogEntry(modelDestroy,  
    KIM_LOG_VERBOSITY_warning, message,  
    __LINE__, __FILE__)
```

Definition at line 70 of file KIM_ModelDestroyLogMacros.h.

12.24.1.10 WARNING_VERBOSITY

```
#define WARNING_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_WARNING_)
```

Definition at line 65 of file KIM_ModelDestroyLogMacros.h.

12.25 kim-api-v2.0.0-beta.0/c/include/KIM_ModelDriverCreate.h File Reference

```
#include "KIM_func.h"
```

Macros

- #define [KIM_LOG_VERBOSITY_DEFINED_](#)
- #define [KIM_LANGUAGE_NAME_DEFINED_](#)
- #define [KIM_NUMBERING_DEFINED_](#)
- #define [KIM_SPECIES_NAME_DEFINED_](#)
- #define [KIM_SUPPORT_STATUS_DEFINED_](#)
- #define [KIM_LENGTH_UNIT_DEFINED_](#)
- #define [KIM_ENERGY_UNIT_DEFINED_](#)
- #define [KIM_CHARGE_UNIT_DEFINED_](#)
- #define [KIM_TEMPERATURE_UNIT_DEFINED_](#)
- #define [KIM_TIME_UNIT_DEFINED_](#)
- #define [KIM_MODEL_DRIVER_CREATE_DEFINED_](#)

Typedefs

- typedef struct [KIM_LogVerbosity](#) KIM_LogVerbosity
- typedef struct [KIM_LanguageName](#) KIM_LanguageName
- typedef struct [KIM_Numbering](#) KIM_Numbering
- typedef struct [KIM_SpeciesName](#) KIM_SpeciesName
- typedef struct [KIM_SupportStatus](#) KIM_SupportStatus
- typedef struct [KIM_LengthUnit](#) KIM_LengthUnit
- typedef struct [KIM_EnergyUnit](#) KIM_EnergyUnit
- typedef struct [KIM_ChargeUnit](#) KIM_ChargeUnit
- typedef struct [KIM_TemperatureUnit](#) KIM_TemperatureUnit
- typedef struct [KIM_TimeUnit](#) KIM_TimeUnit
- typedef struct [KIM_ModelDriverCreate](#) KIM_ModelDriverCreate

Functions

- void [KIM_ModelDriverCreate_GetNumberOfParameterFiles](#) ([KIM_ModelDriverCreate](#) *const modelDriverCreate, int *const numberOfParameterFiles)
- int [KIM_ModelDriverCreate_GetParameterFileName](#) ([KIM_ModelDriverCreate](#) *const modelDriverCreate, int const index, char const **const parameterFileName)
- int [KIM_ModelDriverCreate_SetModelNumbering](#) ([KIM_ModelDriverCreate](#) *const modelDriverCreate, [KIM_Numbering](#) const numbering)
- void [KIM_ModelDriverCreate_SetInfluenceDistancePointer](#) ([KIM_ModelDriverCreate](#) *const modelDriverCreate, double *const influenceDistance)
- void [KIM_ModelDriverCreate_SetNeighborListCutoffsPointer](#) ([KIM_ModelDriverCreate](#) *const modelDriverCreate, int const numberOfCutoffs, double const *const cutoffs)
- int [KIM_ModelDriverCreate_SetRefreshPointer](#) ([KIM_ModelDriverCreate](#) *const modelDriverCreate, [KIM_LanguageName](#) const languageName, func *const fptr)
- int [KIM_ModelDriverCreate_SetDestroyPointer](#) ([KIM_ModelDriverCreate](#) *const modelDriverCreate, [KIM_LanguageName](#) const languageName, func *const fptr)
- int [KIM_ModelDriverCreate_SetComputeArgumentsCreatePointer](#) ([KIM_ModelDriverCreate](#) *const modelDriverCreate, [KIM_LanguageName](#) const languageName, func *const fptr)
- int [KIM_ModelDriverCreate_SetComputeArgumentsDestroyPointer](#) ([KIM_ModelDriverCreate](#) *const modelDriverCreate, [KIM_LanguageName](#) const languageName, func *const fptr)
- int [KIM_ModelDriverCreate_SetComputePointer](#) ([KIM_ModelDriverCreate](#) *const modelDriverCreate, [KIM_LanguageName](#) const languageName, func *const fptr)
- int [KIM_ModelDriverCreate_SetSpeciesCode](#) ([KIM_ModelDriverCreate](#) *const modelDriverCreate, [KIM_SpeciesName](#) const speciesName, int const code)
- int [KIM_ModelDriverCreate_SetParameterPointerInteger](#) ([KIM_ModelDriverCreate](#) *const modelDriverCreate, int const extent, int *const ptr, char const *const description)
- int [KIM_ModelDriverCreate_SetParameterPointerDouble](#) ([KIM_ModelDriverCreate](#) *const modelDriverCreate, int const extent, double *const ptr, char const *const description)
- void [KIM_ModelDriverCreate_SetModelBufferPointer](#) ([KIM_ModelDriverCreate](#) *const modelDriverCreate, void *const ptr)
- int [KIM_ModelDriverCreate_SetUnits](#) ([KIM_ModelDriverCreate](#) *const modelDriverCreate, [KIM_LengthUnit](#) const lengthUnit, [KIM_EnergyUnit](#) const energyUnit, [KIM_ChargeUnit](#) const chargeUnit, [KIM_TemperatureUnit](#) const temperatureUnit, [KIM_TimeUnit](#) const timeUnit)
- int [KIM_ModelDriverCreate_ConvertUnit](#) ([KIM_ModelDriverCreate](#) const *const modelDriverCreate, [KIM_LengthUnit](#) const fromLengthUnit, [KIM_EnergyUnit](#) const fromEnergyUnit, [KIM_ChargeUnit](#) const fromChargeUnit, [KIM_TemperatureUnit](#) const fromTemperatureUnit, [KIM_TimeUnit](#) const fromTimeUnit, [KIM_LengthUnit](#) const toLengthUnit, [KIM_EnergyUnit](#) const toEnergyUnit, [KIM_ChargeUnit](#) const toChargeUnit, [KIM_TemperatureUnit](#) const toTemperatureUnit, [KIM_TimeUnit](#) const toTimeUnit, double const lengthExponent, double const energyExponent, double const chargeExponent, double const temperatureExponent, double const timeExponent, double *const conversionFactor)
- void [KIM_ModelDriverCreate_LogEntry](#) ([KIM_ModelDriverCreate](#) const *const modelDriverCreate, [KIM_LogVerbosity](#) const logVerbosity, char const *const message, int const lineNumber, char const *const fileName)
- char const *const [KIM_ModelDriverCreate_String](#) ([KIM_ModelDriverCreate](#) const *const modelDriverCreate)

12.25.1 Macro Definition Documentation

12.25.1.1 KIM_CHARGE_UNIT_DEFINED_

```
#define KIM_CHARGE_UNIT_DEFINED_
```

Definition at line 80 of file [KIM_ModelDriverCreate.h](#).

12.25.1.2 KIM_ENERGY_UNIT_DEFINED_

```
#define KIM_ENERGY_UNIT_DEFINED_
```

Definition at line 75 of file KIM_ModelDriverCreate.h.

12.25.1.3 KIM_LANGUAGE_NAME_DEFINED_

```
#define KIM_LANGUAGE_NAME_DEFINED_
```

Definition at line 50 of file KIM_ModelDriverCreate.h.

12.25.1.4 KIM_LENGTH_UNIT_DEFINED_

```
#define KIM_LENGTH_UNIT_DEFINED_
```

Definition at line 70 of file KIM_ModelDriverCreate.h.

12.25.1.5 KIM_LOG_VERBOSITY_DEFINED_

```
#define KIM_LOG_VERBOSITY_DEFINED_
```

Definition at line 45 of file KIM_ModelDriverCreate.h.

12.25.1.6 KIM_MODEL_DRIVER_CREATE_DEFINED_

```
#define KIM_MODEL_DRIVER_CREATE_DEFINED_
```

Definition at line 98 of file KIM_ModelDriverCreate.h.

12.25.1.7 KIM_NUMBERING_DEFINED_

```
#define KIM_NUMBERING_DEFINED_
```

Definition at line 55 of file KIM_ModelDriverCreate.h.

12.25.1.8 KIM_SPECIES_NAME_DEFINED_

```
#define KIM_SPECIES_NAME_DEFINED_
```

Definition at line 60 of file KIM_ModelDriverCreate.h.

12.25.1.9 KIM_SUPPORT_STATUS_DEFINED_

```
#define KIM_SUPPORT_STATUS_DEFINED_
```

Definition at line 65 of file KIM_ModelDriverCreate.h.

12.25.1.10 KIM_TEMPERATURE_UNIT_DEFINED_

```
#define KIM_TEMPERATURE_UNIT_DEFINED_
```

Definition at line 85 of file KIM_ModelDriverCreate.h.

12.25.1.11 KIM_TIME_UNIT_DEFINED_

```
#define KIM_TIME_UNIT_DEFINED_
```

Definition at line 90 of file KIM_ModelDriverCreate.h.

12.25.2 Typedef Documentation

12.25.2.1 KIM_ChargeUnit

```
typedef struct KIM_ChargeUnit KIM_ChargeUnit
```

Definition at line 81 of file KIM_ModelDriverCreate.h.

12.25.2.2 KIM_EnergyUnit

```
typedef struct KIM_EnergyUnit KIM_EnergyUnit
```

Definition at line 76 of file KIM_ModelDriverCreate.h.

12.25.2.3 KIM_LanguageName

```
typedef struct KIM_LanguageName KIM_LanguageName
```

Definition at line 51 of file KIM_ModelDriverCreate.h.

12.25.2.4 KIM_LengthUnit

```
typedef struct KIM_LengthUnit KIM_LengthUnit
```

Definition at line 71 of file KIM_ModelDriverCreate.h.

12.25.2.5 KIM_LogVerbosity

```
typedef struct KIM_LogVerbosity KIM_LogVerbosity
```

Definition at line 46 of file KIM_ModelDriverCreate.h.

12.25.2.6 KIM_ModelDriverCreate

```
typedef struct KIM_ModelDriverCreate KIM_ModelDriverCreate
```

Definition at line 99 of file KIM_ModelDriverCreate.h.

12.25.2.7 KIM_Numbering

```
typedef struct KIM_Numbering KIM_Numbering
```

Definition at line 56 of file KIM_ModelDriverCreate.h.

12.25.2.8 KIM_SpeciesName

```
typedef struct KIM_SpeciesName KIM_SpeciesName
```

Definition at line 61 of file KIM_ModelDriverCreate.h.

12.25.2.9 KIM_SupportStatus

```
typedef struct KIM_SupportStatus KIM_SupportStatus
```

Definition at line 66 of file KIM_ModelDriverCreate.h.

12.25.2.10 KIM_TemperatureUnit

```
typedef struct KIM_TemperatureUnit KIM_TemperatureUnit
```

Definition at line 86 of file KIM_ModelDriverCreate.h.

12.25.2.11 KIM_TimeUnit

```
typedef struct KIM_TimeUnit KIM_TimeUnit
```

Definition at line 91 of file KIM_ModelDriverCreate.h.

12.25.3 Function Documentation

12.25.3.1 KIM_ModelDriverCreate_ConvertUnit()

```
int KIM_ModelDriverCreate_ConvertUnit (
    KIM_ModelDriverCreate const *const modelDriverCreate,
    KIM_LengthUnit const fromLengthUnit,
    KIM_EnergyUnit const fromEnergyUnit,
    KIM_ChargeUnit const fromChargeUnit,
    KIM_TemperatureUnit const fromTemperatureUnit,
    KIM_TimeUnit const fromTimeUnit,
    KIM_LengthUnit const toLengthUnit,
    KIM_EnergyUnit const toEnergyUnit,
    KIM_ChargeUnit const toChargeUnit,
    KIM_TemperatureUnit const toTemperatureUnit,
    KIM_TimeUnit const toTimeUnit,
    double const lengthExponent,
    double const energyExponent,
    double const chargeExponent,
    double const temperatureExponent,
    double const timeExponent,
    double *const conversionFactor )
```

12.25.3.2 KIM_ModelDriverCreate_GetNumberOfParameterFiles()

```
void KIM_ModelDriverCreate_GetNumberOfParameterFiles (
    KIM_ModelDriverCreate *const modelDriverCreate,
    int *const numberOfParameterFiles )
```

12.25.3.3 KIM_ModelDriverCreate_GetParameterFileName()

```
int KIM_ModelDriverCreate_GetParameterFileName (
    KIM_ModelDriverCreate *const modelDriverCreate,
    int const index,
    char const **const parameterFileName )
```

12.25.3.4 KIM_ModelDriverCreate_LogEntry()

```
void KIM_ModelDriverCreate_LogEntry (
    KIM_ModelDriverCreate const *const modelDriverCreate,
    KIM_LogVerbosity const logVerbosity,
    char const *const message,
    int const lineNumber,
    char const *const fileName )
```

12.25.3.5 KIM_ModelDriverCreate_SetComputeArgumentsCreatePointer()

```
int KIM_ModelDriverCreate_SetComputeArgumentsCreatePointer (
    KIM_ModelDriverCreate *const modelDriverCreate,
    KIM_LanguageName const languageName,
    func *const fptr )
```

12.25.3.6 KIM_ModelDriverCreate_SetComputeArgumentsDestroyPointer()

```
int KIM_ModelDriverCreate_SetComputeArgumentsDestroyPointer (
    KIM_ModelDriverCreate *const modelDriverCreate,
    KIM_LanguageName const languageName,
    func *const fptr )
```

12.25.3.7 KIM_ModelDriverCreate_SetComputePointer()

```
int KIM_ModelDriverCreate_SetComputePointer (
    KIM_ModelDriverCreate *const modelDriverCreate,
    KIM_LanguageName const languageName,
    func *const fptr )
```

12.25.3.8 KIM_ModelDriverCreate_SetDestroyPointer()

```
int KIM_ModelDriverCreate_SetDestroyPointer (
    KIM_ModelDriverCreate *const modelDriverCreate,
    KIM_LanguageName const languageName,
    func *const fptr )
```

12.25.3.9 KIM_ModelDriverCreate_SetInfluenceDistancePointer()

```
void KIM_ModelDriverCreate_SetInfluenceDistancePointer (
    KIM_ModelDriverCreate *const modelDriverCreate,
    double *const influenceDistance )
```

12.25.3.10 KIM_ModelDriverCreate_SetModelBufferPointer()

```
void KIM_ModelDriverCreate_SetModelBufferPointer (
    KIM_ModelDriverCreate *const modelDriverCreate,
    void *const ptr )
```

12.25.3.11 KIM_ModelDriverCreate_SetModelNumbering()

```
int KIM_ModelDriverCreate_SetModelNumbering (
    KIM_ModelDriverCreate *const modelDriverCreate,
    KIM_Numbering const numbering )
```

12.25.3.12 KIM_ModelDriverCreate_SetNeighborListCutoffsPointer()

```
void KIM_ModelDriverCreate_SetNeighborListCutoffsPointer (
    KIM_ModelDriverCreate *const modelDriverCreate,
    int const numberOfCutoffs,
    double const *const cutoffs )
```

12.25.3.13 KIM_ModelDriverCreate_SetParameterPointerDouble()

```
int KIM_ModelDriverCreate_SetParameterPointerDouble (
    KIM_ModelDriverCreate *const modelDriverCreate,
    int const extent,
    double *const ptr,
    char const *const description )
```

12.25.3.14 KIM_ModelDriverCreate_SetParameterPointerInteger()

```
int KIM_ModelDriverCreate_SetParameterPointerInteger (
    KIM_ModelDriverCreate *const modelDriverCreate,
    int const extent,
    int *const ptr,
    char const *const description )
```

12.25.3.15 KIM_ModelDriverCreate_SetRefreshPointer()

```
int KIM_ModelDriverCreate_SetRefreshPointer (
    KIM_ModelDriverCreate *const modelDriverCreate,
    KIM_LanguageName const languageName,
    func *const fptr )
```

12.25.3.16 KIM_ModelDriverCreate_SetSpeciesCode()

```
int KIM_ModelDriverCreate_SetSpeciesCode (
    KIM_ModelDriverCreate *const modelDriverCreate,
    KIM_SpeciesName const speciesName,
    int const code )
```

12.25.3.17 KIM_ModelDriverCreate_SetUnits()

```
int KIM_ModelDriverCreate_SetUnits (
    KIM_ModelDriverCreate *const modelDriverCreate,
    KIM_LengthUnit const lengthUnit,
    KIM_EnergyUnit const energyUnit,
    KIM_ChargeUnit const chargeUnit,
    KIM_TemperatureUnit const temperatureUnit,
    KIM_TimeUnit const timeUnit )
```

12.25.3.18 KIM_ModelDriverCreate_String()

```
char const* const KIM_ModelDriverCreate_String (
    KIM_ModelDriverCreate const *const modelDriverCreate )
```

12.26 kim-api-v2.0.0-beta.0/c/include/KIM_ModelDriverCreateLogMacros.h File Reference

Macros

- #define [FATAL_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_FATAL_)
- #define [LOG_FATAL](#)(message)
- #define [ERROR_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_ERROR_)
- #define [LOG_ERROR](#)(message)
- #define [WARNING_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_WARNING_)
- #define [LOG_WARNING](#)(message)
- #define [INFORMATION_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_INFORMATION_)
- #define [LOG_INFORMATION](#)(message)
- #define [DEBUG_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_DEBUG_)
- #define [LOG_DEBUG](#)(message)

12.26.1 Macro Definition Documentation

12.26.1.1 DEBUG_VERBOSITY

```
#define DEBUG_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_DEBUG_)
```

Definition at line 93 of file KIM_ModelDriverCreateLogMacros.h.

12.26.1.2 ERROR_VERBOSITY

```
#define ERROR_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_ERROR_)
```

Definition at line 51 of file KIM_ModelDriverCreateLogMacros.h.

12.26.1.3 FATAL_VERBOSITY

```
#define FATAL_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_FATAL_)
```

Definition at line 37 of file KIM_ModelDriverCreateLogMacros.h.

12.26.1.4 INFORMATION_VERBOSITY

```
#define INFORMATION_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_INFORMATION_)
```

Definition at line 79 of file KIM_ModelDriverCreateLogMacros.h.

12.26.1.5 LOG_DEBUG

```
#define LOG_DEBUG(  
    message )
```

Value:

```
KIM_ModelDriverCreate_LogEntry(modelDriverCreate,  
    KIM_LOG_VERBOSITY_debug, message, \  
    __LINE__, __FILE__)
```

Definition at line 98 of file KIM_ModelDriverCreateLogMacros.h.

12.26.1.6 LOG_ERROR

```
#define LOG_ERROR(  
    message )
```

Value:

```
KIM_ModelDriverCreate_LogEntry(modelDriverCreate,  
    KIM_LOG_VERBOSITY_error, message, \  
    __LINE__, __FILE__)
```

Definition at line 56 of file KIM_ModelDriverCreateLogMacros.h.

12.26.1.7 LOG_FATAL

```
#define LOG_FATAL(  
    message )
```

Value:

```
KIM_ModelDriverCreate_LogEntry(modelDriverCreate,  
    KIM_LOG_VERBOSITY_fatal, message, \  
    __LINE__, __FILE__)
```

Definition at line 42 of file KIM_ModelDriverCreateLogMacros.h.

12.26.1.8 LOG_INFORMATION

```
#define LOG_INFORMATION(  
    message )
```

Value:

```
KIM_ModelDriverCreate_LogEntry(modelDriverCreate,  
    KIM_LOG_VERBOSITY_information, message, \  
    __LINE__, __FILE__)
```

Definition at line 84 of file KIM_ModelDriverCreateLogMacros.h.

12.26.1.9 LOG_WARNING

```
#define LOG_WARNING(  
    message )
```

Value:

```
KIM_ModelDriverCreate_LogEntry(modelDriverCreate,  
    KIM_LOG_VERBOSITY_warning, message, \  
    __LINE__, __FILE__)
```

Definition at line 70 of file KIM_ModelDriverCreateLogMacros.h.

12.26.1.10 WARNING_VERBOSITY

```
#define WARNING_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_WARNING_)
```

Definition at line 65 of file KIM_ModelDriverCreateLogMacros.h.

12.27 kim-api-v2.0.0-beta.0/c/include/KIM_ModelDriverHeaders.h File Reference

```
#include "KIM_ModelDriverCreate.h"  
#include "KIM_LogVerbosity.h"  
#include "KIM_LanguageName.h"  
#include "KIM_Numbering.h"  
#include "KIM_SpeciesName.h"  
#include "KIM_SupportStatus.h"  
#include "KIM_UnitSystem.h"  
#include "KIM_ModelComputeArgumentsCreate.h"  
#include "KIM_ComputeArgumentName.h"  
#include "KIM_DataType.h"  
#include "KIM_ComputeCallbackName.h"  
#include "KIM_ModelComputeArguments.h"  
#include "KIM_ModelComputeArgumentsDestroy.h"  
#include "KIM_ModelCompute.h"  
#include "KIM_ModelRefresh.h"  
#include "KIM_ModelDestroy.h"
```


12.28 kim-api-v2.0.0-beta.0/c/include/KIM_ModelHeaders.h File Reference

```
#include "KIM_ModelCreate.h"
#include "KIM_LogVerbosity.h"
#include "KIM_LanguageName.h"
#include "KIM_Numbering.h"
#include "KIM_SpeciesName.h"
#include "KIM_SupportStatus.h"
#include "KIM_UnitSystem.h"
#include "KIM_ModelComputeArgumentsCreate.h"
#include "KIM_ComputeArgumentName.h"
#include "KIM_DataType.h"
#include "KIM_ComputeCallbackName.h"
#include "KIM_ModelComputeArguments.h"
#include "KIM_ModelComputeArgumentsDestroy.h"
#include "KIM_ModelCompute.h"
#include "KIM_ModelRefresh.h"
#include "KIM_ModelDestroy.h"
```

12.29 kim-api-v2.0.0-beta.0/c/include/KIM_ModelRefresh.h File Reference

Macros

- `#define KIM_LOG_VERBOSITY_DEFINED_`
- `#define KIM_MODEL_REFRESH_DEFINED_`

Typedefs

- `typedef struct KIM_LogVerbosity KIM_LogVerbosity`
- `typedef struct KIM_ModelRefresh KIM_ModelRefresh`

Functions

- `void KIM_ModelRefresh_SetInfluenceDistancePointer (KIM_ModelRefresh *const modelRefresh, double *const influenceDistance)`
- `void KIM_ModelRefresh_SetNeighborListCutoffsPointer (KIM_ModelRefresh *const modelRefresh, int const numberOfCutoffs, double const *const cutoffs)`
- `void KIM_ModelRefresh_GetModelBufferPointer (KIM_ModelRefresh const *const modelRefresh, void **const ptr)`
- `void KIM_ModelRefresh_LogEntry (KIM_ModelRefresh const *const modelRefresh, KIM_LogVerbosity const logVerbosity, char const *const message, int const lineNumber, char const *const fileName)`
- `char const *const KIM_ModelRefresh_String (KIM_ModelRefresh const *const modelRefresh)`

12.29.1 Macro Definition Documentation

12.29.1.1 KIM_LOG_VERBOSITY_DEFINED_

```
#define KIM_LOG_VERBOSITY_DEFINED_
```

Definition at line 42 of file KIM_ModelRefresh.h.

12.29.1.2 KIM_MODEL_REFRESH_DEFINED_

```
#define KIM_MODEL_REFRESH_DEFINED_
```

Definition at line 47 of file KIM_ModelRefresh.h.

12.29.2 Typedef Documentation

12.29.2.1 KIM_LogVerbosity

```
typedef struct KIM_LogVerbosity KIM_LogVerbosity
```

Definition at line 43 of file KIM_ModelRefresh.h.

12.29.2.2 KIM_ModelRefresh

```
typedef struct KIM_ModelRefresh KIM_ModelRefresh
```

Definition at line 48 of file KIM_ModelRefresh.h.

12.29.3 Function Documentation

12.29.3.1 KIM_ModelRefresh_GetModelBufferPointer()

```
void KIM_ModelRefresh_GetModelBufferPointer (
    KIM_ModelRefresh const *const modelRefresh,
    void **const ptr )
```

12.29.3.2 KIM_ModelRefresh_LogEntry()

```
void KIM_ModelRefresh_LogEntry (
    KIM_ModelRefresh const *const modelRefresh,
    KIM_LogVerbosity const logVerbosity,
    char const *const message,
    int const lineNumber,
    char const *const fileName )
```

12.29.3.3 KIM_ModelRefresh_SetInfluenceDistancePointer()

```
void KIM_ModelRefresh_SetInfluenceDistancePointer (
    KIM_ModelRefresh *const modelRefresh,
    double *const influenceDistance )
```

12.29.3.4 KIM_ModelRefresh_SetNeighborListCutoffsPointer()

```
void KIM_ModelRefresh_SetNeighborListCutoffsPointer (
    KIM_ModelRefresh *const modelRefresh,
    int const numberOfCutoffs,
    double const *const cutoffs )
```

12.29.3.5 KIM_ModelRefresh_String()

```
char const* const KIM_ModelRefresh_String (
    KIM_ModelRefresh const *const modelRefresh )
```

12.30 kim-api-v2.0.0-beta.0/c/include/KIM_ModelRefreshLogMacros.h File Reference

Macros

- #define **FATAL_VERBOSITY** (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_FATAL_)
- #define **LOG_FATAL**(message)
- #define **ERROR_VERBOSITY** (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_ERROR_)
- #define **LOG_ERROR**(message)
- #define **WARNING_VERBOSITY** (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_WARNING_↵
_)
- #define **LOG_WARNING**(message)
- #define **INFORMATION_VERBOSITY** (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_INFO_↵
RMATION_)
- #define **LOG_INFORMATION**(message)
- #define **DEBUG_VERBOSITY** (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_DEBUG_)
- #define **LOG_DEBUG**(message)

12.30.1 Macro Definition Documentation

12.30.1.1 DEBUG_VERBOSITY

```
#define DEBUG_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_DEBUG_)
```

Definition at line 93 of file KIM_ModelRefreshLogMacros.h.

12.30.1.2 ERROR_VERBOSITY

```
#define ERROR_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_ERROR_)
```

Definition at line 51 of file KIM_ModelRefreshLogMacros.h.

12.30.1.3 FATAL_VERBOSITY

```
#define FATAL_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_FATAL_)
```

Definition at line 37 of file KIM_ModelRefreshLogMacros.h.

12.30.1.4 INFORMATION_VERBOSITY

```
#define INFORMATION_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_INFORMATION_)
```

Definition at line 79 of file KIM_ModelRefreshLogMacros.h.

12.30.1.5 LOG_DEBUG

```
#define LOG_DEBUG(  
    message )
```

Value:

```
KIM_ModelRefresh_LogEntry(modelRefresh,  
    KIM_LOG_VERBOSITY_debug, message,  
    __LINE__, __FILE__)
```

Definition at line 98 of file KIM_ModelRefreshLogMacros.h.

12.30.1.6 LOG_ERROR

```
#define LOG_ERROR(  
    message )
```

Value:

```
KIM_ModelRefresh_LogEntry(modelRefresh,  
    KIM_LOG_VERBOSITY_error, message,  
    __LINE__, __FILE__)
```

Definition at line 56 of file KIM_ModelRefreshLogMacros.h.

12.30.1.7 LOG_FATAL

```
#define LOG_FATAL(  
    message )
```

Value:

```
KIM_ModelRefresh_LogEntry(modelRefresh,  
    KIM_LOG_VERBOSITY_fatal, message,  
    __LINE__, __FILE__)
```

Definition at line 42 of file KIM_ModelRefreshLogMacros.h.

12.30.1.8 LOG_INFORMATION

```
#define LOG_INFORMATION(  
    message )
```

Value:

```
KIM_ModelRefresh_LogEntry(modelRefresh,  
    KIM_LOG_VERBOSITY_information, message,  
    __LINE__, __FILE__)
```

Definition at line 84 of file KIM_ModelRefreshLogMacros.h.

12.30.1.9 LOG_WARNING

```
#define LOG_WARNING(  
    message )
```

Value:

```
KIM_ModelRefresh_LogEntry (modelRefresh,  
    KIM_LOG_VERBOSITY_warning, message,  
    __LINE__, __FILE__)
```

Definition at line 70 of file KIM_ModelRefreshLogMacros.h.

12.30.1.10 WARNING_VERBOSITY

```
#define WARNING_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_WARNING)
```

Definition at line 65 of file KIM_ModelRefreshLogMacros.h.

12.31 kim-api-v2.0.0-beta.0/c/include/KIM_Numbering.h File Reference

Classes

- struct [KIM_Numbering](#)

Macros

- `#define` [KIM_NUMBERING_DEFINED_](#)

Typedefs

- typedef struct [KIM_Numbering](#) [KIM_Numbering](#)

Functions

- [KIM_Numbering KIM_Numbering_FromString](#) (char const *const str)
- int [KIM_Numbering_Equal](#) (KIM_Numbering const left, KIM_Numbering const right)
- int [KIM_Numbering_NotEqual](#) (KIM_Numbering const left, KIM_Numbering const right)
- char const *const [KIM_Numbering_String](#) (KIM_Numbering const numbering)
- void [KIM_NUMBERING_GetNumberOfNumberings](#) (int *const numberOfNumberings)
- int [KIM_NUMBERING_GetNumbering](#) (int const index, KIM_Numbering *const numbering)

Variables

- [KIM_Numbering](#) const [KIM_NUMBERING_zeroBased](#)
- [KIM_Numbering](#) const [KIM_NUMBERING_oneBased](#)

12.31.1 Macro Definition Documentation

12.31.1.1 KIM_NUMBERING_DEFINED_

```
#define KIM_NUMBERING_DEFINED_
```

Definition at line 44 of file KIM_Numbering.h.

12.31.2 Typedef Documentation

12.31.2.1 KIM_Numbering

```
typedef struct KIM_Numbering KIM_Numbering
```

Definition at line 45 of file KIM_Numbering.h.

12.31.3 Function Documentation

12.31.3.1 KIM_Numbering_Equal()

```
int KIM_Numbering_Equal (
    KIM_Numbering const left,
    KIM_Numbering const right )
```

12.31.3.2 KIM_Numbering_FromString()

```
KIM_Numbering KIM_Numbering_FromString (
    char const *const str )
```

12.31.3.3 KIM_NUMBERING_GetNumbering()

```
int KIM_NUMBERING_GetNumbering (
    int const index,
    KIM_Numbering *const numbering )
```

12.31.3.4 KIM_NUMBERING_GetNumberOfNumberings()

```
void KIM_NUMBERING_GetNumberOfNumberings (
    int *const numberOfNumberings )
```

12.31.3.5 KIM_Numbering_NotEqual()

```
int KIM_Numbering_NotEqual (
    KIM_Numbering const left,
    KIM_Numbering const right )
```

12.31.3.6 KIM_Numbering_String()

```
char const* const KIM_Numbering_String (
    KIM_Numbering const numbering )
```

12.31.4 Variable Documentation

12.31.4.1 KIM_NUMBERING_oneBased

```
KIM_Numbering const KIM_NUMBERING_oneBased
```

12.31.4.2 KIM_NUMBERING_zeroBased

```
KIM_Numbering const KIM_NUMBERING_zeroBased
```

12.32 kim-api-v2.0.0-beta.0/c/include/KIM_SemVer.h File Reference

Functions

- void [KIM_SEM_VER_GetSemVer](#) (char const **const version)
- int [KIM_SEM_VER_IsLessThan](#) (char const *const versionA, char const *const versionB, int *const isLessThan)
- int [KIM_SEM_VER_ParseSemVer](#) (char const *const version, int *const major, int *const minor, int *const patch, char *const prerelease, int const prereleaseLength, char *const buildMetadata, int const buildMetadataLength)

12.32.1 Function Documentation

12.32.1.1 KIM_SEM_VER_GetSemVer()

```
void KIM_SEM_VER_GetSemVer (
    char const **const version )
```

12.32.1.2 KIM_SEM_VER_IsLessThan()

```
int KIM_SEM_VER_IsLessThan (
    char const *const versionA,
    char const *const versionB,
    int *const isLessThan )
```

12.32.1.3 KIM_SEM_VER_ParseSemVer()

```
int KIM_SEM_VER_ParseSemVer (
    char const *const version,
    int *const major,
    int *const minor,
    int *const patch,
    char *const prerelease,
    int const prereleaseLength,
    char *const buildMetadata,
    int const buildMetadataLength )
```

12.33 kim-api-v2.0.0-beta.0/c/include/KIM_SimulatorHeaders.h File Reference

```
#include "KIM_Model.h"
#include "KIM_LogVerbosity.h"
#include "KIM_DataType.h"
#include "KIM_LanguageName.h"
#include "KIM_SpeciesName.h"
#include "KIM_Numbering.h"
#include "KIM_UnitSystem.h"
#include "KIM_ComputeArguments.h"
#include "KIM_ComputeArgumentName.h"
#include "KIM_ComputeCallbackName.h"
#include "KIM_SupportStatus.h"
```

12.34 kim-api-v2.0.0-beta.0/c/include/KIM_SpeciesName.h File Reference

Classes

- struct [KIM_SpeciesName](#)

Macros

- `#define` [KIM_SPECIES_NAME_DEFINED_](#)

Typedefs

- typedef struct [KIM_SpeciesName](#) [KIM_SpeciesName](#)

Functions

- [KIM_SpeciesName](#) [KIM_SpeciesName_FromString](#) (char const *const str)
- int [KIM_SpeciesName_Equal](#) ([KIM_SpeciesName](#) const left, [KIM_SpeciesName](#) const right)
- int [KIM_SpeciesName_NotEqual](#) ([KIM_SpeciesName](#) const left, [KIM_SpeciesName](#) const right)
- char const *const [KIM_SpeciesName_String](#) ([KIM_SpeciesName](#) const speciesName)
- void [KIM_SPECIES_NAME_GetNumberOfSpeciesNames](#) (int *const numberOfSpeciesNames)
- int [KIM_SPECIES_NAME_GetSpeciesName](#) (int const index, [KIM_SpeciesName](#) *const speciesName)

Variables

- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_electron](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_H](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_He](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Li](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Be](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_B](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_C](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_N](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_O](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_F](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Ne](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Na](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Mg](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Al](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Si](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_P](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_S](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Cl](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Ar](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_K](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Ca](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Sc](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Ti](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_V](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Cr](#)

- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Mn](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Fe](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Co](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Ni](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Cu](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Zn](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Ga](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Ge](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_As](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Se](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Br](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Kr](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Rb](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Sr](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Y](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Zr](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Nb](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Mo](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Tc](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Ru](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Rh](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Pd](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Ag](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Cd](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_In](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Sn](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Sb](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Te](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_I](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Xe](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Cs](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Ba](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_La](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Ce](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Pr](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Nd](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Pm](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Sm](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Eu](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Gd](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Tb](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Dy](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Ho](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Er](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Tm](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Yb](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Lu](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Hf](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME-Ta](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_W](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Re](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Os](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Ir](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Pt](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Au](#)

- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Hg](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Tl](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Pb](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Bi](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Po](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_At](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Rn](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Fr](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Ra](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Ac](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Th](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Pa](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_U](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Np](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Pu](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Am](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Cm](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Bk](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Cf](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Es](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Fm](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Md](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_No](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Lr](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Rf](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Db](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Sg](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Bh](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Hs](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Mt](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Ds](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Rg](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Cn](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Uut](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Fl](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Uup](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Lv](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Uus](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_Uuo](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_user01](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_user02](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_user03](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_user04](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_user05](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_user06](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_user07](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_user08](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_user09](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_user10](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_user11](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_user12](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_user13](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_user14](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_user15](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_user16](#)

- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_user17](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_user18](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_user19](#)
- [KIM_SpeciesName](#) const [KIM_SPECIES_NAME_user20](#)

12.34.1 Macro Definition Documentation

12.34.1.1 KIM_SPECIES_NAME_DEFINED_

```
#define KIM_SPECIES_NAME_DEFINED_
```

Definition at line 45 of file [KIM_SpeciesName.h](#).

12.34.2 Typedef Documentation

12.34.2.1 KIM_SpeciesName

```
typedef struct KIM\_SpeciesName KIM\_SpeciesName
```

Definition at line 46 of file [KIM_SpeciesName.h](#).

12.34.3 Function Documentation

12.34.3.1 KIM_SPECIES_NAME_GetNumberOfSpeciesNames()

```
void KIM_SPECIES_NAME_GetNumberOfSpeciesNames (
    int *const numberOfSpeciesNames )
```

12.34.3.2 KIM_SPECIES_NAME_GetSpeciesName()

```
int KIM_SPECIES_NAME_GetSpeciesName (
    int const index,
    KIM\_SpeciesName *const speciesName )
```

12.34.3.3 KIM_SpeciesName_Equal()

```
int KIM_SpeciesName_Equal (
    KIM_SpeciesName const left,
    KIM_SpeciesName const right )
```

12.34.3.4 KIM_SpeciesName_FromString()

```
KIM_SpeciesName KIM_SpeciesName_FromString (
    char const *const str )
```

12.34.3.5 KIM_SpeciesName_NotEqual()

```
int KIM_SpeciesName_NotEqual (
    KIM_SpeciesName const left,
    KIM_SpeciesName const right )
```

12.34.3.6 KIM_SpeciesName_String()

```
char const* const KIM_SpeciesName_String (
    KIM_SpeciesName const speciesName )
```

12.34.4 Variable Documentation

12.34.4.1 KIM_SPECIES_NAME_Ac

```
KIM_SpeciesName const KIM_SPECIES_NAME_Ac
```

12.34.4.2 KIM_SPECIES_NAME_Ag

```
KIM_SpeciesName const KIM_SPECIES_NAME_Ag
```

12.34.4.3 KIM_SPECIES_NAME_Al

`KIM_SpeciesName` const KIM_SPECIES_NAME_Al

12.34.4.4 KIM_SPECIES_NAME_Am

`KIM_SpeciesName` const KIM_SPECIES_NAME_Am

12.34.4.5 KIM_SPECIES_NAME_Ar

`KIM_SpeciesName` const KIM_SPECIES_NAME_Ar

12.34.4.6 KIM_SPECIES_NAME_As

`KIM_SpeciesName` const KIM_SPECIES_NAME_As

12.34.4.7 KIM_SPECIES_NAME_At

`KIM_SpeciesName` const KIM_SPECIES_NAME_At

12.34.4.8 KIM_SPECIES_NAME_Au

`KIM_SpeciesName` const KIM_SPECIES_NAME_Au

12.34.4.9 KIM_SPECIES_NAME_B

`KIM_SpeciesName` const KIM_SPECIES_NAME_B

12.34.4.10 KIM_SPECIES_NAME_Ba

`KIM_SpeciesName` const KIM_SPECIES_NAME_Ba

12.34.4.11 KIM_SPECIES_NAME_Be

`KIM_SpeciesName` const KIM_SPECIES_NAME_Be

12.34.4.12 KIM_SPECIES_NAME_Bh

`KIM_SpeciesName` const KIM_SPECIES_NAME_Bh

12.34.4.13 KIM_SPECIES_NAME_Bi

`KIM_SpeciesName` const KIM_SPECIES_NAME_Bi

12.34.4.14 KIM_SPECIES_NAME_Bk

`KIM_SpeciesName` const KIM_SPECIES_NAME_Bk

12.34.4.15 KIM_SPECIES_NAME_Br

`KIM_SpeciesName` const KIM_SPECIES_NAME_Br

12.34.4.16 KIM_SPECIES_NAME_C

`KIM_SpeciesName` const KIM_SPECIES_NAME_C

12.34.4.17 KIM_SPECIES_NAME_Ca

`KIM_SpeciesName` const KIM_SPECIES_NAME_Ca

12.34.4.18 KIM_SPECIES_NAME_Cd

`KIM_SpeciesName` const KIM_SPECIES_NAME_Cd

12.34.4.19 KIM_SPECIES_NAME_Ce

`KIM_SpeciesName` const KIM_SPECIES_NAME_Ce

12.34.4.20 KIM_SPECIES_NAME_Cf

`KIM_SpeciesName` const KIM_SPECIES_NAME_Cf

12.34.4.21 KIM_SPECIES_NAME_Cl

`KIM_SpeciesName` const KIM_SPECIES_NAME_Cl

12.34.4.22 KIM_SPECIES_NAME_Cm

`KIM_SpeciesName` const KIM_SPECIES_NAME_Cm

12.34.4.23 KIM_SPECIES_NAME_Cn

`KIM_SpeciesName` const KIM_SPECIES_NAME_Cn

12.34.4.24 KIM_SPECIES_NAME_Co

`KIM_SpeciesName` const KIM_SPECIES_NAME_Co

12.34.4.25 KIM_SPECIES_NAME_Cr

`KIM_SpeciesName` const KIM_SPECIES_NAME_Cr

12.34.4.26 KIM_SPECIES_NAME-Cs

`KIM_SpeciesName` const KIM_SPECIES_NAME-Cs

12.34.4.27 KIM_SPECIES_NAME_Cu

`KIM_SpeciesName` const KIM_SPECIES_NAME_Cu

12.34.4.28 KIM_SPECIES_NAME_Db

`KIM_SpeciesName` const KIM_SPECIES_NAME_Db

12.34.4.29 KIM_SPECIES_NAME_Ds

`KIM_SpeciesName` const KIM_SPECIES_NAME_Ds

12.34.4.30 KIM_SPECIES_NAME_Dy

`KIM_SpeciesName` const KIM_SPECIES_NAME_Dy

12.34.4.31 KIM_SPECIES_NAME_electron

`KIM_SpeciesName` const KIM_SPECIES_NAME_electron

12.34.4.32 KIM_SPECIES_NAME_Er

`KIM_SpeciesName` const KIM_SPECIES_NAME_Er

12.34.4.33 KIM_SPECIES_NAME_Es

`KIM_SpeciesName` const KIM_SPECIES_NAME_Es

12.34.4.34 KIM_SPECIES_NAME_Eu

`KIM_SpeciesName` const KIM_SPECIES_NAME_Eu

12.34.4.35 KIM_SPECIES_NAME_F

`KIM_SpeciesName` const KIM_SPECIES_NAME_F

12.34.4.36 KIM_SPECIES_NAME_Fe

`KIM_SpeciesName` const KIM_SPECIES_NAME_Fe

12.34.4.37 KIM_SPECIES_NAME_Fl

`KIM_SpeciesName` const KIM_SPECIES_NAME_Fl

12.34.4.38 KIM_SPECIES_NAME_Fm

`KIM_SpeciesName` const KIM_SPECIES_NAME_Fm

12.34.4.39 KIM_SPECIES_NAME_Fr

`KIM_SpeciesName` const KIM_SPECIES_NAME_Fr

12.34.4.40 KIM_SPECIES_NAME_Ga

`KIM_SpeciesName` const KIM_SPECIES_NAME_Ga

12.34.4.41 KIM_SPECIES_NAME_Gd

`KIM_SpeciesName` const KIM_SPECIES_NAME_Gd

12.34.4.42 KIM_SPECIES_NAME_Ge

`KIM_SpeciesName` const KIM_SPECIES_NAME_Ge

12.34.4.43 KIM_SPECIES_NAME_H

`KIM_SpeciesName` const KIM_SPECIES_NAME_H

12.34.4.44 KIM_SPECIES_NAME_He

`KIM_SpeciesName` const KIM_SPECIES_NAME_He

12.34.4.45 KIM_SPECIES_NAME_Hf

`KIM_SpeciesName` const KIM_SPECIES_NAME_Hf

12.34.4.46 KIM_SPECIES_NAME_Hg

`KIM_SpeciesName` const KIM_SPECIES_NAME_Hg

12.34.4.47 KIM_SPECIES_NAME_Ho

`KIM_SpeciesName` const KIM_SPECIES_NAME_Ho

12.34.4.48 KIM_SPECIES_NAME_Hs

`KIM_SpeciesName` const KIM_SPECIES_NAME_Hs

12.34.4.49 KIM_SPECIES_NAME_I

`KIM_SpeciesName` const KIM_SPECIES_NAME_I

12.34.4.50 KIM_SPECIES_NAME_In

`KIM_SpeciesName` const KIM_SPECIES_NAME_In

12.34.4.51 KIM_SPECIES_NAME_Ir

`KIM_SpeciesName` const KIM_SPECIES_NAME_Ir

12.34.4.52 KIM_SPECIES_NAME_K

`KIM_SpeciesName` const KIM_SPECIES_NAME_K

12.34.4.53 KIM_SPECIES_NAME_Kr

`KIM_SpeciesName` const KIM_SPECIES_NAME_Kr

12.34.4.54 KIM_SPECIES_NAME_La

`KIM_SpeciesName` const KIM_SPECIES_NAME_La

12.34.4.55 KIM_SPECIES_NAME_Li

`KIM_SpeciesName` const KIM_SPECIES_NAME_Li

12.34.4.56 KIM_SPECIES_NAME_Lr

`KIM_SpeciesName` const KIM_SPECIES_NAME_Lr

12.34.4.57 KIM_SPECIES_NAME_Lu

`KIM_SpeciesName` const KIM_SPECIES_NAME_Lu

12.34.4.58 KIM_SPECIES_NAME_Lv

`KIM_SpeciesName` const KIM_SPECIES_NAME_Lv

12.34.4.59 KIM_SPECIES_NAME_Md

`KIM_SpeciesName` const KIM_SPECIES_NAME_Md

12.34.4.60 KIM_SPECIES_NAME_Mg

`KIM_SpeciesName` const KIM_SPECIES_NAME_Mg

12.34.4.61 KIM_SPECIES_NAME_Mn

`KIM_SpeciesName` const KIM_SPECIES_NAME_Mn

12.34.4.62 KIM_SPECIES_NAME_Mo

`KIM_SpeciesName` const KIM_SPECIES_NAME_Mo

12.34.4.63 KIM_SPECIES_NAME_Mt

`KIM_SpeciesName` const KIM_SPECIES_NAME_Mt

12.34.4.64 KIM_SPECIES_NAME_N

`KIM_SpeciesName` const KIM_SPECIES_NAME_N

12.34.4.65 KIM_SPECIES_NAME_Na

`KIM_SpeciesName` const KIM_SPECIES_NAME_Na

12.34.4.66 KIM_SPECIES_NAME_Nb

`KIM_SpeciesName` const KIM_SPECIES_NAME_Nb

12.34.4.67 KIM_SPECIES_NAME_Nd

`KIM_SpeciesName` const KIM_SPECIES_NAME_Nd

12.34.4.68 KIM_SPECIES_NAME_Ne

`KIM_SpeciesName` const KIM_SPECIES_NAME_Ne

12.34.4.69 KIM_SPECIES_NAME_Ni

`KIM_SpeciesName` const KIM_SPECIES_NAME_Ni

12.34.4.70 KIM_SPECIES_NAME_No

`KIM_SpeciesName` const KIM_SPECIES_NAME_No

12.34.4.71 KIM_SPECIES_NAME_Np

`KIM_SpeciesName` const KIM_SPECIES_NAME_Np

12.34.4.72 KIM_SPECIES_NAME_O

`KIM_SpeciesName` const KIM_SPECIES_NAME_O

12.34.4.73 KIM_SPECIES_NAME_Os

`KIM_SpeciesName` const KIM_SPECIES_NAME_Os

12.34.4.74 KIM_SPECIES_NAME_P

`KIM_SpeciesName` const KIM_SPECIES_NAME_P

12.34.4.75 KIM_SPECIES_NAME_Pa

`KIM_SpeciesName` const KIM_SPECIES_NAME_Pa

12.34.4.76 KIM_SPECIES_NAME_Pb

`KIM_SpeciesName` const KIM_SPECIES_NAME_Pb

12.34.4.77 KIM_SPECIES_NAME_Pd

`KIM_SpeciesName` const KIM_SPECIES_NAME_Pd

12.34.4.78 KIM_SPECIES_NAME_Pm

`KIM_SpeciesName` const KIM_SPECIES_NAME_Pm

12.34.4.79 KIM_SPECIES_NAME_Po

`KIM_SpeciesName` const KIM_SPECIES_NAME_Po

12.34.4.80 KIM_SPECIES_NAME_Pr

`KIM_SpeciesName` const KIM_SPECIES_NAME_Pr

12.34.4.81 KIM_SPECIES_NAME_Pt

`KIM_SpeciesName` const KIM_SPECIES_NAME_Pt

12.34.4.82 KIM_SPECIES_NAME_Pu

`KIM_SpeciesName` const KIM_SPECIES_NAME_Pu

12.34.4.83 KIM_SPECIES_NAME_Ra

`KIM_SpeciesName` const KIM_SPECIES_NAME_Ra

12.34.4.84 KIM_SPECIES_NAME_Rb

`KIM_SpeciesName` const KIM_SPECIES_NAME_Rb

12.34.4.85 KIM_SPECIES_NAME_Re

`KIM_SpeciesName` const KIM_SPECIES_NAME_Re

12.34.4.86 KIM_SPECIES_NAME_Rf

`KIM_SpeciesName` const KIM_SPECIES_NAME_Rf

12.34.4.87 KIM_SPECIES_NAME_Rg

`KIM_SpeciesName` const KIM_SPECIES_NAME_Rg

12.34.4.88 KIM_SPECIES_NAME_Rh

`KIM_SpeciesName` const KIM_SPECIES_NAME_Rh

12.34.4.89 KIM_SPECIES_NAME_Rn

`KIM_SpeciesName` const KIM_SPECIES_NAME_Rn

12.34.4.90 KIM_SPECIES_NAME_Ru

`KIM_SpeciesName` const KIM_SPECIES_NAME_Ru

12.34.4.91 KIM_SPECIES_NAME_S

`KIM_SpeciesName` const KIM_SPECIES_NAME_S

12.34.4.92 KIM_SPECIES_NAME_Sb

`KIM_SpeciesName` const KIM_SPECIES_NAME_Sb

12.34.4.93 KIM_SPECIES_NAME_Sc

`KIM_SpeciesName` const KIM_SPECIES_NAME_Sc

12.34.4.94 KIM_SPECIES_NAME_Se

`KIM_SpeciesName` const KIM_SPECIES_NAME_Se

12.34.4.95 KIM_SPECIES_NAME_Sg

`KIM_SpeciesName` const KIM_SPECIES_NAME_Sg

12.34.4.96 KIM_SPECIES_NAME_Si

`KIM_SpeciesName` const KIM_SPECIES_NAME_Si

12.34.4.97 KIM_SPECIES_NAME_Sm

`KIM_SpeciesName` const KIM_SPECIES_NAME_Sm

12.34.4.98 KIM_SPECIES_NAME_Sn

`KIM_SpeciesName` const KIM_SPECIES_NAME_Sn

12.34.4.99 KIM_SPECIES_NAME_Sr

`KIM_SpeciesName` const KIM_SPECIES_NAME_Sr

12.34.4.100 KIM_SPECIES_NAME-Ta

`KIM_SpeciesName` const KIM_SPECIES_NAME-Ta

12.34.4.101 KIM_SPECIES_NAME_Tb

`KIM_SpeciesName` const KIM_SPECIES_NAME_Tb

12.34.4.102 KIM_SPECIES_NAME_Tc

`KIM_SpeciesName` const KIM_SPECIES_NAME_Tc

12.34.4.103 KIM_SPECIES_NAME_Te

`KIM_SpeciesName` const KIM_SPECIES_NAME_Te

12.34.4.104 KIM_SPECIES_NAME_Th

`KIM_SpeciesName` const KIM_SPECIES_NAME_Th

12.34.4.105 KIM_SPECIES_NAME_Ti

`KIM_SpeciesName` const KIM_SPECIES_NAME_Ti

12.34.4.106 KIM_SPECIES_NAME_Tl

`KIM_SpeciesName` const KIM_SPECIES_NAME_Tl

12.34.4.107 KIM_SPECIES_NAME_Tm

`KIM_SpeciesName` const KIM_SPECIES_NAME_Tm

12.34.4.108 KIM_SPECIES_NAME_U

`KIM_SpeciesName` const KIM_SPECIES_NAME_U

12.34.4.109 KIM_SPECIES_NAME_user01

`KIM_SpeciesName` const KIM_SPECIES_NAME_user01

12.34.4.110 KIM_SPECIES_NAME_user02

`KIM_SpeciesName` const KIM_SPECIES_NAME_user02

12.34.4.111 KIM_SPECIES_NAME_user03

`KIM_SpeciesName` const KIM_SPECIES_NAME_user03

12.34.4.112 KIM_SPECIES_NAME_user04

`KIM_SpeciesName` const KIM_SPECIES_NAME_user04

12.34.4.113 KIM_SPECIES_NAME_user05

`KIM_SpeciesName` const KIM_SPECIES_NAME_user05

12.34.4.114 KIM_SPECIES_NAME_user06

`KIM_SpeciesName` const KIM_SPECIES_NAME_user06

12.34.4.115 KIM_SPECIES_NAME_user07

`KIM_SpeciesName` const KIM_SPECIES_NAME_user07

12.34.4.116 KIM_SPECIES_NAME_user08

`KIM_SpeciesName` const KIM_SPECIES_NAME_user08

12.34.4.117 KIM_SPECIES_NAME_user09

`KIM_SpeciesName` const KIM_SPECIES_NAME_user09

12.34.4.118 KIM_SPECIES_NAME_user10

`KIM_SpeciesName` const KIM_SPECIES_NAME_user10

12.34.4.119 KIM_SPECIES_NAME_user11

`KIM_SpeciesName` const KIM_SPECIES_NAME_user11

12.34.4.120 KIM_SPECIES_NAME_user12

`KIM_SpeciesName` const KIM_SPECIES_NAME_user12

12.34.4.121 KIM_SPECIES_NAME_user13

`KIM_SpeciesName` const KIM_SPECIES_NAME_user13

12.34.4.122 KIM_SPECIES_NAME_user14

`KIM_SpeciesName` const KIM_SPECIES_NAME_user14

12.34.4.123 KIM_SPECIES_NAME_user15

`KIM_SpeciesName` const KIM_SPECIES_NAME_user15

12.34.4.124 KIM_SPECIES_NAME_user16

`KIM_SpeciesName` const KIM_SPECIES_NAME_user16

12.34.4.125 KIM_SPECIES_NAME_user17

`KIM_SpeciesName` const KIM_SPECIES_NAME_user17

12.34.4.126 KIM_SPECIES_NAME_user18

`KIM_SpeciesName` const KIM_SPECIES_NAME_user18

12.34.4.127 KIM_SPECIES_NAME_user19

`KIM_SpeciesName` const KIM_SPECIES_NAME_user19

12.34.4.128 KIM_SPECIES_NAME_user20

`KIM_SpeciesName` const KIM_SPECIES_NAME_user20

12.34.4.129 KIM_SPECIES_NAME_Uuo

`KIM_SpeciesName` const KIM_SPECIES_NAME_Uuo

12.34.4.130 KIM_SPECIES_NAME_Uup

`KIM_SpeciesName` const KIM_SPECIES_NAME_Uup

12.34.4.131 KIM_SPECIES_NAME_Uus

`KIM_SpeciesName` const KIM_SPECIES_NAME_Uus

12.34.4.132 KIM_SPECIES_NAME_Uut

`KIM_SpeciesName` const KIM_SPECIES_NAME_Uut

12.34.4.133 KIM_SPECIES_NAME_V

`KIM_SpeciesName` const KIM_SPECIES_NAME_V

12.34.4.134 KIM_SPECIES_NAME_W

`KIM_SpeciesName` const KIM_SPECIES_NAME_W

12.34.4.135 KIM_SPECIES_NAME_Xe

`KIM_SpeciesName` const KIM_SPECIES_NAME_Xe

12.34.4.136 KIM_SPECIES_NAME_Y

`KIM_SpeciesName` const KIM_SPECIES_NAME_Y

12.34.4.137 KIM_SPECIES_NAME_Yb

`KIM_SpeciesName` const KIM_SPECIES_NAME_Yb

12.34.4.138 KIM_SPECIES_NAME_Zn

`KIM_SpeciesName` const KIM_SPECIES_NAME_Zn

12.34.4.139 KIM_SPECIES_NAME_Zr

```
KIM_SpeciesName const KIM_SPECIES_NAME_Zr
```

12.35 kim-api-v2.0.0-beta.0/c/include/KIM_SupportStatus.h File Reference

Classes

- struct [KIM_SupportStatus](#)

Macros

- `#define` [KIM_SUPPORT_STATUS_DEFINED_](#)

Typedefs

- typedef struct [KIM_SupportStatus](#) [KIM_SupportStatus](#)

Functions

- [KIM_SupportStatus KIM_SupportStatus_FromString](#) (char const *const str)
- int [KIM_SupportStatus_Equal](#) (KIM_SupportStatus const left, [KIM_SupportStatus](#) const right)
- int [KIM_SupportStatus_NotEqual](#) (KIM_SupportStatus const left, [KIM_SupportStatus](#) const right)
- char const *const [KIM_SupportStatus_String](#) (KIM_SupportStatus const supportStatus)
- void [KIM_SUPPORT_STATUS_GetNumberOfSupportStatuses](#) (int *const numberOfSupportStatuses)
- int [KIM_SUPPORT_STATUS_GetSupportStatus](#) (int const index, [KIM_SupportStatus](#) *const supportStatus)

Variables

- [KIM_SupportStatus](#) const [KIM_SUPPORT_STATUS_requiredByAPI](#)
- [KIM_SupportStatus](#) const [KIM_SUPPORT_STATUS_notSupported](#)
- [KIM_SupportStatus](#) const [KIM_SUPPORT_STATUS_required](#)
- [KIM_SupportStatus](#) const [KIM_SUPPORT_STATUS_optional](#)

12.35.1 Macro Definition Documentation

12.35.1.1 KIM_SUPPORT_STATUS_DEFINED_

```
#define KIM_SUPPORT_STATUS_DEFINED_
```

Definition at line 44 of file [KIM_SupportStatus.h](#).

12.35.2 Typedef Documentation

12.35.2.1 KIM_SupportStatus

```
typedef struct KIM_SupportStatus KIM_SupportStatus
```

Definition at line 45 of file KIM_SupportStatus.h.

12.35.3 Function Documentation

12.35.3.1 KIM_SUPPORT_STATUS_GetNumberOfSupportStatuses()

```
void KIM_SUPPORT_STATUS_GetNumberOfSupportStatuses (
    int *const numberOfSupportStatuses )
```

12.35.3.2 KIM_SUPPORT_STATUS_GetSupportStatus()

```
int KIM_SUPPORT_STATUS_GetSupportStatus (
    int const index,
    KIM_SupportStatus *const supportStatus )
```

12.35.3.3 KIM_SupportStatus_Equal()

```
int KIM_SupportStatus_Equal (
    KIM_SupportStatus const left,
    KIM_SupportStatus const right )
```

12.35.3.4 KIM_SupportStatus_FromString()

```
KIM_SupportStatus KIM_SupportStatus_FromString (
    char const *const str )
```

12.35.3.5 KIM_SupportStatus_NotEqual()

```
int KIM_SupportStatus_NotEqual (
    KIM_SupportStatus const left,
    KIM_SupportStatus const right )
```

12.35.3.6 KIM_SupportStatus_String()

```
char const* const KIM_SupportStatus_String (
    KIM_SupportStatus const supportStatus )
```

12.35.4 Variable Documentation

12.35.4.1 KIM_SUPPORT_STATUS_notSupported

```
KIM_SupportStatus const KIM_SUPPORT_STATUS_notSupported
```

12.35.4.2 KIM_SUPPORT_STATUS_optional

```
KIM_SupportStatus const KIM_SUPPORT_STATUS_optional
```

12.35.4.3 KIM_SUPPORT_STATUS_required

```
KIM_SupportStatus const KIM_SUPPORT_STATUS_required
```

12.35.4.4 KIM_SUPPORT_STATUS_requiredByAPI

```
KIM_SupportStatus const KIM_SUPPORT_STATUS_requiredByAPI
```

12.36 kim-api-v2.0.0-beta.0/c/include/KIM_TemperatureUnit.h File Reference

Classes

- struct [KIM_TemperatureUnit](#)

Macros

- `#define KIM_TEMPERATURE_UNIT_DEFINED_`

Typedefs

- `typedef struct KIM_TemperatureUnit KIM_TemperatureUnit`

Functions

- `KIM_TemperatureUnit KIM_TemperatureUnit_FromString` (char const *const str)
- `int KIM_TemperatureUnit_Equal` (KIM_TemperatureUnit const left, KIM_TemperatureUnit const right)
- `int KIM_TemperatureUnit_NotEqual` (KIM_TemperatureUnit const left, KIM_TemperatureUnit const right)
- `char const *const KIM_TemperatureUnit_String` (KIM_TemperatureUnit const temperatureUnit)
- `void KIM_TEMPERATURE_UNIT_GetNumberOfTemperatureUnits` (int *const numberOfTemperatureUnits)
- `int KIM_TEMPERATURE_UNIT_GetTemperatureUnit` (int const index, KIM_TemperatureUnit *const temperatureUnit)

Variables

- `KIM_TemperatureUnit const KIM_TEMPERATURE_UNIT_unused`
- `KIM_TemperatureUnit const KIM_TEMPERATURE_UNIT_K`

12.36.1 Macro Definition Documentation

12.36.1.1 KIM_TEMPERATURE_UNIT_DEFINED_

```
#define KIM_TEMPERATURE_UNIT_DEFINED_
```

Definition at line 44 of file KIM_TemperatureUnit.h.

12.36.2 Typedef Documentation

12.36.2.1 KIM_TemperatureUnit

```
typedef struct KIM_TemperatureUnit KIM_TemperatureUnit
```

Definition at line 45 of file KIM_TemperatureUnit.h.

12.36.3 Function Documentation

12.36.3.1 KIM_TEMPERATURE_UNIT_GetNumberOfTemperatureUnits()

```
void KIM_TEMPERATURE_UNIT_GetNumberOfTemperatureUnits (
    int *const numberOfTemperatureUnits )
```

12.36.3.2 KIM_TEMPERATURE_UNIT_GetTemperatureUnit()

```
int KIM_TEMPERATURE_UNIT_GetTemperatureUnit (
    int const index,
    KIM_TemperatureUnit *const temperatureUnit )
```

12.36.3.3 KIM_TemperatureUnit_Equal()

```
int KIM_TemperatureUnit_Equal (
    KIM_TemperatureUnit const left,
    KIM_TemperatureUnit const right )
```

12.36.3.4 KIM_TemperatureUnit_FromString()

```
KIM_TemperatureUnit KIM_TemperatureUnit_FromString (
    char const *const str )
```

12.36.3.5 KIM_TemperatureUnit_NotEqual()

```
int KIM_TemperatureUnit_NotEqual (
    KIM_TemperatureUnit const left,
    KIM_TemperatureUnit const right )
```

12.36.3.6 KIM_TemperatureUnit_String()

```
char const* const KIM_TemperatureUnit_String (
    KIM_TemperatureUnit const temperatureUnit )
```

12.36.4 Variable Documentation

12.36.4.1 KIM_TEMPERATURE_UNIT_K

`KIM_TemperatureUnit` const KIM_TEMPERATURE_UNIT_K

12.36.4.2 KIM_TEMPERATURE_UNIT_unused

`KIM_TemperatureUnit` const KIM_TEMPERATURE_UNIT_unused

12.37 kim-api-v2.0.0-beta.0/c/include/KIM_TimeUnit.h File Reference

Classes

- struct `KIM_TimeUnit`

Macros

- `#define KIM_TIME_UNIT_DEFINED_`

Typedefs

- typedef struct `KIM_TimeUnit` `KIM_TimeUnit`

Functions

- `KIM_TimeUnit KIM_TimeUnit_FromString` (char const *const str)
- int `KIM_TimeUnit_Equal` (KIM_TimeUnit const left, `KIM_TimeUnit` right)
- int `KIM_TimeUnit_NotEqual` (KIM_TimeUnit const left, `KIM_TimeUnit` right)
- char const *const `KIM_TimeUnit_String` (KIM_TimeUnit const timeUnit)
- void `KIM_TIME_UNIT_GetNumberOfTimeUnits` (int *const numberOfTimeUnits)
- int `KIM_TIME_UNIT_GetTimeUnit` (int const index, `KIM_TimeUnit` *const timeUnit)

Variables

- `KIM_TimeUnit` const `KIM_TIME_UNIT_unused`
- `KIM_TimeUnit` const `KIM_TIME_UNIT_fs`
- `KIM_TimeUnit` const `KIM_TIME_UNIT_ps`
- `KIM_TimeUnit` const `KIM_TIME_UNIT_ns`
- `KIM_TimeUnit` const `KIM_TIME_UNIT_s`

12.37.1 Macro Definition Documentation

12.37.1.1 KIM_TIME_UNIT_DEFINED_

```
#define KIM_TIME_UNIT_DEFINED_
```

Definition at line 44 of file KIM_TimeUnit.h.

12.37.2 Typedef Documentation

12.37.2.1 KIM_TimeUnit

```
typedef struct KIM_TimeUnit KIM_TimeUnit
```

Definition at line 45 of file KIM_TimeUnit.h.

12.37.3 Function Documentation

12.37.3.1 KIM_TIME_UNIT_GetNumberOfTimeUnits()

```
void KIM_TIME_UNIT_GetNumberOfTimeUnits (
    int *const numberOfTimeUnits )
```

12.37.3.2 KIM_TIME_UNIT_GetTimeUnit()

```
int KIM_TIME_UNIT_GetTimeUnit (
    int const index,
    KIM_TimeUnit *const timeUnit )
```

12.37.3.3 KIM_TimeUnit_Equal()

```
int KIM_TimeUnit_Equal (
    KIM_TimeUnit const left,
    KIM_TimeUnit right )
```

12.37.3.4 KIM_TimeUnit_FromString()

```
KIM_TimeUnit KIM_TimeUnit_FromString (
    char const *const str )
```

12.37.3.5 KIM_TimeUnit_NotEqual()

```
int KIM_TimeUnit_NotEqual (
    KIM_TimeUnit const left,
    KIM_TimeUnit right )
```

12.37.3.6 KIM_TimeUnit_String()

```
char const* const KIM_TimeUnit_String (
    KIM_TimeUnit const timeUnit )
```

12.37.4 Variable Documentation

12.37.4.1 KIM_TIME_UNIT_fs

```
KIM_TimeUnit const KIM_TIME_UNIT_fs
```

12.37.4.2 KIM_TIME_UNIT_ns

```
KIM_TimeUnit const KIM_TIME_UNIT_ns
```

12.37.4.3 KIM_TIME_UNIT_ps

```
KIM_TimeUnit const KIM_TIME_UNIT_ps
```

12.37.4.4 KIM_TIME_UNIT_s

```
KIM_TimeUnit const KIM_TIME_UNIT_s
```

12.37.4.5 KIM_TIME_UNIT_unused

```
KIM_TimeUnit const KIM_TIME_UNIT_unused
```

12.38 kim-api-v2.0.0-beta.0/c/include/KIM_UnitSystem.h File Reference

```
#include "KIM_LengthUnit.h"  
#include "KIM_EnergyUnit.h"  
#include "KIM_ChargeUnit.h"  
#include "KIM_TemperatureUnit.h"  
#include "KIM_TimeUnit.h"
```

12.39 kim-api-v2.0.0-beta.0/c/include/KIM_Version.h.tpl File Reference

12.40 kim-api-v2.0.0-beta.0/cpp/include/KIM_ChargeUnit.hpp File Reference

```
#include <string>
```

Classes

- class [KIM::ChargeUnit](#)
- struct [KIM::CHARGE_UNIT::Comparator](#)

Namespaces

- [KIM](#)
- [KIM::CHARGE_UNIT](#)

Functions

- void [KIM::CHARGE_UNIT::GetNumberOfChargeUnits](#) (int *const numberOfChargeUnits)
- int [KIM::CHARGE_UNIT::GetChargeUnit](#) (int const index, ChargeUnit *const chargeUnit)

Variables

- ChargeUnit const [KIM::CHARGE_UNIT::unused](#)
- ChargeUnit const [KIM::CHARGE_UNIT::C](#)
- ChargeUnit const [KIM::CHARGE_UNIT::e](#)
- ChargeUnit const [KIM::CHARGE_UNIT::statC](#)

12.41 kim-api-v2.0.0-beta.0/cpp/include/KIM_ChargeUnit.inc File Reference

12.42 kim-api-v2.0.0-beta.0/cpp/include/KIM_ComputeArgumentName.hpp File Reference

```
#include <string>
```

Classes

- class [KIM::ComputeArgumentName](#)
- struct [KIM::COMPUTE_ARGUMENT_NAME::Comparator](#)

Namespaces

- [KIM](#)
- [KIM::COMPUTE_ARGUMENT_NAME](#)

Functions

- void [KIM::COMPUTE_ARGUMENT_NAME::GetNumberOfComputeArgumentNames](#) (int *const number↔ OfComputeArgumentNames)
- int [KIM::COMPUTE_ARGUMENT_NAME::GetComputeArgumentName](#) (int const index, Compute↔ ArgumentName *const computeArgumentName)
- int [KIM::COMPUTE_ARGUMENT_NAME::GetComputeArgumentDataType](#) (ComputeArgumentName const computeArgumentName, DataType *const dataType)

Variables

- ComputeArgumentName const [KIM::COMPUTE_ARGUMENT_NAME::numberOfParticles](#)
- ComputeArgumentName const [KIM::COMPUTE_ARGUMENT_NAME::particleSpeciesCodes](#)
- ComputeArgumentName const [KIM::COMPUTE_ARGUMENT_NAME::particleContributing](#)
- ComputeArgumentName const [KIM::COMPUTE_ARGUMENT_NAME::coordinates](#)
- ComputeArgumentName const [KIM::COMPUTE_ARGUMENT_NAME::partialEnergy](#)
- ComputeArgumentName const [KIM::COMPUTE_ARGUMENT_NAME::partialForces](#)
- ComputeArgumentName const [KIM::COMPUTE_ARGUMENT_NAME::partialParticleEnergy](#)
- ComputeArgumentName const [KIM::COMPUTE_ARGUMENT_NAME::partialVirial](#)
- ComputeArgumentName const [KIM::COMPUTE_ARGUMENT_NAME::partialParticleVirial](#)

12.43 kim-api-v2.0.0-beta.0/cpp/include/KIM_ComputeArgumentName.inc File Reference

12.44 kim-api-v2.0.0-beta.0/cpp/include/KIM_ComputeArguments.hpp File Reference

```
#include <string>
#include "KIM_func.hpp"
```

Classes

- class [KIM::ComputeArguments](#)

Namespaces

- [KIM](#)

12.45 kim-api-v2.0.0-beta.0/cpp/include/KIM_ComputeCallbackName.hpp File Reference

```
#include <string>
```

Classes

- class [KIM::ComputeCallbackName](#)
- struct [KIM::COMPUTE_CALLBACK_NAME::Comparator](#)

Namespaces

- [KIM](#)
- [KIM::COMPUTE_CALLBACK_NAME](#)

Functions

- void [KIM::COMPUTE_CALLBACK_NAME::GetNumberOfComputeCallbackNames](#) (int *const numberOfComputeCallbackNames)
- int [KIM::COMPUTE_CALLBACK_NAME::GetComputeCallbackName](#) (int const index, ComputeCallbackName *const computeCallbackName)

Variables

- ComputeCallbackName const [KIM::COMPUTE_CALLBACK_NAME::GetNeighborList](#)
- ComputeCallbackName const [KIM::COMPUTE_CALLBACK_NAME::ProcessDEDrTerm](#)
- ComputeCallbackName const [KIM::COMPUTE_CALLBACK_NAME::ProcessD2EDr2Term](#)

12.46 kim-api-v2.0.0-beta.0/cpp/include/KIM_ComputeCallbackName.inc File Reference

12.47 kim-api-v2.0.0-beta.0/cpp/include/KIM_DataType.hpp File Reference

```
#include <string>
```

Classes

- class [KIM::DataType](#)
- struct [KIM::DATA_TYPE::Comparator](#)

Namespaces

- [KIM](#)
- [KIM::DATA_TYPE](#)

Functions

- void [KIM::DATA_TYPE::GetNumberOfDataTypes](#) (int *const numberOfDataTypes)
- int [KIM::DATA_TYPE::GetDataType](#) (int const index, DataType *const dataType)

Variables

- DataType const [KIM::DATA_TYPE::Integer](#)
- DataType const [KIM::DATA_TYPE::Double](#)

12.48 kim-api-v2.0.0-beta.0/cpp/include/KIM_DataType.inc File Reference

12.49 kim-api-v2.0.0-beta.0/cpp/include/KIM_EnergyUnit.hpp File Reference

```
#include <string>
```

Classes

- class [KIM::EnergyUnit](#)
- struct [KIM::ENERGY_UNIT::Comparator](#)

Namespaces

- [KIM](#)
- [KIM::ENERGY_UNIT](#)

Functions

- void [KIM::ENERGY_UNIT::GetNumberOfEnergyUnits](#) (int *const numberOfEnergyUnits)
- int [KIM::ENERGY_UNIT::GetEnergyUnit](#) (int const index, EnergyUnit *const energyUnit)

Variables

- EnergyUnit const [KIM::ENERGY_UNIT::unused](#)
- EnergyUnit const [KIM::ENERGY_UNIT::amu_A2_per_ps2](#)
- EnergyUnit const [KIM::ENERGY_UNIT::erg](#)
- EnergyUnit const [KIM::ENERGY_UNIT::eV](#)
- EnergyUnit const [KIM::ENERGY_UNIT::Hartree](#)
- EnergyUnit const [KIM::ENERGY_UNIT::J](#)
- EnergyUnit const [KIM::ENERGY_UNIT::kcal_mol](#)

12.50 kim-api-v2.0.0-beta.0/cpp/include/KIM_EnergyUnit.inc File Reference

12.51 kim-api-v2.0.0-beta.0/cpp/include/KIM_func.hpp File Reference

Namespaces

- [KIM](#)

Typedefs

- typedef void() [KIM::func\(\)](#)

12.52 kim-api-v2.0.0-beta.0/cpp/include/KIM_LanguageName.hpp File Reference

```
#include <string>
```

Classes

- class [KIM::LanguageName](#)
- struct [KIM::LANGUAGE_NAME::Comparator](#)

Namespaces

- [KIM](#)
- [KIM::LANGUAGE_NAME](#)

Functions

- void [KIM::LANGUAGE_NAME::GetNumberOfLanguageNames](#) (int *const numberOfLanguageNames)
- int [KIM::LANGUAGE_NAME::GetLanguageName](#) (int const index, LanguageName *const languageName)

Variables

- LanguageName const [KIM::LANGUAGE_NAME::cpp](#)
- LanguageName const [KIM::LANGUAGE_NAME::c](#)
- LanguageName const [KIM::LANGUAGE_NAME::fortran](#)

12.53 kim-api-v2.0.0-beta.0/cpp/include/KIM_LanguageName.inc File Reference

12.54 kim-api-v2.0.0-beta.0/cpp/include/KIM_LengthUnit.hpp File Reference

```
#include <string>
```

Classes

- class [KIM::LengthUnit](#)
- struct [KIM::LENGTH_UNIT::Comparator](#)

Namespaces

- [KIM](#)
- [KIM::LENGTH_UNIT](#)

Functions

- void [KIM::LENGTH_UNIT::GetNumberOfLengthUnits](#) (int *const numberOfLengthUnits)
- int [KIM::LENGTH_UNIT::GetLengthUnit](#) (int const index, LengthUnit *const lengthUnit)

Variables

- LengthUnit const [KIM::LENGTH_UNIT::unused](#)
- LengthUnit const [KIM::LENGTH_UNIT::A](#)
- LengthUnit const [KIM::LENGTH_UNIT::Bohr](#)
- LengthUnit const [KIM::LENGTH_UNIT::cm](#)
- LengthUnit const [KIM::LENGTH_UNIT::m](#)
- LengthUnit const [KIM::LENGTH_UNIT::nm](#)

12.55 kim-api-v2.0.0-beta.0/cpp/include/KIM_LengthUnit.inc File Reference

12.56 kim-api-v2.0.0-beta.0/cpp/include/KIM_Log.hpp File Reference

```
#include <string>
#include <sstream>
```

Classes

- class [KIM::Log](#)

Namespaces

- [KIM](#)

12.57 kim-api-v2.0.0-beta.0/cpp/include/KIM_LOG_DEFINES.inc File Reference

```
#include "KIM_LOG_MAXIMUM_LEVEL.inc"
```

12.58 kim-api-v2.0.0-beta.0/cpp/include/KIM_LogVerbosity.hpp File Reference

```
#include <string>
#include "KIM_LOG_DEFINES.inc"
```

Classes

- class [KIM::LogVerbosity](#)
- struct [KIM::LOG_VERBOSITY::Comparator](#)

Namespaces

- [KIM](#)
- [KIM::LOG_VERBOSITY](#)

Functions

- void [KIM::LOG_VERBOSITY::GetNumberOfLogVerbsities](#) (int *const numberOfLogVerbsities)
- int [KIM::LOG_VERBOSITY::GetLogVerbosity](#) (int const index, LogVerbosity *const logVerbosity)

Variables

- LogVerbosity const [KIM::LOG_VERBOSITY::silent](#)
- LogVerbosity const [KIM::LOG_VERBOSITY::fatal](#)
- LogVerbosity const [KIM::LOG_VERBOSITY::error](#)
- LogVerbosity const [KIM::LOG_VERBOSITY::warning](#)
- LogVerbosity const [KIM::LOG_VERBOSITY::information](#)
- LogVerbosity const [KIM::LOG_VERBOSITY::debug](#)

12.59 kim-api-v2.0.0-beta.0/cpp/include/KIM_Model.hpp File Reference

```
#include <string>
#include "KIM_func.hpp"
```

Classes

- class [KIM::Model](#)

Namespaces

- [KIM](#)

12.60 kim-api-v2.0.0-beta.0/cpp/include/KIM_ModelCompute.hpp File Reference

```
#include <string>
#include <sstream>
```

Classes

- class [KIM::ModelCompute](#)

Namespaces

- [KIM](#)

12.61 kim-api-v2.0.0-beta.0/cpp/include/KIM_ModelComputeArguments.hpp File Reference

```
#include <string>
#include <sstream>
```

Classes

- class [KIM::ModelComputeArguments](#)

Namespaces

- [KIM](#)

12.62 kim-api-v2.0.0-beta.0/cpp/include/KIM_ModelComputeArgumentsCreate.hpp File Reference

```
#include <string>
#include <sstream>
#include "KIM_func.hpp"
```

Classes

- class [KIM::ModelComputeArgumentsCreate](#)

Namespaces

- [KIM](#)

12.63 kim-api-v2.0.0-beta.0/cpp/include/KIM_ModelComputeArgumentsCreateLogMacros.hpp File Reference

Macros

- #define [FATAL_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_FATAL_)
- #define [LOG_FATAL](#)(message)
- #define [ERROR_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_ERROR_)
- #define [LOG_ERROR](#)(message)
- #define [WARNING_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_WARNING_↵
_)
- #define [LOG_WARNING](#)(message)
- #define [INFORMATION_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_INFO_↵
RMATION_)
- #define [LOG_INFORMATION](#)(message)
- #define [DEBUG_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_DEBUG_)
- #define [LOG_DEBUG](#)(message)

12.63.1 Macro Definition Documentation

12.63.1.1 DEBUG_VERBOSITY

```
#define DEBUG_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_DEBUG_)
```

Definition at line 87 of file KIM_ModelComputeArgumentsCreateLogMacros.hpp.

12.63.1.2 ERROR_VERBOSITY

```
#define ERROR_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_ERROR_)
```

Definition at line 48 of file KIM_ModelComputeArgumentsCreateLogMacros.hpp.

12.63.1.3 FATAL_VERBOSITY

```
#define FATAL_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_FATAL_)
```

Definition at line 35 of file KIM_ModelComputeArgumentsCreateLogMacros.hpp.

12.63.1.4 INFORMATION_VERBOSITY

```
#define INFORMATION_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_INFORMATION_)
```

Definition at line 74 of file KIM_ModelComputeArgumentsCreateLogMacros.hpp.

12.63.1.5 LOG_DEBUG

```
#define LOG_DEBUG(  
    message )
```

Value:

```
modelComputeArgumentsCreate->LogEntry(KIM::LOG_VERBOSITY::debug, message, \  
    __LINE__, __FILE__)
```

Definition at line 92 of file KIM_ModelComputeArgumentsCreateLogMacros.hpp.

12.63.1.6 LOG_ERROR

```
#define LOG_ERROR(  
    message )
```

Value:

```
modelComputeArgumentsCreate->LogEntry(KIM::LOG_VERBOSITY::error, message, \  
    __LINE__, __FILE__)
```

Definition at line 53 of file KIM_ModelComputeArgumentsCreateLogMacros.hpp.

12.63.1.7 LOG_FATAL

```
#define LOG_FATAL(  
    message )
```

Value:

```
modelComputeArgumentsCreate->LogEntry(KIM::LOG\_VERBOSITY::fatal, message, \  
    __LINE__, __FILE__)
```

Definition at line 40 of file KIM_ModelComputeArgumentsCreateLogMacros.hpp.

12.63.1.8 LOG_INFORMATION

```
#define LOG_INFORMATION(  
    message )
```

Value:

```
modelComputeArgumentsCreate->LogEntry(KIM::LOG\_VERBOSITY::information, \  
    message, __LINE__, __FILE__)
```

Definition at line 79 of file KIM_ModelComputeArgumentsCreateLogMacros.hpp.

12.63.1.9 LOG_WARNING

```
#define LOG_WARNING(  
    message )
```

Value:

```
modelComputeArgumentsCreate->LogEntry(KIM::LOG\_VERBOSITY::warning, message, \  
    __LINE__, __FILE__)
```

Definition at line 66 of file KIM_ModelComputeArgumentsCreateLogMacros.hpp.

12.63.1.10 WARNING_VERBOSITY

```
#define WARNING_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_WARNING_)
```

Definition at line 61 of file KIM_ModelComputeArgumentsCreateLogMacros.hpp.

12.64 kim-api-v2.0.0-beta.0/cpp/include/KIM_ModelComputeArgumentsDestroy.hpp File Reference

```
#include <string>
#include <sstream>
```

Classes

- class [KIM::ModelComputeArgumentsDestroy](#)

Namespaces

- [KIM](#)

12.65 kim-api-v2.0.0-beta.0/cpp/include/KIM_ModelComputeArgumentsDestroyLogMacros.hpp File Reference

Macros

- #define [FATAL_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_FATAL_)
- #define [LOG_FATAL](#)(message)
- #define [ERROR_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_ERROR_)
- #define [LOG_ERROR](#)(message)
- #define [WARNING_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_WARNING_)
- #define [LOG_WARNING](#)(message)
- #define [INFORMATION_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_INFORMATION_)
- #define [LOG_INFORMATION](#)(message)
- #define [DEBUG_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_DEBUG_)
- #define [LOG_DEBUG](#)(message)

12.65.1 Macro Definition Documentation

12.65.1.1 DEBUG_VERBOSITY

```
#define DEBUG_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_DEBUG_)
```

Definition at line 87 of file KIM_ModelComputeArgumentsDestroyLogMacros.hpp.

12.65.1.2 ERROR_VERBOSITY

```
#define ERROR_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_ERROR_)
```

Definition at line 48 of file KIM_ModelComputeArgumentsDestroyLogMacros.hpp.

12.65.1.3 FATAL_VERBOSITY

```
#define FATAL_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_FATAL_)
```

Definition at line 35 of file KIM_ModelComputeArgumentsDestroyLogMacros.hpp.

12.65.1.4 INFORMATION_VERBOSITY

```
#define INFORMATION_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_INFORMATION_)
```

Definition at line 74 of file KIM_ModelComputeArgumentsDestroyLogMacros.hpp.

12.65.1.5 LOG_DEBUG

```
#define LOG_DEBUG(  
    message )
```

Value:

```
modelComputeArgumentsDestroy->LogEntry(KIM::LOG_VERBOSITY::debug, message, \  
    __LINE__, __FILE__)
```

Definition at line 92 of file KIM_ModelComputeArgumentsDestroyLogMacros.hpp.

12.65.1.6 LOG_ERROR

```
#define LOG_ERROR(  
    message )
```

Value:

```
modelComputeArgumentsDestroy->LogEntry(KIM::LOG_VERBOSITY::error, message, \  
    __LINE__, __FILE__)
```

Definition at line 53 of file KIM_ModelComputeArgumentsDestroyLogMacros.hpp.

12.65.1.7 LOG_FATAL

```
#define LOG_FATAL(  
    message )
```

Value:

```
modelComputeArgumentsDestroy->LogEntry (KIM::LOG_VERBOSITY::fatal, message, \  
    __LINE__, __FILE__)
```

Definition at line 40 of file KIM_ModelComputeArgumentsDestroyLogMacros.hpp.

12.65.1.8 LOG_INFORMATION

```
#define LOG_INFORMATION(  
    message )
```

Value:

```
modelComputeArgumentsDestroy->LogEntry (KIM::LOG_VERBOSITY::information, \  
    message, __LINE__, __FILE__)
```

Definition at line 79 of file KIM_ModelComputeArgumentsDestroyLogMacros.hpp.

12.65.1.9 LOG_WARNING

```
#define LOG_WARNING(  
    message )
```

Value:

```
modelComputeArgumentsDestroy->LogEntry (KIM::LOG_VERBOSITY::warning, message, \  
    __LINE__, __FILE__)
```

Definition at line 66 of file KIM_ModelComputeArgumentsDestroyLogMacros.hpp.

12.65.1.10 WARNING_VERBOSITY

```
#define WARNING_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_WARNING_)
```

Definition at line 61 of file KIM_ModelComputeArgumentsDestroyLogMacros.hpp.

12.66 kim-api-v2.0.0-beta.0/cpp/include/KIM_ModelComputeArgumentsLogMacros.hpp File Reference

Macros

- `#define FATAL_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_FATAL_)`
- `#define LOG_FATAL(message)`
- `#define ERROR_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_ERROR_)`
- `#define LOG_ERROR(message)`
- `#define WARNING_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_WARNING_)`
- `#define LOG_WARNING(message)`
- `#define INFORMATION_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_INFORMATION_)`
- `#define LOG_INFORMATION(message)`
- `#define DEBUG_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_DEBUG_)`
- `#define LOG_DEBUG(message)`

12.66.1 Macro Definition Documentation

12.66.1.1 DEBUG_VERBOSITY

```
#define DEBUG_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_DEBUG_)
```

Definition at line 87 of file KIM_ModelComputeArgumentsLogMacros.hpp.

12.66.1.2 ERROR_VERBOSITY

```
#define ERROR_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_ERROR_)
```

Definition at line 48 of file KIM_ModelComputeArgumentsLogMacros.hpp.

12.66.1.3 FATAL_VERBOSITY

```
#define FATAL_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_FATAL_)
```

Definition at line 35 of file KIM_ModelComputeArgumentsLogMacros.hpp.

12.66.1.4 INFORMATION_VERBOSITY

```
#define INFORMATION_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_INFORMATION_)
```

Definition at line 74 of file KIM_ModelComputeArgumentsLogMacros.hpp.

12.66.1.5 LOG_DEBUG

```
#define LOG_DEBUG(  
    message )
```

Value:

```
modelComputeArguments->LogEntry(KIM::LOG_VERBOSITY::debug, message, \  
    __LINE__, __FILE__)
```

Definition at line 92 of file KIM_ModelComputeArgumentsLogMacros.hpp.

12.66.1.6 LOG_ERROR

```
#define LOG_ERROR(  
    message )
```

Value:

```
modelComputeArguments->LogEntry(KIM::LOG_VERBOSITY::error, message, \  
    __LINE__, __FILE__)
```

Definition at line 53 of file KIM_ModelComputeArgumentsLogMacros.hpp.

12.66.1.7 LOG_FATAL

```
#define LOG_FATAL(  
    message )
```

Value:

```
modelComputeArguments->LogEntry(KIM::LOG_VERBOSITY::fatal, message, \  
    __LINE__, __FILE__)
```

Definition at line 40 of file KIM_ModelComputeArgumentsLogMacros.hpp.

12.66.1.8 LOG_INFORMATION

```
#define LOG_INFORMATION(  
    message )
```

Value:

```
modelComputeArguments->LogEntry (KIM::LOG_VERBOSITY::information, message, \  
    __LINE__, __FILE__)
```

Definition at line 79 of file KIM_ModelComputeArgumentsLogMacros.hpp.

12.66.1.9 LOG_WARNING

```
#define LOG_WARNING(  
    message )
```

Value:

```
modelComputeArguments->LogEntry (KIM::LOG_VERBOSITY::warning, message, \  
    __LINE__, __FILE__)
```

Definition at line 66 of file KIM_ModelComputeArgumentsLogMacros.hpp.

12.66.1.10 WARNING_VERBOSITY

```
#define WARNING_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_WARNING_)
```

Definition at line 61 of file KIM_ModelComputeArgumentsLogMacros.hpp.

12.67 kim-api-v2.0.0-beta.0/cpp/include/KIM_ModelComputeLogMacros.hpp File Reference

Macros

- #define [FATAL_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_FATAL_)
- #define [LOG_FATAL](#)(message)
- #define [ERROR_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_ERROR_)
- #define [LOG_ERROR](#)(message)
- #define [WARNING_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_WARNING_)
- #define [LOG_WARNING](#)(message)
- #define [INFORMATION_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_INFORMATION_)
- #define [LOG_INFORMATION](#)(message)
- #define [DEBUG_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_DEBUG_)
- #define [LOG_DEBUG](#)(message)

12.67.1 Macro Definition Documentation

12.67.1.1 DEBUG_VERBOSITY

```
#define DEBUG_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_DEBUG_)
```

Definition at line 87 of file KIM_ModelComputeLogMacros.hpp.

12.67.1.2 ERROR_VERBOSITY

```
#define ERROR_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_ERROR_)
```

Definition at line 48 of file KIM_ModelComputeLogMacros.hpp.

12.67.1.3 FATAL_VERBOSITY

```
#define FATAL_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_FATAL_)
```

Definition at line 35 of file KIM_ModelComputeLogMacros.hpp.

12.67.1.4 INFORMATION_VERBOSITY

```
#define INFORMATION_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_INFORMATION_)
```

Definition at line 74 of file KIM_ModelComputeLogMacros.hpp.

12.67.1.5 LOG_DEBUG

```
#define LOG_DEBUG(  
    message )
```

Value:

```
modelCompute->LogEntry (KIM::LOG_VERBOSITY::debug, message, \n    __LINE__, __FILE__)
```

Definition at line 92 of file KIM_ModelComputeLogMacros.hpp.

12.67.1.6 LOG_ERROR

```
#define LOG_ERROR(  
    message )
```

Value:

```
modelCompute->LogEntry (KIM::LOG_VERBOSITY::error, message, \  
    __LINE__, __FILE__)
```

Definition at line 53 of file KIM_ModelComputeLogMacros.hpp.

12.67.1.7 LOG_FATAL

```
#define LOG_FATAL(  
    message )
```

Value:

```
modelCompute->LogEntry (KIM::LOG_VERBOSITY::fatal, message, \  
    __LINE__, __FILE__)
```

Definition at line 40 of file KIM_ModelComputeLogMacros.hpp.

12.67.1.8 LOG_INFORMATION

```
#define LOG_INFORMATION(  
    message )
```

Value:

```
modelCompute->LogEntry (KIM::LOG_VERBOSITY::information, message, \  
    __LINE__, __FILE__)
```

Definition at line 79 of file KIM_ModelComputeLogMacros.hpp.

12.67.1.9 LOG_WARNING

```
#define LOG_WARNING(  
    message )
```

Value:

```
modelCompute->LogEntry (KIM::LOG_VERBOSITY::warning, message, \  
    __LINE__, __FILE__)
```

Definition at line 66 of file KIM_ModelComputeLogMacros.hpp.

12.67.1.10 WARNING_VERBOSITY

```
#define WARNING_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_WARNING_)
```

Definition at line 61 of file KIM_ModelComputeLogMacros.hpp.

12.68 kim-api-v2.0.0-beta.0/cpp/include/KIM_ModelCreate.hpp File Reference

```
#include <string>
#include <sstream>
#include "KIM_func.hpp"
```

Classes

- class [KIM::ModelCreate](#)

Namespaces

- [KIM](#)

12.69 kim-api-v2.0.0-beta.0/cpp/include/KIM_ModelCreateLogMacros.hpp File Reference

Macros

- #define [FATAL_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_FATAL_)
- #define [LOG_FATAL](#)(message)
- #define [ERROR_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_ERROR_)
- #define [LOG_ERROR](#)(message)
- #define [WARNING_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_WARNING_)
- #define [LOG_WARNING](#)(message)
- #define [INFORMATION_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_INFORMATION_)
- #define [LOG_INFORMATION](#)(message)
- #define [DEBUG_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_DEBUG_)
- #define [LOG_DEBUG](#)(message)

12.69.1 Macro Definition Documentation

12.69.1.1 DEBUG_VERBOSITY

```
#define DEBUG_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_DEBUG_)
```

Definition at line 87 of file KIM_ModelCreateLogMacros.hpp.

12.69.1.2 ERROR_VERBOSITY

```
#define ERROR_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_ERROR_)
```

Definition at line 48 of file KIM_ModelCreateLogMacros.hpp.

12.69.1.3 FATAL_VERBOSITY

```
#define FATAL_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_FATAL_)
```

Definition at line 35 of file KIM_ModelCreateLogMacros.hpp.

12.69.1.4 INFORMATION_VERBOSITY

```
#define INFORMATION_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_INFORMATION_)
```

Definition at line 74 of file KIM_ModelCreateLogMacros.hpp.

12.69.1.5 LOG_DEBUG

```
#define LOG_DEBUG(  
    message )
```

Value:

```
modelCreate->LogEntry(KIM::LOG_VERBOSITY::debug, message, \n    __LINE__, __FILE__)
```

Definition at line 92 of file KIM_ModelCreateLogMacros.hpp.

12.69.1.6 LOG_ERROR

```
#define LOG_ERROR(  
    message )
```

Value:

```
modelCreate->LogEntry (KIM::LOG_VERBOSITY::error, message, \  
    __LINE__, __FILE__)
```

Definition at line 53 of file KIM_ModelCreateLogMacros.hpp.

12.69.1.7 LOG_FATAL

```
#define LOG_FATAL(  
    message )
```

Value:

```
modelCreate->LogEntry (KIM::LOG_VERBOSITY::fatal, message, \  
    __LINE__, __FILE__)
```

Definition at line 40 of file KIM_ModelCreateLogMacros.hpp.

12.69.1.8 LOG_INFORMATION

```
#define LOG_INFORMATION(  
    message )
```

Value:

```
modelCreate->LogEntry (KIM::LOG_VERBOSITY::information, message, \  
    __LINE__, __FILE__)
```

Definition at line 79 of file KIM_ModelCreateLogMacros.hpp.

12.69.1.9 LOG_WARNING

```
#define LOG_WARNING(  
    message )
```

Value:

```
modelCreate->LogEntry (KIM::LOG_VERBOSITY::warning, message, \  
    __LINE__, __FILE__)
```

Definition at line 66 of file KIM_ModelCreateLogMacros.hpp.

12.69.1.10 WARNING_VERBOSITY

```
#define WARNING_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_WARNING_)
```

Definition at line 61 of file KIM_ModelCreateLogMacros.hpp.

12.70 kim-api-v2.0.0-beta.0/cpp/include/KIM_ModelDestroy.hpp File Reference

```
#include <string>
#include <sstream>
```

Classes

- class [KIM::ModelDestroy](#)

Namespaces

- [KIM](#)

12.71 kim-api-v2.0.0-beta.0/cpp/include/KIM_ModelDestroyLogMacros.hpp File Reference

Macros

- #define [FATAL_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_FATAL_)
- #define [LOG_FATAL](#)(message)
- #define [ERROR_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_ERROR_)
- #define [LOG_ERROR](#)(message)
- #define [WARNING_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_WARNING_)
- #define [LOG_WARNING](#)(message)
- #define [INFORMATION_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_INFORMATION_)
- #define [LOG_INFORMATION](#)(message)
- #define [DEBUG_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_DEBUG_)
- #define [LOG_DEBUG](#)(message)

12.71.1 Macro Definition Documentation

12.71.1.1 DEBUG_VERBOSITY

```
#define DEBUG_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_DEBUG_)
```

Definition at line 87 of file KIM_ModelDestroyLogMacros.hpp.

12.71.1.2 ERROR_VERBOSITY

```
#define ERROR_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_ERROR_)
```

Definition at line 48 of file KIM_ModelDestroyLogMacros.hpp.

12.71.1.3 FATAL_VERBOSITY

```
#define FATAL_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_FATAL_)
```

Definition at line 35 of file KIM_ModelDestroyLogMacros.hpp.

12.71.1.4 INFORMATION_VERBOSITY

```
#define INFORMATION_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_INFORMATION_)
```

Definition at line 74 of file KIM_ModelDestroyLogMacros.hpp.

12.71.1.5 LOG_DEBUG

```
#define LOG_DEBUG(  
    message )
```

Value:

```
modelDestroy->LogEntry(KIM::LOG\_VERBOSITY::debug, message, \
    __LINE__, __FILE__)
```

Definition at line 92 of file KIM_ModelDestroyLogMacros.hpp.

12.71.1.6 LOG_ERROR

```
#define LOG_ERROR(  
    message )
```

Value:

```
modelDestroy->LogEntry(KIM::LOG_VERBOSITY::error, message, \  
    __LINE__, __FILE__)
```

Definition at line 53 of file KIM_ModelDestroyLogMacros.hpp.

12.71.1.7 LOG_FATAL

```
#define LOG_FATAL(  
    message )
```

Value:

```
modelDestroy->LogEntry(KIM::LOG_VERBOSITY::fatal, message, \  
    __LINE__, __FILE__)
```

Definition at line 40 of file KIM_ModelDestroyLogMacros.hpp.

12.71.1.8 LOG_INFORMATION

```
#define LOG_INFORMATION(  
    message )
```

Value:

```
modelDestroy->LogEntry(KIM::LOG_VERBOSITY::information, message, \  
    __LINE__, __FILE__)
```

Definition at line 79 of file KIM_ModelDestroyLogMacros.hpp.

12.71.1.9 LOG_WARNING

```
#define LOG_WARNING(  
    message )
```

Value:

```
modelDestroy->LogEntry(KIM::LOG_VERBOSITY::warning, message, \  
    __LINE__, __FILE__)
```

Definition at line 66 of file KIM_ModelDestroyLogMacros.hpp.

12.71.1.10 WARNING_VERBOSITY

```
#define WARNING_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_WARNING_)
```

Definition at line 61 of file KIM_ModelDestroyLogMacros.hpp.

12.72 kim-api-v2.0.0-beta.0/cpp/include/KIM_ModelDriverCreate.hpp File Reference

```
#include <string>
#include <sstream>
#include "KIM_func.hpp"
```

Classes

- class [KIM::ModelDriverCreate](#)

Namespaces

- [KIM](#)

12.73 kim-api-v2.0.0-beta.0/cpp/include/KIM_ModelDriverCreateLogMacros.hpp File Reference

Macros

- #define [FATAL_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_FATAL_)
- #define [LOG_FATAL](#)(message)
- #define [ERROR_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_ERROR_)
- #define [LOG_ERROR](#)(message)
- #define [WARNING_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_WARNING_)
- #define [LOG_WARNING](#)(message)
- #define [INFORMATION_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_INFORMATION_)
- #define [LOG_INFORMATION](#)(message)
- #define [DEBUG_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_DEBUG_)
- #define [LOG_DEBUG](#)(message)

12.73.1 Macro Definition Documentation

12.73.1.1 DEBUG_VERBOSITY

```
#define DEBUG_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_DEBUG_)
```

Definition at line 88 of file KIM_ModelDriverCreateLogMacros.hpp.

12.73.1.2 ERROR_VERBOSITY

```
#define ERROR_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_ERROR_)
```

Definition at line 49 of file KIM_ModelDriverCreateLogMacros.hpp.

12.73.1.3 FATAL_VERBOSITY

```
#define FATAL_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_FATAL_)
```

Definition at line 35 of file KIM_ModelDriverCreateLogMacros.hpp.

12.73.1.4 INFORMATION_VERBOSITY

```
#define INFORMATION_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_INFORMATION_)
```

Definition at line 75 of file KIM_ModelDriverCreateLogMacros.hpp.

12.73.1.5 LOG_DEBUG

```
#define LOG_DEBUG(  
    message )
```

Value:

```
modelDriverCreate->LogEntry(KIM::LOG_VERBOSITY::debug, message, \  
    __LINE__, __FILE__)
```

Definition at line 93 of file KIM_ModelDriverCreateLogMacros.hpp.

12.73.1.6 LOG_ERROR

```
#define LOG_ERROR(  
    message )
```

Value:

```
modelDriverCreate->LogEntry(KIM::LOG_VERBOSITY::error, message, \  
    __LINE__, __FILE__)
```

Definition at line 54 of file KIM_ModelDriverCreateLogMacros.hpp.

12.73.1.7 LOG_FATAL

```
#define LOG_FATAL(  
    message )
```

Value:

```
modelDriverCreate->LogEntry(KIM::LOG_VERBOSITY::fatal, message, \  
    __LINE__, __FILE__)
```

Definition at line 40 of file KIM_ModelDriverCreateLogMacros.hpp.

12.73.1.8 LOG_INFORMATION

```
#define LOG_INFORMATION(  
    message )
```

Value:

```
modelDriverCreate->LogEntry(KIM::LOG_VERBOSITY::information, message, \  
    __LINE__, __FILE__)
```

Definition at line 80 of file KIM_ModelDriverCreateLogMacros.hpp.

12.73.1.9 LOG_WARNING

```
#define LOG_WARNING(  
    message )
```

Value:

```
modelDriverCreate->LogEntry(KIM::LOG_VERBOSITY::warning, message, \  
    __LINE__, __FILE__)
```

Definition at line 67 of file KIM_ModelDriverCreateLogMacros.hpp.

12.73.1.10 WARNING_VERBOSITY

```
#define WARNING_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_WARNING_)
```

Definition at line 62 of file KIM_ModelDriverCreateLogMacros.hpp.

12.74 kim-api-v2.0.0-beta.0/cpp/include/KIM_ModelDriverHeaders.hpp File Reference

```
#include "KIM_ModelDriverCreate.hpp"
#include "KIM_LogVerbosity.hpp"
#include "KIM_LanguageName.hpp"
#include "KIM_Numbering.hpp"
#include "KIM_SpeciesName.hpp"
#include "KIM_SupportStatus.hpp"
#include "KIM_UnitSystem.hpp"
#include "KIM_ModelComputeArgumentsCreate.hpp"
#include "KIM_ComputeArgumentName.hpp"
#include "KIM_DataType.hpp"
#include "KIM_ComputeCallbackName.hpp"
#include "KIM_ModelComputeArguments.hpp"
#include "KIM_ModelComputeArgumentsDestroy.hpp"
#include "KIM_ModelCompute.hpp"
#include "KIM_ModelRefresh.hpp"
#include "KIM_ModelDestroy.hpp"
```

12.75 kim-api-v2.0.0-beta.0/cpp/include/KIM_ModelHeaders.hpp File Reference

```
#include "KIM_ModelCreate.hpp"
#include "KIM_LogVerbosity.hpp"
#include "KIM_LanguageName.hpp"
#include "KIM_Numbering.hpp"
#include "KIM_SpeciesName.hpp"
#include "KIM_SupportStatus.hpp"
#include "KIM_UnitSystem.hpp"
#include "KIM_ModelComputeArgumentsCreate.hpp"
#include "KIM_ComputeArgumentName.hpp"
#include "KIM_DataType.hpp"
#include "KIM_ComputeCallbackName.hpp"
#include "KIM_ModelComputeArguments.hpp"
#include "KIM_ModelComputeArgumentsDestroy.hpp"
#include "KIM_ModelCompute.hpp"
#include "KIM_ModelRefresh.hpp"
#include "KIM_ModelDestroy.hpp"
```

12.76 kim-api-v2.0.0-beta.0/cpp/include/KIM_ModelRefresh.hpp File Reference

```
#include <string>
#include <sstream>
```

Classes

- class [KIM::ModelRefresh](#)

Namespaces

- [KIM](#)

12.77 kim-api-v2.0.0-beta.0/cpp/include/KIM_ModelRefreshLogMacros.hpp File Reference

Macros

- #define [FATAL_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_FATAL_)
- #define [LOG_FATAL](#)(message)
- #define [ERROR_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_ERROR_)
- #define [LOG_ERROR](#)(message)
- #define [WARNING_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_WARNING_)
- #define [LOG_WARNING](#)(message)
- #define [INFORMATION_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_INFORMATION_)
- #define [LOG_INFORMATION](#)(message)
- #define [DEBUG_VERBOSITY](#) (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_DEBUG_)
- #define [LOG_DEBUG](#)(message)

12.77.1 Macro Definition Documentation

12.77.1.1 [DEBUG_VERBOSITY](#)

```
#define DEBUG_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_DEBUG_)
```

Definition at line 87 of file `KIM_ModelRefreshLogMacros.hpp`.

12.77.1.2 [ERROR_VERBOSITY](#)

```
#define ERROR_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_ERROR_)
```

Definition at line 48 of file `KIM_ModelRefreshLogMacros.hpp`.

12.77.1.3 FATAL_VERBOSITY

```
#define FATAL_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_FATAL_)
```

Definition at line 35 of file KIM_ModelRefreshLogMacros.hpp.

12.77.1.4 INFORMATION_VERBOSITY

```
#define INFORMATION_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_INFORMATION_)
```

Definition at line 74 of file KIM_ModelRefreshLogMacros.hpp.

12.77.1.5 LOG_DEBUG

```
#define LOG_DEBUG(  
    message )
```

Value:

```
modelRefresh->LogEntry (KIM::LOG_VERBOSITY::debug, message, \n                        __LINE__, __FILE__)
```

Definition at line 92 of file KIM_ModelRefreshLogMacros.hpp.

12.77.1.6 LOG_ERROR

```
#define LOG_ERROR(  
    message )
```

Value:

```
modelRefresh->LogEntry (KIM::LOG_VERBOSITY::error, message, \n                        __LINE__, __FILE__)
```

Definition at line 53 of file KIM_ModelRefreshLogMacros.hpp.

12.77.1.7 LOG_FATAL

```
#define LOG_FATAL(  
    message )
```

Value:

```
modelRefresh->LogEntry(KIM::LOG\_VERBOSITY::fatal, message, \br/>    __LINE__, __FILE__)
```

Definition at line 40 of file KIM_ModelRefreshLogMacros.hpp.

12.77.1.8 LOG_INFORMATION

```
#define LOG_INFORMATION(  
    message )
```

Value:

```
modelRefresh->LogEntry(KIM::LOG\_VERBOSITY::information, message, \br/>    __LINE__, __FILE__)
```

Definition at line 79 of file KIM_ModelRefreshLogMacros.hpp.

12.77.1.9 LOG_WARNING

```
#define LOG_WARNING(  
    message )
```

Value:

```
modelRefresh->LogEntry(KIM::LOG\_VERBOSITY::warning, message, \br/>    __LINE__, __FILE__)
```

Definition at line 66 of file KIM_ModelRefreshLogMacros.hpp.

12.77.1.10 WARNING_VERBOSITY

```
#define WARNING_VERBOSITY (KIM_LOG_MAXIMUM_LEVEL >= KIM_LOG_VERBOSITY_WARNING_)
```

Definition at line 61 of file KIM_ModelRefreshLogMacros.hpp.

12.78 kim-api-v2.0.0-beta.0/cpp/include/KIM_Numbering.hpp File Reference

```
#include <string>
```

Classes

- class [KIM::Numbering](#)
- struct [KIM::NUMBERING::Comparator](#)

Namespaces

- [KIM](#)
- [KIM::NUMBERING](#)

Functions

- void [KIM::NUMBERING::GetNumberOfNumberings](#) (int *const numberOfNumberings)
- int [KIM::NUMBERING::GetNumbering](#) (int const index, Numbering *const numbering)

Variables

- Numbering const [KIM::NUMBERING::zeroBased](#)
- Numbering const [KIM::NUMBERING::oneBased](#)

12.79 kim-api-v2.0.0-beta.0/cpp/include/KIM_Numbering.inc File Reference

12.80 kim-api-v2.0.0-beta.0/cpp/include/KIM_SemVer.hpp File Reference

```
#include <string>
```

Namespaces

- [KIM](#)
- [KIM::SEM_VER](#)

Functions

- void [KIM::SEM_VER::GetSemVer](#) (std::string const **const version)
- int [KIM::SEM_VER::IsLessThan](#) (std::string const &versionA, std::string const &versionB, int *const isLessThan)
- int [KIM::SEM_VER::ParseSemVer](#) (std::string const &version, int *const major, int *const minor, int *const patch, std::string *const prerelease, std::string *const buildMetadata)

12.81 kim-api-v2.0.0-beta.0/cpp/include/KIM_SimulatorHeaders.hpp File Reference

```
#include "KIM_Model.hpp"
#include "KIM_LogVerbosity.hpp"
#include "KIM_DataType.hpp"
#include "KIM_LanguageName.hpp"
#include "KIM_SpeciesName.hpp"
#include "KIM_Numbering.hpp"
#include "KIM_UnitSystem.hpp"
#include "KIM_ComputeArguments.hpp"
#include "KIM_ComputeArgumentName.hpp"
#include "KIM_ComputeCallbackName.hpp"
#include "KIM_SupportStatus.hpp"
```

12.82 kim-api-v2.0.0-beta.0/cpp/include/KIM_SpeciesName.hpp File Reference

```
#include <string>
```

Classes

- class [KIM::SpeciesName](#)
- struct [KIM::SPECIES_NAME::Comparator](#)

Namespaces

- [KIM](#)
- [KIM::SPECIES_NAME](#)

Functions

- void [KIM::SPECIES_NAME::GetNumberOfSpeciesNames](#) (int *const numberOfSpeciesNames)
- int [KIM::SPECIES_NAME::GetSpeciesName](#) (int const index, SpeciesName *const speciesName)

Variables

- SpeciesName const [KIM::SPECIES_NAME::electron](#)
- SpeciesName const [KIM::SPECIES_NAME::H](#)
- SpeciesName const [KIM::SPECIES_NAME::He](#)
- SpeciesName const [KIM::SPECIES_NAME::Li](#)
- SpeciesName const [KIM::SPECIES_NAME::Be](#)
- SpeciesName const [KIM::SPECIES_NAME::B](#)
- SpeciesName const [KIM::SPECIES_NAME::C](#)
- SpeciesName const [KIM::SPECIES_NAME::N](#)
- SpeciesName const [KIM::SPECIES_NAME::O](#)
- SpeciesName const [KIM::SPECIES_NAME::F](#)
- SpeciesName const [KIM::SPECIES_NAME::Ne](#)

- SpeciesName const [KIM::SPECIES_NAME::Na](#)
- SpeciesName const [KIM::SPECIES_NAME::Mg](#)
- SpeciesName const [KIM::SPECIES_NAME::Al](#)
- SpeciesName const [KIM::SPECIES_NAME::Si](#)
- SpeciesName const [KIM::SPECIES_NAME::P](#)
- SpeciesName const [KIM::SPECIES_NAME::S](#)
- SpeciesName const [KIM::SPECIES_NAME::Cl](#)
- SpeciesName const [KIM::SPECIES_NAME::Ar](#)
- SpeciesName const [KIM::SPECIES_NAME::K](#)
- SpeciesName const [KIM::SPECIES_NAME::Ca](#)
- SpeciesName const [KIM::SPECIES_NAME::Sc](#)
- SpeciesName const [KIM::SPECIES_NAME::Ti](#)
- SpeciesName const [KIM::SPECIES_NAME::V](#)
- SpeciesName const [KIM::SPECIES_NAME::Cr](#)
- SpeciesName const [KIM::SPECIES_NAME::Mn](#)
- SpeciesName const [KIM::SPECIES_NAME::Fe](#)
- SpeciesName const [KIM::SPECIES_NAME::Co](#)
- SpeciesName const [KIM::SPECIES_NAME::Ni](#)
- SpeciesName const [KIM::SPECIES_NAME::Cu](#)
- SpeciesName const [KIM::SPECIES_NAME::Zn](#)
- SpeciesName const [KIM::SPECIES_NAME::Ga](#)
- SpeciesName const [KIM::SPECIES_NAME::Ge](#)
- SpeciesName const [KIM::SPECIES_NAME::As](#)
- SpeciesName const [KIM::SPECIES_NAME::Se](#)
- SpeciesName const [KIM::SPECIES_NAME::Br](#)
- SpeciesName const [KIM::SPECIES_NAME::Kr](#)
- SpeciesName const [KIM::SPECIES_NAME::Rb](#)
- SpeciesName const [KIM::SPECIES_NAME::Sr](#)
- SpeciesName const [KIM::SPECIES_NAME::Y](#)
- SpeciesName const [KIM::SPECIES_NAME::Zr](#)
- SpeciesName const [KIM::SPECIES_NAME::Nb](#)
- SpeciesName const [KIM::SPECIES_NAME::Mo](#)
- SpeciesName const [KIM::SPECIES_NAME::Tc](#)
- SpeciesName const [KIM::SPECIES_NAME::Ru](#)
- SpeciesName const [KIM::SPECIES_NAME::Rh](#)
- SpeciesName const [KIM::SPECIES_NAME::Pd](#)
- SpeciesName const [KIM::SPECIES_NAME::Ag](#)
- SpeciesName const [KIM::SPECIES_NAME::Cd](#)
- SpeciesName const [KIM::SPECIES_NAME::In](#)
- SpeciesName const [KIM::SPECIES_NAME::Sn](#)
- SpeciesName const [KIM::SPECIES_NAME::Sb](#)
- SpeciesName const [KIM::SPECIES_NAME::Te](#)
- SpeciesName const [KIM::SPECIES_NAME::I](#)
- SpeciesName const [KIM::SPECIES_NAME::Xe](#)
- SpeciesName const [KIM::SPECIES_NAME::Cs](#)
- SpeciesName const [KIM::SPECIES_NAME::Ba](#)
- SpeciesName const [KIM::SPECIES_NAME::La](#)
- SpeciesName const [KIM::SPECIES_NAME::Ce](#)
- SpeciesName const [KIM::SPECIES_NAME::Pr](#)
- SpeciesName const [KIM::SPECIES_NAME::Nd](#)
- SpeciesName const [KIM::SPECIES_NAME::Pm](#)
- SpeciesName const [KIM::SPECIES_NAME::Sm](#)
- SpeciesName const [KIM::SPECIES_NAME::Eu](#)
- SpeciesName const [KIM::SPECIES_NAME::Gd](#)
- SpeciesName const [KIM::SPECIES_NAME::Tb](#)

- SpeciesName const [KIM::SPECIES_NAME::Dy](#)
- SpeciesName const [KIM::SPECIES_NAME::Ho](#)
- SpeciesName const [KIM::SPECIES_NAME::Er](#)
- SpeciesName const [KIM::SPECIES_NAME::Tm](#)
- SpeciesName const [KIM::SPECIES_NAME::Yb](#)
- SpeciesName const [KIM::SPECIES_NAME::Lu](#)
- SpeciesName const [KIM::SPECIES_NAME::Hf](#)
- SpeciesName const [KIM::SPECIES_NAME::Ta](#)
- SpeciesName const [KIM::SPECIES_NAME::W](#)
- SpeciesName const [KIM::SPECIES_NAME::Re](#)
- SpeciesName const [KIM::SPECIES_NAME::Os](#)
- SpeciesName const [KIM::SPECIES_NAME::Ir](#)
- SpeciesName const [KIM::SPECIES_NAME::Pt](#)
- SpeciesName const [KIM::SPECIES_NAME::Au](#)
- SpeciesName const [KIM::SPECIES_NAME::Hg](#)
- SpeciesName const [KIM::SPECIES_NAME::Tl](#)
- SpeciesName const [KIM::SPECIES_NAME::Pb](#)
- SpeciesName const [KIM::SPECIES_NAME::Bi](#)
- SpeciesName const [KIM::SPECIES_NAME::Po](#)
- SpeciesName const [KIM::SPECIES_NAME::At](#)
- SpeciesName const [KIM::SPECIES_NAME::Rn](#)
- SpeciesName const [KIM::SPECIES_NAME::Fr](#)
- SpeciesName const [KIM::SPECIES_NAME::Ra](#)
- SpeciesName const [KIM::SPECIES_NAME::Ac](#)
- SpeciesName const [KIM::SPECIES_NAME::Th](#)
- SpeciesName const [KIM::SPECIES_NAME::Pa](#)
- SpeciesName const [KIM::SPECIES_NAME::U](#)
- SpeciesName const [KIM::SPECIES_NAME::Np](#)
- SpeciesName const [KIM::SPECIES_NAME::Pu](#)
- SpeciesName const [KIM::SPECIES_NAME::Am](#)
- SpeciesName const [KIM::SPECIES_NAME::Cm](#)
- SpeciesName const [KIM::SPECIES_NAME::Bk](#)
- SpeciesName const [KIM::SPECIES_NAME::Cf](#)
- SpeciesName const [KIM::SPECIES_NAME::Es](#)
- SpeciesName const [KIM::SPECIES_NAME::Fm](#)
- SpeciesName const [KIM::SPECIES_NAME::Md](#)
- SpeciesName const [KIM::SPECIES_NAME::No](#)
- SpeciesName const [KIM::SPECIES_NAME::Lr](#)
- SpeciesName const [KIM::SPECIES_NAME::Rf](#)
- SpeciesName const [KIM::SPECIES_NAME::Db](#)
- SpeciesName const [KIM::SPECIES_NAME::Sg](#)
- SpeciesName const [KIM::SPECIES_NAME::Bh](#)
- SpeciesName const [KIM::SPECIES_NAME::Hs](#)
- SpeciesName const [KIM::SPECIES_NAME::Mt](#)
- SpeciesName const [KIM::SPECIES_NAME::Ds](#)
- SpeciesName const [KIM::SPECIES_NAME::Rg](#)
- SpeciesName const [KIM::SPECIES_NAME::Cn](#)
- SpeciesName const [KIM::SPECIES_NAME::Uut](#)
- SpeciesName const [KIM::SPECIES_NAME::Fl](#)
- SpeciesName const [KIM::SPECIES_NAME::Uup](#)
- SpeciesName const [KIM::SPECIES_NAME::Lv](#)
- SpeciesName const [KIM::SPECIES_NAME::Uus](#)
- SpeciesName const [KIM::SPECIES_NAME::Uuo](#)
- SpeciesName const [KIM::SPECIES_NAME::user01](#)
- SpeciesName const [KIM::SPECIES_NAME::user02](#)

- SpeciesName const [KIM::SPECIES_NAME::user03](#)
- SpeciesName const [KIM::SPECIES_NAME::user04](#)
- SpeciesName const [KIM::SPECIES_NAME::user05](#)
- SpeciesName const [KIM::SPECIES_NAME::user06](#)
- SpeciesName const [KIM::SPECIES_NAME::user07](#)
- SpeciesName const [KIM::SPECIES_NAME::user08](#)
- SpeciesName const [KIM::SPECIES_NAME::user09](#)
- SpeciesName const [KIM::SPECIES_NAME::user10](#)
- SpeciesName const [KIM::SPECIES_NAME::user11](#)
- SpeciesName const [KIM::SPECIES_NAME::user12](#)
- SpeciesName const [KIM::SPECIES_NAME::user13](#)
- SpeciesName const [KIM::SPECIES_NAME::user14](#)
- SpeciesName const [KIM::SPECIES_NAME::user15](#)
- SpeciesName const [KIM::SPECIES_NAME::user16](#)
- SpeciesName const [KIM::SPECIES_NAME::user17](#)
- SpeciesName const [KIM::SPECIES_NAME::user18](#)
- SpeciesName const [KIM::SPECIES_NAME::user19](#)
- SpeciesName const [KIM::SPECIES_NAME::user20](#)

12.83 kim-api-v2.0.0-beta.0/cpp/include/KIM_SpeciesName.inc File Reference

12.84 kim-api-v2.0.0-beta.0/cpp/include/KIM_SupportStatus.hpp File Reference

```
#include <string>
```

Classes

- class [KIM::SupportStatus](#)
- struct [KIM::SUPPORT_STATUS::Comparator](#)

Namespaces

- [KIM](#)
- [KIM::SUPPORT_STATUS](#)

Functions

- void [KIM::SUPPORT_STATUS::GetNumberOfSupportStatuses](#) (int *const numberOfSupportStatuses)
- int [KIM::SUPPORT_STATUS::GetSupportStatus](#) (int const index, SupportStatus *const supportStatus)

Variables

- SupportStatus const [KIM::SUPPORT_STATUS::requiredByAPI](#)
- SupportStatus const [KIM::SUPPORT_STATUS::notSupported](#)
- SupportStatus const [KIM::SUPPORT_STATUS::required](#)
- SupportStatus const [KIM::SUPPORT_STATUS::optional](#)

12.85 kim-api-v2.0.0-beta.0/cpp/include/KIM_SupportStatus.inc File Reference

12.86 kim-api-v2.0.0-beta.0/cpp/include/KIM_TemperatureUnit.hpp File Reference

```
#include <string>
```

Classes

- class [KIM::TemperatureUnit](#)
- struct [KIM::TEMPERATURE_UNIT::Comparator](#)

Namespaces

- [KIM](#)
- [KIM::TEMPERATURE_UNIT](#)

Functions

- void [KIM::TEMPERATURE_UNIT::GetNumberOfTemperatureUnits](#) (int *const numberOfTemperatureUnits)
- int [KIM::TEMPERATURE_UNIT::GetTemperatureUnit](#) (int const index, TemperatureUnit *const temperature↔Unit)

Variables

- TemperatureUnit const [KIM::TEMPERATURE_UNIT::unused](#)
- TemperatureUnit const [KIM::TEMPERATURE_UNIT::K](#)

12.87 kim-api-v2.0.0-beta.0/cpp/include/KIM_TemperatureUnit.inc File Reference

12.88 kim-api-v2.0.0-beta.0/cpp/include/KIM_TimeUnit.hpp File Reference

```
#include <string>
```

Classes

- class [KIM::TimeUnit](#)
- struct [KIM::TIME_UNIT::Comparator](#)

Namespaces

- [KIM](#)
- [KIM::TIME_UNIT](#)

Functions

- void [KIM::TIME_UNIT::GetNumberOfTimeUnits](#) (int *const numberOfTimeUnits)
- int [KIM::TIME_UNIT::GetTimeUnit](#) (int const index, TimeUnit *const timeUnit)

Variables

- TimeUnit const [KIM::TIME_UNIT::unused](#)
- TimeUnit const [KIM::TIME_UNIT::fs](#)
- TimeUnit const [KIM::TIME_UNIT::ps](#)
- TimeUnit const [KIM::TIME_UNIT::ns](#)
- TimeUnit const [KIM::TIME_UNIT::s](#)

12.89 kim-api-v2.0.0-beta.0/cpp/include/KIM_TimeUnit.inc File Reference

12.90 kim-api-v2.0.0-beta.0/cpp/include/KIM_UnitSystem.hpp File Reference

```
#include "KIM_LengthUnit.hpp"
#include "KIM_EnergyUnit.hpp"
#include "KIM_ChargeUnit.hpp"
#include "KIM_TemperatureUnit.hpp"
#include "KIM_TimeUnit.hpp"
```

12.91 kim-api-v2.0.0-beta.0/cpp/include/KIM_Version.hpp.tpl File Reference

12.92 kim-api-v2.0.0-beta.0/cpp/include/Makefile.dependencies File Reference

12.93 kim-api-v2.0.0-beta.0/c/include/Makefile.dependencies File Reference

12.94 kim-api-v2.0.0-beta.0/fortran/include/Makefile.dependencies File Reference

12.95 kim-api-v2.0.0-beta.0/docs/porting-content-from-v1-to-v2-examples/models/step0/ex↔ _model_Ar_P_MLJ_F03/ex_model_Ar_P_MLJ_F03.F03 File Reference

```
#include "KIM_API_status.h"
```

Modules

- module [ex_model_ar_p_ml_j_f03](#)

Macros

- #define [THIS_FILE_NAME](#) __FILE__
- #define [TRUEFALSE](#)(TRUTH) merge(1,0,(TRUTH))

Functions/Subroutines

- integer(c_int) function, public [ex_model_ar_p_mlj_f03::compute_energy_forces](#) (pkim)

Variables

- real(c_double), parameter, public [ex_model_ar_p_mlj_f03::model_cutoff](#) = 8.15_cd

12.95.1 Macro Definition Documentation

12.95.1.1 THIS_FILE_NAME

```
#define THIS_FILE_NAME __FILE__
```

12.95.1.2 TRUEFALSE

```
#define TRUEFALSE(  
    TRUTH ) merge(1,0,(TRUTH))
```

12.96 kim-api-v2.0.0-beta.0/docs/porting-content-from-v1-to-v2-examples/models/step1/ex_model_Ar_P_MLJ_F03/ex_model_Ar_P_MLJ_F03.F03 File Reference

```
#include "KIM_API_status.h"
```

Modules

- module [ex_model_ar_p_mlj_f03](#)

Macros

- #define [THIS_FILE_NAME](#) __FILE__
- #define [TRUEFALSE](#)(TRUTH) merge(1,0,(TRUTH))

Functions/Subroutines

- integer(c_int) function, public [ex_model_ar_p_mlj_f03::compute_energy_forces](#) (pkim)

12.96.1 Macro Definition Documentation

12.96.1.1 THIS_FILE_NAME

```
#define THIS_FILE_NAME __FILE__
```

12.96.1.2 TRUEFALSE

```
#define TRUEFALSE(  
    TRUTH ) merge(1,0,(TRUTH))
```

12.97 [kim-api-v2.0.0-beta.0/docs/porting-content-from-v1-to-v2-examples/models/step3/ex_model_Ar_P_MLJ_F03/ex_model_Ar_P_MLJ_F03.F03](#) File Reference

```
#include "kim_model_create_log_macros.fd"
```

Modules

- module [ex_model_ar_p_mlj_f03](#)

12.98 [kim-api-v2.0.0-beta.0/docs/porting-content-from-v1-to-v2-examples/models/step4/ex_model_Ar_P_MLJ_F03/ex_model_Ar_P_MLJ_F03.F03](#) File Reference

```
#include "kim_model_compute_arguments_create_log_macros.fd"  
#include "kim_model_compute_arguments_destroy_log_macros.fd"  
#include "kim_model_create_log_macros.fd"
```

Modules

- module [ex_model_ar_p_mlj_f03](#)

- subroutine, public [ex_model_ar_p_mlj_f03::model_compute_arguments_create](#) (model_compute_handle, model_compute_arguments_create_handle, ierr)
- subroutine, public [ex_model_ar_p_mlj_f03::model_compute_arguments_destroy](#) (model_compute_handle, model_compute_arguments_destroy_handle, ierr)
- subroutine [model_create_routine](#) (model_create_handle, requested_length_unit, requested_energy_unit, requested_charge_unit, requested_temperature_unit, requested_time_unit, ierr)

12.98.1 Function/Subroutine Documentation

12.98.1.1 model_create_routine()

```
subroutine model_create_routine (
    type(kim_model_create_handle_type), intent(inout) model_create_handle,
    type(kim_length_unit_type), intent(in) requested_length_unit,
    type(kim_energy_unit_type), intent(in) requested_energy_unit,
    type(kim_charge_unit_type), intent(in) requested_charge_unit,
    type(kim_temperature_unit_type), intent(in) requested_temperature_unit,
    type(kim_time_unit_type), intent(in) requested_time_unit,
    integer(c_int), intent(out) ierr )
```

Definition at line 439 of file ex_model_Ar_P_MLJ_F03.F03.

12.99 kim-api-v2.0.0-beta.0/docs/porting-content-from-v1-to-v2-examples/models/step5/ex_model_Ar_P_MLJ_F03/ex_model_Ar_P_MLJ_F03.F03 File Reference

```
#include "kim_model_destroy_log_macros.fd"
#include "kim_model_refresh_log_macros.fd"
#include "kim_model_compute_arguments_create_log_macros.fd"
#include "kim_model_compute_arguments_destroy_log_macros.fd"
#include "kim_model_create_log_macros.fd"
```

Modules

- module [ex_model_ar_p_mlj_f03](#)

Functions/Subroutines

- subroutine, public [ex_model_ar_p_mlj_f03::model_destroy_func](#) (model_destroy_handle, ierr)
- subroutine, public [ex_model_ar_p_mlj_f03::model_refresh_func](#) (model_refresh_handle, ierr)
- subroutine, public [ex_model_ar_p_mlj_f03::model_compute_arguments_create](#) (model_compute_handle, model_compute_arguments_create_handle, ierr)
- subroutine, public [ex_model_ar_p_mlj_f03::model_compute_arguments_destroy](#) (model_compute_handle, model_compute_arguments_destroy_handle, ierr)
- subroutine [model_create_routine](#) (model_create_handle, requested_length_unit, requested_energy_unit, requested_charge_unit, requested_temperature_unit, requested_time_unit, ierr)

12.99.1 Function/Subroutine Documentation

12.99.1.1 `model_create_routine()`

```
subroutine model_create_routine (
    type(kim_model_create_handle_type), intent(inout) model_create_handle,
    type(kim_length_unit_type), intent(in) requested_length_unit,
    type(kim_energy_unit_type), intent(in) requested_energy_unit,
    type(kim_charge_unit_type), intent(in) requested_charge_unit,
    type(kim_temperature_unit_type), intent(in) requested_temperature_unit,
    type(kim_time_unit_type), intent(in) requested_time_unit,
    integer(c_int), intent(out) ierr )
```

Definition at line 493 of file `ex_model_Ar_P_MLJ_F03.F03`.

12.100 `kim-api-v2.0.0-beta.0/docs/porting-content-from-v1-to-v2-examples/models/step6/ex_model_Ar_P_MLJ_F03/ex_model_Ar_P_MLJ_F03.F03` File Reference

```
#include "kim_model_compute_log_macros.fd"
#include "kim_model_destroy_log_macros.fd"
#include "kim_model_refresh_log_macros.fd"
#include "kim_model_compute_arguments_create_log_macros.fd"
#include "kim_model_compute_arguments_destroy_log_macros.fd"
#include "kim_model_create_log_macros.fd"
```

Modules

- module [ex_model_ar_p_mlj_f03](#)

Functions/Subroutines

- subroutine, public [ex_model_ar_p_mlj_f03::compute_energy_forces](#) (model_compute_handle, model_compute_arguments_handle, ierr)
- subroutine, public [ex_model_ar_p_mlj_f03::model_destroy_func](#) (model_destroy_handle, ierr)
- subroutine, public [ex_model_ar_p_mlj_f03::model_refresh_func](#) (model_refresh_handle, ierr)
- subroutine, public [ex_model_ar_p_mlj_f03::model_compute_arguments_create](#) (model_compute_handle, model_compute_arguments_create_handle, ierr)
- subroutine, public [ex_model_ar_p_mlj_f03::model_compute_arguments_destroy](#) (model_compute_handle, model_compute_arguments_destroy_handle, ierr)
- subroutine [model_create_routine](#) (model_create_handle, requested_length_unit, requested_energy_unit, requested_charge_unit, requested_temperature_unit, requested_time_unit, ierr)

12.100.1 Function/Subroutine Documentation

12.100.1.1 `model_create_routine()`

```
subroutine model_create_routine (
    type(kim_model_create_handle_type), intent(inout) model_create_handle,
    type(kim_length_unit_type), intent(in) requested_length_unit,
    type(kim_energy_unit_type), intent(in) requested_energy_unit,
    type(kim_charge_unit_type), intent(in) requested_charge_unit,
    type(kim_temperature_unit_type), intent(in) requested_temperature_unit,
    type(kim_time_unit_type), intent(in) requested_time_unit,
    integer(c_int), intent(out) ierr )
```

Definition at line 524 of file `ex_model_Ar_P_MLJ_F03.F03`.

12.101 kim-api-v2.0.0-beta.0/examples/models/ex_model_Ar_P_MLJ_F03/ex_model_Ar_P_MLJ_F03.F03 File Reference

```
#include "kim_model_compute_log_macros.fd"
#include "kim_model_destroy_log_macros.fd"
#include "kim_model_refresh_log_macros.fd"
#include "kim_model_compute_arguments_create_log_macros.fd"
#include "kim_model_compute_arguments_destroy_log_macros.fd"
#include "kim_model_create_log_macros.fd"
```

Modules

- module [ex_model_ar_p_mlj_f03](#)

Functions/Subroutines

- subroutine, public [ex_model_ar_p_mlj_f03::compute_energy_forces](#) (model_compute_handle, model_compute_arguments_handle, ierr)
- subroutine, public [ex_model_ar_p_mlj_f03::model_destroy_func](#) (model_destroy_handle, ierr)
- subroutine, public [ex_model_ar_p_mlj_f03::model_refresh_func](#) (model_refresh_handle, ierr)
- subroutine, public [ex_model_ar_p_mlj_f03::model_compute_arguments_create](#) (model_compute_handle, model_compute_arguments_create_handle, ierr)
- subroutine, public [ex_model_ar_p_mlj_f03::model_compute_arguments_destroy](#) (model_compute_handle, model_compute_arguments_destroy_handle, ierr)
- subroutine [model_create_routine](#) (model_create_handle, requested_length_unit, requested_energy_unit, requested_charge_unit, requested_temperature_unit, requested_time_unit, ierr)

12.101.1 Function/Subroutine Documentation

12.101.1.1 model_create_routine()

```

subroutine model_create_routine (
    type(kim_model_create_handle_type), intent(inout) model_create_handle,
    type(kim_length_unit_type), intent(in) requested_length_unit,
    type(kim_energy_unit_type), intent(in) requested_energy_unit,
    type(kim_charge_unit_type), intent(in) requested_charge_unit,
    type(kim_temperature_unit_type), intent(in) requested_temperature_unit,
    type(kim_time_unit_type), intent(in) requested_time_unit,
    integer(c_int), intent(out) ierr )

```

Definition at line 524 of file ex_model_Ar_P_MLJ_F03.F03.

12.102 [kim-api-v2.0.0-beta.0/docs/porting-content-from-v1-to-v2-examples/models/step0/ex_model_Ar_P_MLJ_F03/Makefile](#) File Reference ↩

12.103 [kim-api-v2.0.0-beta.0/docs/porting-content-from-v1-to-v2-examples/models/step0/ex_model_Ar_P_Morse_07C/Makefile](#) File Reference ↩

12.104 [kim-api-v2.0.0-beta.0/docs/porting-content-from-v1-to-v2-examples/models/step1/ex_model_Ar_P_MLJ_F03/Makefile](#) File Reference ↩

12.105 [kim-api-v2.0.0-beta.0/docs/porting-content-from-v1-to-v2-examples/models/step1/ex_model_Ar_P_Morse_07C/Makefile](#) File Reference ↩

12.106 [kim-api-v2.0.0-beta.0/docs/porting-content-from-v1-to-v2-examples/models/step3/ex_model_Ar_P_MLJ_F03/Makefile](#) File Reference ↩

12.107 [kim-api-v2.0.0-beta.0/docs/porting-content-from-v1-to-v2-examples/models/step3/ex_model_Ar_P_Morse_07C/Makefile](#) File Reference ↩

12.108 [kim-api-v2.0.0-beta.0/docs/porting-content-from-v1-to-v2-examples/models/step4/ex_model_Ar_P_MLJ_F03/Makefile](#) File Reference ↩

12.109 [kim-api-v2.0.0-beta.0/docs/porting-content-from-v1-to-v2-examples/models/step4/ex_model_Ar_P_Morse_07C/Makefile](#) File Reference ↩

12.110 [kim-api-v2.0.0-beta.0/docs/porting-content-from-v1-to-v2-examples/models/step5/ex_model_Ar_P_MLJ_F03/Makefile](#) File Reference ↩

12.111 kim-api-v2.0.0-beta.0/docs/porting-content-from-v1-to-v2-examples/models/step5/ex_model_Ar_P_Morse_07C/Makefile File

Reference

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12.111 kim-api-v2.0.0-beta.0/docs/porting-content-from-v1-to-v2-examples/models/step5/ex_model_Ar_P_Morse_07C/Makefile File Reference

12.112 kim-api-v2.0.0-beta.0/docs/porting-content-from-v1-to-v2-examples/models/step6/ex_model_Ar_P_MLJ_F03/Makefile File Reference

12.113 kim-api-v2.0.0-beta.0/docs/porting-content-from-v1-to-v2-examples/models/step6/ex_model_Ar_P_Morse_07C/Makefile File Reference

12.114 kim-api-v2.0.0-beta.0/docs/porting-content-from-v1-to-v2-examples/simulators/step0/ex_test_Ar_fcc_cluster/Makefile File Reference

12.115 kim-api-v2.0.0-beta.0/docs/porting-content-from-v1-to-v2-examples/simulators/step0/ex_test_Ar_fcc_cluster_cpp/Makefile File Reference

12.116 kim-api-v2.0.0-beta.0/docs/porting-content-from-v1-to-v2-examples/simulators/step0/ex_test_Ar_fcc_cluster_fortran/Makefile File Reference

12.117 kim-api-v2.0.0-beta.0/docs/porting-content-from-v1-to-v2-examples/simulators/step1/ex_test_Ar_fcc_cluster/Makefile File Reference

12.118 kim-api-v2.0.0-beta.0/docs/porting-content-from-v1-to-v2-examples/simulators/step1/ex_test_Ar_fcc_cluster_cpp/Makefile File Reference

12.119 kim-api-v2.0.0-beta.0/docs/porting-content-from-v1-to-v2-examples/simulators/step1/ex_test_Ar_fcc_cluster_fortran/Makefile File Reference

12.120 kim-api-v2.0.0-beta.0/docs/porting-content-from-v1-to-v2-examples/simulators/step3/ex_test_Ar_fcc_cluster/Makefile File Reference

12.121 kim-api-v2.0.0-beta.0/docs/porting-content-from-v1-to-v2-examples/simulators/step3/ex_test_Ar_fcc_cluster_cpp/Makefile File Reference

12.122 kim-api-v2.0.0-beta.0/docs/porting-content-from-v1-to-v2-examples/simulators/step3/ex_test_Ar_fcc_cluster_fortran/Makefile File Reference

- 12.123 [kim-api-v2.0.0-beta.0/docs/porting-content-from-v1-to-v2-examples/simulators/step4/ex↵
_test_Ar_fcc_cluster/Makefile File Reference](#)
- 12.124 [kim-api-v2.0.0-beta.0/docs/porting-content-from-v1-to-v2-examples/simulators/step4/ex↵
_test_Ar_fcc_cluster_cpp/Makefile File Reference](#)
- 12.125 [kim-api-v2.0.0-beta.0/docs/porting-content-from-v1-to-v2-examples/simulators/step4/ex↵
_test_Ar_fcc_cluster_fortran/Makefile File Reference](#)
- 12.126 [kim-api-v2.0.0-beta.0/docs/porting-content-from-v1-to-v2-examples/simulators/step5/ex↵
_test_Ar_fcc_cluster/Makefile File Reference](#)
- 12.127 [kim-api-v2.0.0-beta.0/docs/porting-content-from-v1-to-v2-examples/simulators/step5/ex↵
_test_Ar_fcc_cluster_cpp/Makefile File Reference](#)
- 12.128 [kim-api-v2.0.0-beta.0/docs/porting-content-from-v1-to-v2-examples/simulators/step5/ex↵
_test_Ar_fcc_cluster_fortran/Makefile File Reference](#)
- 12.129 [kim-api-v2.0.0-beta.0/cpp/include/Makefile File Reference](#)
- 12.130 [kim-api-v2.0.0-beta.0/c/include/Makefile File Reference](#)
- 12.131 [kim-api-v2.0.0-beta.0/fortran/include/Makefile File Reference](#)
- 12.132 [kim-api-v2.0.0-beta.0/examples/model_drivers/ex_model_driver_P_LJ/Makefile
File Reference](#)
- 12.133 [kim-api-v2.0.0-beta.0/examples/model_drivers/ex_model_driver_P_Morse/↵
Makefile File Reference](#)
- 12.134 [kim-api-v2.0.0-beta.0/examples/model_drivers/LennardJones612__MD_414112407348↵
_003/Makefile File Reference](#)
- 12.135 [kim-api-v2.0.0-beta.0/examples/model_drivers/Makefile File Reference](#)

- 12.136 kim-api-v2.0.0-beta.0/examples/models/ex_model_Ar_P_LJ/Makefile File Reference
- 12.137 kim-api-v2.0.0-beta.0/examples/models/ex_model_Ar_P_MLJ_F03/Makefile File Reference
- 12.138 kim-api-v2.0.0-beta.0/examples/models/ex_model_Ar_P_Morse/Makefile File Reference
- 12.139 kim-api-v2.0.0-beta.0/examples/models/ex_model_Ar_P_Morse_07C/Makefile File Reference
- 12.140 kim-api-v2.0.0-beta.0/examples/models/LennardJones612_UniversalShifted__M↵
O_959249795837_003/Makefile File Reference
- 12.141 kim-api-v2.0.0-beta.0/examples/models/Makefile File Reference
- 12.142 kim-api-v2.0.0-beta.0/examples/simulators/ex_test_Ar_fcc_cluster/Makefile File Reference
- 12.143 kim-api-v2.0.0-beta.0/examples/simulators/ex_test_Ar_fcc_cluster_cpp/Makefile File Reference
- 12.144 kim-api-v2.0.0-beta.0/examples/simulators/ex_test_Ar_fcc_cluster_fortran/↵
Makefile File Reference
- 12.145 kim-api-v2.0.0-beta.0/examples/simulators/Makefile File Reference
- 12.146 kim-api-v2.0.0-beta.0/examples/simulators/utility_forces_numer_deriv/Makefile File Reference
- 12.147 kim-api-v2.0.0-beta.0/docs/porting-content-from-v1-to-v2-examples/models/step0/ex↵
_model_Ar_P_Morse_07C/ex_model_Ar_P_Morse_07C.c File Reference

```
#include <stdlib.h>
#include <stdio.h>
#include <string.h>
#include <math.h>
#include "KIM_API_C.h"
#include "KIM_API_status.h"
```

Macros

- `#define DIM 3 /* dimensionality of space */`
- `#define SPECCODE 1 /* internal species code */`
- `#define CUTOFF 8.15 /* Angstroms */`
- `#define EPSILON -0.0134783698072604 /* eV */`
- `#define PARAM_C 1.545 /* 1/Angstroms */`
- `#define RZERO 3.786 /* Angstroms */`

Functions

- `int model_init (void *km)`
- `static int compute (void *km)`
- `static void calc_phi (double *epsilon, double *C, double *Rzero, double *shift, double *cutoff, double r, double *phi)`
- `static void calc_phi_dphi (double *epsilon, double *C, double *Rzero, double *shift, double *cutoff, double r, double *phi, double *dphi)`
- `static void calc_phi_d2phi (double *epsilon, double *C, double *Rzero, double *shift, double *cutoff, double r, double *phi, double *dphi, double *d2phi)`

12.147.1 Macro Definition Documentation

12.147.1.1 CUTOFF

```
#define CUTOFF 8.15 /* Angstroms */
```

Definition at line 55 of file `ex_model_Ar_P_Morse_07C.c`.

12.147.1.2 DIM

```
#define DIM 3 /* dimensionality of space */
```

Definition at line 53 of file `ex_model_Ar_P_Morse_07C.c`.

12.147.1.3 EPSILON

```
#define EPSILON -0.0134783698072604 /* eV */
```

Definition at line 56 of file `ex_model_Ar_P_Morse_07C.c`.

12.147.1.4 PARAM_C

```
#define PARAM_C 1.545 /* 1/Angstroms */
```

Definition at line 57 of file ex_model_Ar_P_Morse_07C.c.

12.147.1.5 RZERO

```
#define RZERO 3.786 /* Angstroms */
```

Definition at line 58 of file ex_model_Ar_P_Morse_07C.c.

12.147.1.6 SPECCODE

```
#define SPECCODE 1 /* internal species code */
```

Definition at line 54 of file ex_model_Ar_P_Morse_07C.c.

12.147.2 Function Documentation

12.147.2.1 calc_phi()

```
static void calc_phi (
    double * epsilon,
    double * C,
    double * Rzero,
    double * shift,
    double * cutoff,
    double r,
    double * phi ) [static]
```

Definition at line 88 of file ex_model_Ar_P_Morse_07C.c.

12.147.2.2 calc_phi_d2phi()

```
static void calc_phi_d2phi (
    double * epsilon,
    double * C,
    double * Rzero,
    double * shift,
    double * cutoff,
    double r,
    double * phi,
    double * dphi,
    double * d2phi ) [static]
```

Definition at line 133 of file ex_model_Ar_P_Morse_07C.c.

12.147.2.3 calc_phi_dphi()

```
static void calc_phi_dphi (
    double * epsilon,
    double * C,
    double * Rzero,
    double * shift,
    double * cutoff,
    double r,
    double * phi,
    double * dphi ) [static]
```

Definition at line 109 of file `ex_model_Ar_P_Morse_07C.c`.

12.147.2.4 compute()

```
static int compute (
    void * km ) [static]
```

Definition at line 159 of file `ex_model_Ar_P_Morse_07C.c`.

12.147.2.5 model_init()

```
int model_init (
    void * km )
```

Definition at line 494 of file `ex_model_Ar_P_Morse_07C.c`.

12.148 kim-api-v2.0.0-beta.0/docs/porting-content-from-v1-to-v2-examples/models/step1/ex_model_Ar_P_Morse_07C/ex_model_Ar_P_Morse_07C.c File Reference

```
#include <stdlib.h>
#include <stdio.h>
#include <string.h>
#include <math.h>
#include "KIM_API_C.h"
#include "KIM_API_status.h"
```

Macros

- `#define DIM 3` /* dimensionality of space */
- `#define SPECCODE 1` /* internal species code */
- `#define CUTOFF 8.15` /* Angstroms */
- `#define EPSILON -0.0134783698072604` /* eV */
- `#define PARAM_C 1.545` /* 1/Angstroms */
- `#define RZERO 3.786` /* Angstroms */

- int [model_init](#) (void *km)
- static int [compute](#) (void *km)
- static void [calc_phi](#) (double *epsilon, double *C, double *Rzero, double *shift, double *cutoff, double r, double *phi)
- static void [calc_phi_dphi](#) (double *epsilon, double *C, double *Rzero, double *shift, double *cutoff, double r, double *phi, double *dphi)
- static void [calc_phi_d2phi](#) (double *epsilon, double *C, double *Rzero, double *shift, double *cutoff, double r, double *phi, double *dphi, double *d2phi)

12.148.1 Macro Definition Documentation

12.148.1.1 CUTOFF

```
#define CUTOFF 8.15 /* Angstroms */
```

Definition at line 55 of file ex_model_Ar_P_Morse_07C.c.

12.148.1.2 DIM

```
#define DIM 3 /* dimensionality of space */
```

Definition at line 53 of file ex_model_Ar_P_Morse_07C.c.

12.148.1.3 EPSILON

```
#define EPSILON -0.0134783698072604 /* eV */
```

Definition at line 56 of file ex_model_Ar_P_Morse_07C.c.

12.148.1.4 PARAM_C

```
#define PARAM_C 1.545 /* 1/Angstroms */
```

Definition at line 57 of file ex_model_Ar_P_Morse_07C.c.

12.148.1.5 RZERO

```
#define RZERO 3.786 /* Angstroms */
```

Definition at line 58 of file `ex_model_Ar_P_Morse_07C.c`.

12.148.1.6 SPECCODE

```
#define SPECCODE 1 /* internal species code */
```

Definition at line 54 of file `ex_model_Ar_P_Morse_07C.c`.

12.148.2 Function Documentation

12.148.2.1 `calc_phi()`

```
static void calc_phi (  
    double * epsilon,  
    double * C,  
    double * Rzero,  
    double * shift,  
    double * cutoff,  
    double r,  
    double * phi ) [static]
```

Definition at line 88 of file `ex_model_Ar_P_Morse_07C.c`.

12.148.2.2 `calc_phi_d2phi()`

```
static void calc_phi_d2phi (  
    double * epsilon,  
    double * C,  
    double * Rzero,  
    double * shift,  
    double * cutoff,  
    double r,  
    double * phi,  
    double * dphi,  
    double * d2phi ) [static]
```

Definition at line 133 of file `ex_model_Ar_P_Morse_07C.c`.

12.148.2.3 calc_phi_dphi()

```
static void calc_phi_dphi (
    double * epsilon,
    double * C,
    double * Rzero,
    double * shift,
    double * cutoff,
    double r,
    double * phi,
    double * dphi ) [static]
```

Definition at line 109 of file ex_model_Ar_P_Morse_07C.c.

12.148.2.4 compute()

```
static int compute (
    void * km ) [static]
```

Definition at line 159 of file ex_model_Ar_P_Morse_07C.c.

12.148.2.5 model_init()

```
int model_init (
    void * km )
```

Definition at line 366 of file ex_model_Ar_P_Morse_07C.c.

12.149 kim-api-v2.0.0-beta.0/docs/porting-content-from-v1-to-v2-examples/models/step3/ex_model_Ar_P_Morse_07C/ex_model_Ar_P_Morse_07C.c File Reference

```
#include <stdlib.h>
#include <stdio.h>
#include <string.h>
#include <math.h>
#include "KIM_ModelHeaders.h"
#include "KIM_ModelCreateLogMacros.h"
```

Macros

- `#define TRUE 1`
- `#define FALSE 0`
- `#define DIM 3 /* dimensionality of space */`
- `#define SPECCODE 1 /* internal species code */`
- `#define CUTOFF 8.15 /* Angstroms */`
- `#define EPSILON -0.0134783698072604 /* eV */`
- `#define PARAM_C 1.545 /* 1/Angstroms */`
- `#define RZERO 3.786 /* Angstroms */`

Typedefs

- typedef struct buffer [buffer](#)

Functions

- int [model_create](#) ([KIM_ModelCreate](#) *const modelCreate, [KIM_LengthUnit](#) const requestedLengthUnit, [KIM_EnergyUnit](#) const requestedEnergyUnit, [KIM_ChargeUnit](#) const requestedChargeUnit, [KIM_TemperatureUnit](#) const requestedTemperatureUnit, [KIM_TimeUnit](#) const requestedTimeUnit)
- static int [compute](#) (void *km)
- static void [calc_phi](#) (double *epsilon, double *C, double *Rzero, double *shift, double *cutoff, double r, double *phi)
- static void [calc_phi_dphi](#) (double *epsilon, double *C, double *Rzero, double *shift, double *cutoff, double r, double *phi, double *dphi)
- static void [calc_phi_d2phi](#) (double *epsilon, double *C, double *Rzero, double *shift, double *cutoff, double r, double *phi, double *dphi, double *d2phi)

12.149.1 Macro Definition Documentation

12.149.1.1 CUTOFF

```
#define CUTOFF 8.15 /* Angstroms */
```

Definition at line 57 of file `ex_model_Ar_P_Morse_07C.c`.

12.149.1.2 DIM

```
#define DIM 3 /* dimensionality of space */
```

Definition at line 55 of file `ex_model_Ar_P_Morse_07C.c`.

12.149.1.3 EPSILON

```
#define EPSILON -0.0134783698072604 /* eV */
```

Definition at line 58 of file `ex_model_Ar_P_Morse_07C.c`.

12.149.1.4 FALSE

```
#define FALSE 0
```

Definition at line 50 of file ex_model_Ar_P_Morse_07C.c.

12.149.1.5 PARAM_C

```
#define PARAM_C 1.545 /* 1/Angstroms */
```

Definition at line 59 of file ex_model_Ar_P_Morse_07C.c.

12.149.1.6 RZERO

```
#define RZERO 3.786 /* Angstroms */
```

Definition at line 60 of file ex_model_Ar_P_Morse_07C.c.

12.149.1.7 SPECCODE

```
#define SPECCODE 1 /* internal species code */
```

Definition at line 56 of file ex_model_Ar_P_Morse_07C.c.

12.149.1.8 TRUE

```
#define TRUE 1
```

Definition at line 49 of file ex_model_Ar_P_Morse_07C.c.

12.149.2 Typedef Documentation

12.149.2.1 buffer

```
typedef struct buffer buffer
```

Definition at line 68 of file ex_model_Ar_P_Morse_07C.c.

12.149.3 Function Documentation

12.149.3.1 `calc_phi()`

```
static void calc_phi (  
    double * epsilon,  
    double * C,  
    double * Rzero,  
    double * shift,  
    double * cutoff,  
    double r,  
    double * phi ) [static]
```

Definition at line 102 of file `ex_model_Ar_P_Morse_07C.c`.

12.149.3.2 `calc_phi_d2phi()`

```
static void calc_phi_d2phi (  
    double * epsilon,  
    double * C,  
    double * Rzero,  
    double * shift,  
    double * cutoff,  
    double r,  
    double * phi,  
    double * dphi,  
    double * d2phi ) [static]
```

Definition at line 147 of file `ex_model_Ar_P_Morse_07C.c`.

12.149.3.3 `calc_phi_dphi()`

```
static void calc_phi_dphi (  
    double * epsilon,  
    double * C,  
    double * Rzero,  
    double * shift,  
    double * cutoff,  
    double r,  
    double * phi,  
    double * dphi ) [static]
```

Definition at line 123 of file `ex_model_Ar_P_Morse_07C.c`.

12.149.3.4 compute()

```
static int compute (
    void * km ) [static]
```

12.149.3.5 model_create()

```
int model_create (
    KIM_ModelCreate *const modelCreate,
    KIM_LengthUnit const requestedLengthUnit,
    KIM_EnergyUnit const requestedEnergyUnit,
    KIM_ChargeUnit const requestedChargeUnit,
    KIM_TemperatureUnit const requestedTemperatureUnit,
    KIM_TimeUnit const requestedTimeUnit )
```

- compute function */

Definition at line 381 of file ex_model_Ar_P_Morse_07C.c.

12.150 kim-api-v2.0.0-beta.0/docs/porting-content-from-v1-to-v2-examples/models/step4/ex_model_Ar_P_Morse_07C/ex_model_Ar_P_Morse_07C.c File Reference

```
#include <stdlib.h>
#include <stdio.h>
#include <string.h>
#include <math.h>
#include "KIM_ModelHeaders.h"
#include "KIM_ModelCreateLogMacros.h"
#include "KIM_ModelComputeArgumentsCreateLogMacros.h"
#include "KIM_ModelComputeArgumentsDestroyLogMacros.h"
```

Macros

- #define TRUE 1
- #define FALSE 0
- #define DIM 3 /* dimensionality of space */
- #define SPECCODE 1 /* internal species code */
- #define CUTOFF 8.15 /* Angstroms */
- #define EPSILON -0.0134783698072604 /* eV */
- #define PARAM_C 1.545 /* 1/Angstroms */
- #define RZERO 3.786 /* Angstroms */

Typedefs

- typedef struct buffer buffer

Functions

- int [model_create](#) ([KIM_ModelCreate](#) *const modelCreate, [KIM_LengthUnit](#) const requestedLengthUnit, [KIM_EnergyUnit](#) const requestedEnergyUnit, [KIM_ChargeUnit](#) const requestedChargeUnit, [KIM_TemperatureUnit](#) const requestedTemperatureUnit, [KIM_TimeUnit](#) const requestedTimeUnit)
- static int [compute](#) (void *km)
- static int [compute_arguments_create](#) ([KIM_ModelCompute](#) const *const modelCompute, [KIM_ModelComputeArgumentsCreate](#) *const modelComputeArgumentsCreate)
- static int [compute_arguments_destroy](#) ([KIM_ModelCompute](#) const *const modelCompute, [KIM_ModelComputeArgumentsDestroy](#) *const modelComputeArgumentsDestroy)
- static void [calc_phi](#) (double *epsilon, double *C, double *Rzero, double *shift, double *cutoff, double r, double *phi)
- static void [calc_phi_dphi](#) (double *epsilon, double *C, double *Rzero, double *shift, double *cutoff, double r, double *phi, double *dphi)
- static void [calc_phi_d2phi](#) (double *epsilon, double *C, double *Rzero, double *shift, double *cutoff, double r, double *phi, double *dphi, double *d2phi)

12.150.1 Macro Definition Documentation

12.150.1.1 CUTOFF

```
#define CUTOFF 8.15 /* Angstroms */
```

Definition at line 57 of file `ex_model_Ar_P_Morse_07C.c`.

12.150.1.2 DIM

```
#define DIM 3 /* dimensionality of space */
```

Definition at line 55 of file `ex_model_Ar_P_Morse_07C.c`.

12.150.1.3 EPSILON

```
#define EPSILON -0.0134783698072604 /* eV */
```

Definition at line 58 of file `ex_model_Ar_P_Morse_07C.c`.

12.150.1.4 FALSE

```
#define FALSE 0
```

Definition at line 50 of file `ex_model_Ar_P_Morse_07C.c`.

12.150.1.5 PARAM_C

```
#define PARAM_C 1.545 /* 1/Angstroms */
```

Definition at line 59 of file ex_model_Ar_P_Morse_07C.c.

12.150.1.6 RZERO

```
#define RZERO 3.786 /* Angstroms */
```

Definition at line 60 of file ex_model_Ar_P_Morse_07C.c.

12.150.1.7 SPECCODE

```
#define SPECCODE 1 /* internal species code */
```

Definition at line 56 of file ex_model_Ar_P_Morse_07C.c.

12.150.1.8 TRUE

```
#define TRUE 1
```

Definition at line 49 of file ex_model_Ar_P_Morse_07C.c.

12.150.2 Typedef Documentation

12.150.2.1 buffer

```
typedef struct buffer buffer
```

Definition at line 68 of file ex_model_Ar_P_Morse_07C.c.

12.150.3 Function Documentation

12.150.3.1 `calc_phi()`

```
static void calc_phi (
    double * epsilon,
    double * C,
    double * Rzero,
    double * shift,
    double * cutoff,
    double r,
    double * phi ) [static]
```

Definition at line 108 of file `ex_model_Ar_P_Morse_07C.c`.

12.150.3.2 `calc_phi_d2phi()`

```
static void calc_phi_d2phi (
    double * epsilon,
    double * C,
    double * Rzero,
    double * shift,
    double * cutoff,
    double r,
    double * phi,
    double * dphi,
    double * d2phi ) [static]
```

Definition at line 153 of file `ex_model_Ar_P_Morse_07C.c`.

12.150.3.3 `calc_phi_dphi()`

```
static void calc_phi_dphi (
    double * epsilon,
    double * C,
    double * Rzero,
    double * shift,
    double * cutoff,
    double r,
    double * phi,
    double * dphi ) [static]
```

Definition at line 129 of file `ex_model_Ar_P_Morse_07C.c`.

12.150.3.4 `compute()`

```
static int compute (
    void * km ) [static]
```

12.150.3.5 compute_arguments_create()

```
static int compute_arguments_create (
    KIM_ModelCompute const *const modelCompute,
    KIM_ModelComputeArgumentsCreate *const modelComputeArgumentsCreate ) [static]
```

Definition at line 482 of file ex_model_Ar_P_Morse_07C.c.

12.150.3.6 compute_arguments_destroy()

```
static int compute_arguments_destroy (
    KIM_ModelCompute const *const modelCompute,
    KIM_ModelComputeArgumentsDestroy *const modelComputeArgumentsDestroy ) [static]
```

Definition at line 531 of file ex_model_Ar_P_Morse_07C.c.

12.150.3.7 model_create()

```
int model_create (
    KIM_ModelCreate *const modelCreate,
    KIM_LengthUnit const requestedLengthUnit,
    KIM_EnergyUnit const requestedEnergyUnit,
    KIM_ChargeUnit const requestedChargeUnit,
    KIM_TemperatureUnit const requestedTemperatureUnit,
    KIM_TimeUnit const requestedTimeUnit )
```

- compute function */

Definition at line 387 of file ex_model_Ar_P_Morse_07C.c.

12.151 kim-api-v2.0.0-beta.0/docs/porting-content-from-v1-to-v2-examples/models/step5/ex_model_Ar_P_Morse_07C/ex_model_Ar_P_Morse_07C.c File Reference

```
#include <stdlib.h>
#include <stdio.h>
#include <string.h>
#include <math.h>
#include "KIM_ModelHeaders.h"
#include "KIM_ModelCreateLogMacros.h"
#include "KIM_ModelRefreshLogMacros.h"
#include "KIM_ModelDestroyLogMacros.h"
#include "KIM_ModelComputeArgumentsCreateLogMacros.h"
#include "KIM_ModelComputeArgumentsDestroyLogMacros.h"
```

Macros

- `#define TRUE 1`
- `#define FALSE 0`
- `#define DIM 3 /* dimensionality of space */`
- `#define SPECCODE 1 /* internal species code */`
- `#define CUTOFF 8.15 /* Angstroms */`
- `#define EPSILON -0.0134783698072604 /* eV */`
- `#define PARAM_C 1.545 /* 1/Angstroms */`
- `#define RZERO 3.786 /* Angstroms */`

Typedefs

- `typedef struct buffer buffer`

Functions

- `int model_create (KIM_ModelCreate *const modelCreate, KIM_LengthUnit const requestedLengthUnit, KIM_EnergyUnit const requestedEnergyUnit, KIM_ChargeUnit const requestedChargeUnit, KIM_TemperatureUnit const requestedTemperatureUnit, KIM_TimeUnit const requestedTimeUnit)`
- `static int compute (void *km)`
- `static int compute_arguments_create (KIM_ModelCompute const *const modelCompute, KIM_ModelComputeArgumentsCreate *const modelComputeArgumentsCreate)`
- `static int compute_arguments_destroy (KIM_ModelCompute const *const modelCompute, KIM_ModelComputeArgumentsDestroy *const modelComputeArgumentsDestroy)`
- `static int model_refresh (KIM_ModelRefresh *const modelRefresh)`
- `static int model_destroy (KIM_ModelDestroy *const modelDestroy)`
- `static void calc_phi (double *epsilon, double *C, double *Rzero, double *shift, double *cutoff, double r, double *phi)`
- `static void calc_phi_dphi (double *epsilon, double *C, double *Rzero, double *shift, double *cutoff, double r, double *phi, double *dphi)`
- `static void calc_phi_d2phi (double *epsilon, double *C, double *Rzero, double *shift, double *cutoff, double r, double *phi, double *dphi, double *d2phi)`

12.151.1 Macro Definition Documentation

12.151.1.1 CUTOFF

```
#define CUTOFF 8.15 /* Angstroms */
```

Definition at line 57 of file `ex_model_Ar_P_Morse_07C.c`.

12.151.1.2 DIM

```
#define DIM 3 /* dimensionality of space */
```

Definition at line 55 of file ex_model_Ar_P_Morse_07C.c.

12.151.1.3 EPSILON

```
#define EPSILON -0.0134783698072604 /* eV */
```

Definition at line 58 of file ex_model_Ar_P_Morse_07C.c.

12.151.1.4 FALSE

```
#define FALSE 0
```

Definition at line 50 of file ex_model_Ar_P_Morse_07C.c.

12.151.1.5 PARAM_C

```
#define PARAM_C 1.545 /* 1/Angstroms */
```

Definition at line 59 of file ex_model_Ar_P_Morse_07C.c.

12.151.1.6 RZERO

```
#define RZERO 3.786 /* Angstroms */
```

Definition at line 60 of file ex_model_Ar_P_Morse_07C.c.

12.151.1.7 SPECCODE

```
#define SPECCODE 1 /* internal species code */
```

Definition at line 56 of file ex_model_Ar_P_Morse_07C.c.

12.151.1.8 TRUE

```
#define TRUE 1
```

Definition at line 49 of file `ex_model_Ar_P_Morse_07C.c`.

12.151.2 Typedef Documentation

12.151.2.1 buffer

```
typedef struct buffer buffer
```

Definition at line 68 of file `ex_model_Ar_P_Morse_07C.c`.

12.151.3 Function Documentation

12.151.3.1 calc_phi()

```
static void calc_phi (  
    double * epsilon,  
    double * C,  
    double * Rzero,  
    double * shift,  
    double * cutoff,  
    double r,  
    double * phi ) [static]
```

Definition at line 110 of file `ex_model_Ar_P_Morse_07C.c`.

12.151.3.2 calc_phi_d2phi()

```
static void calc_phi_d2phi (  
    double * epsilon,  
    double * C,  
    double * Rzero,  
    double * shift,  
    double * cutoff,  
    double r,  
    double * phi,  
    double * dphi,  
    double * d2phi ) [static]
```

Definition at line 155 of file `ex_model_Ar_P_Morse_07C.c`.

12.151.3.3 calc_phi_dphi()

```
static void calc_phi_dphi (
    double * epsilon,
    double * C,
    double * Rzero,
    double * shift,
    double * cutoff,
    double r,
    double * phi,
    double * dphi ) [static]
```

Definition at line 131 of file ex_model_Ar_P_Morse_07C.c.

12.151.3.4 compute()

```
static int compute (
    void * km ) [static]
```

12.151.3.5 compute_arguments_create()

```
static int compute_arguments_create (
    KIM_ModelCompute const *const modelCompute,
    KIM_ModelComputeArgumentsCreate *const modelComputeArgumentsCreate ) [static]
```

Definition at line 515 of file ex_model_Ar_P_Morse_07C.c.

12.151.3.6 compute_arguments_destroy()

```
static int compute_arguments_destroy (
    KIM_ModelCompute const *const modelCompute,
    KIM_ModelComputeArgumentsDestroy *const modelComputeArgumentsDestroy ) [static]
```

Definition at line 560 of file ex_model_Ar_P_Morse_07C.c.

12.151.3.7 model_create()

```
int model_create (
    KIM_ModelCreate *const modelCreate,
    KIM_LengthUnit const requestedLengthUnit,
    KIM_EnergyUnit const requestedEnergyUnit,
    KIM_ChargeUnit const requestedChargeUnit,
    KIM_TemperatureUnit const requestedTemperatureUnit,
    KIM_TimeUnit const requestedTimeUnit )
```

- compute function */

Definition at line 389 of file ex_model_Ar_P_Morse_07C.c.

12.151.3.8 `model_destroy()`

```
int model_destroy (
    KIM_ModelDestroy *const modelDestroy )    [static]
```

Definition at line 502 of file `ex_model_Ar_P_Morse_07C.c`.

12.151.3.9 `model_refresh()`

```
static int model_refresh (
    KIM_ModelRefresh *const modelRefresh )    [static]
```

Definition at line 481 of file `ex_model_Ar_P_Morse_07C.c`.

12.152 `kim-api-v2.0.0-beta.0/docs/porting-content-from-v1-to-v2-examples/models/step6/ex_model_Ar_P_Morse_07C/ex_model_Ar_P_Morse_07C.c` File Reference

```
#include <stdlib.h>
#include <stdio.h>
#include <string.h>
#include <math.h>
#include "KIM_ModelHeaders.h"
#include "KIM_ModelComputeLogMacros.h"
#include "KIM_ModelCreateLogMacros.h"
#include "KIM_ModelRefreshLogMacros.h"
#include "KIM_ModelDestroyLogMacros.h"
#include "KIM_ModelComputeArgumentsCreateLogMacros.h"
#include "KIM_ModelComputeArgumentsDestroyLogMacros.h"
```

Macros

- `#define TRUE 1`
- `#define FALSE 0`
- `#define DIM 3` /* dimensionality of space */
- `#define SPECCODE 1` /* internal species code */
- `#define CUTOFF 8.15` /* Angstroms */
- `#define EPSILON -0.0134783698072604` /* eV */
- `#define PARAM_C 1.545` /* 1/Angstroms */
- `#define RZERO 3.786` /* Angstroms */

Typedefs

- `typedef struct buffer` `buffer`

- int `model_create` (`KIM_ModelCreate` *const modelCreate, `KIM_LengthUnit` const requestedLengthUnit, `KIM_EnergyUnit` const requestedEnergyUnit, `KIM_ChargeUnit` const requestedChargeUnit, `KIM_TemperatureUnit` const requestedTemperatureUnit, `KIM_TimeUnit` const requestedTimeUnit)
- static int `compute` (`KIM_ModelCompute` const *const modelCompute, `KIM_ModelComputeArguments` const *const modelComputeArguments)
- static int `compute_arguments_create` (`KIM_ModelCompute` const *const modelCompute, `KIM_ModelComputeArgumentsCreate` *const modelComputeArgumentsCreate)
- static int `compute_arguments_destroy` (`KIM_ModelCompute` const *const modelCompute, `KIM_ModelComputeArgumentsDestroy` *const modelComputeArgumentsDestroy)
- static int `model_refresh` (`KIM_ModelRefresh` *const modelRefresh)
- static int `model_destroy` (`KIM_ModelDestroy` *const modelDestroy)
- static void `calc_phi` (double *epsilon, double *C, double *Rzero, double *shift, double *cutoff, double r, double *phi)
- static void `calc_phi_dphi` (double *epsilon, double *C, double *Rzero, double *shift, double *cutoff, double r, double *phi, double *dphi)
- static void `calc_phi_d2phi` (double *epsilon, double *C, double *Rzero, double *shift, double *cutoff, double r, double *phi, double *dphi, double *d2phi)

12.152.1 Macro Definition Documentation

12.152.1.1 CUTOFF

```
#define CUTOFF 8.15 /* Angstroms */
```

Definition at line 57 of file `ex_model_Ar_P_Morse_07C.c`.

12.152.1.2 DIM

```
#define DIM 3 /* dimensionality of space */
```

Definition at line 55 of file `ex_model_Ar_P_Morse_07C.c`.

12.152.1.3 EPSILON

```
#define EPSILON -0.0134783698072604 /* eV */
```

Definition at line 58 of file `ex_model_Ar_P_Morse_07C.c`.

12.152.1.4 FALSE

```
#define FALSE 0
```

Definition at line 50 of file `ex_model_Ar_P_Morse_07C.c`.

12.152.1.5 PARAM_C

```
#define PARAM_C 1.545 /* 1/Angstroms */
```

Definition at line 59 of file `ex_model_Ar_P_Morse_07C.c`.

12.152.1.6 RZERO

```
#define RZERO 3.786 /* Angstroms */
```

Definition at line 60 of file `ex_model_Ar_P_Morse_07C.c`.

12.152.1.7 SPECCODE

```
#define SPECCODE 1 /* internal species code */
```

Definition at line 56 of file `ex_model_Ar_P_Morse_07C.c`.

12.152.1.8 TRUE

```
#define TRUE 1
```

Definition at line 49 of file `ex_model_Ar_P_Morse_07C.c`.

12.152.2 Typedef Documentation

12.152.2.1 buffer

```
typedef struct buffer buffer
```

Definition at line 68 of file `ex_model_Ar_P_Morse_07C.c`.

12.152.3.1 calc_phi()

```
static void calc_phi (
    double * epsilon,
    double * C,
    double * Rzero,
    double * shift,
    double * cutoff,
    double r,
    double * phi ) [static]
```

Definition at line 112 of file ex_model_Ar_P_Morse_07C.c.

12.152.3.2 calc_phi_d2phi()

```
static void calc_phi_d2phi (
    double * epsilon,
    double * C,
    double * Rzero,
    double * shift,
    double * cutoff,
    double r,
    double * phi,
    double * dphi,
    double * d2phi ) [static]
```

Definition at line 157 of file ex_model_Ar_P_Morse_07C.c.

12.152.3.3 calc_phi_dphi()

```
static void calc_phi_dphi (
    double * epsilon,
    double * C,
    double * Rzero,
    double * shift,
    double * cutoff,
    double r,
    double * phi,
    double * dphi ) [static]
```

Definition at line 133 of file ex_model_Ar_P_Morse_07C.c.

12.152.3.4 compute()

```
static int compute (
    KIM_ModelCompute const *const modelCompute,
    KIM_ModelComputeArguments const *const modelComputeArguments ) [static]
```

Definition at line 184 of file ex_model_Ar_P_Morse_07C.c.

12.152.3.5 compute_arguments_create()

```
static int compute_arguments_create (
    KIM_ModelCompute const *const modelCompute,
    KIM_ModelComputeArgumentsCreate *const modelComputeArgumentsCreate ) [static]
```

Definition at line 554 of file ex_model_Ar_P_Morse_07C.c.

12.152.3.6 compute_arguments_destroy()

```
static int compute_arguments_destroy (
    KIM_ModelCompute const *const modelCompute,
    KIM_ModelComputeArgumentsDestroy *const modelComputeArgumentsDestroy ) [static]
```

Definition at line 599 of file ex_model_Ar_P_Morse_07C.c.

12.152.3.7 model_create()

```
int model_create (
    KIM_ModelCreate *const modelCreate,
    KIM_LengthUnit const requestedLengthUnit,
    KIM_EnergyUnit const requestedEnergyUnit,
    KIM_ChargeUnit const requestedChargeUnit,
    KIM_TemperatureUnit const requestedTemperatureUnit,
    KIM_TimeUnit const requestedTimeUnit )
```

Definition at line 428 of file ex_model_Ar_P_Morse_07C.c.

12.152.3.8 model_destroy()

```
int model_destroy (
    KIM_ModelDestroy *const modelDestroy ) [static]
```

Definition at line 541 of file ex_model_Ar_P_Morse_07C.c.

12.152.3.9 model_refresh()

```
static int model_refresh (
    KIM_ModelRefresh *const modelRefresh ) [static]
```

Definition at line 520 of file ex_model_Ar_P_Morse_07C.c.

12.153 kim-api-v2.0.0-beta.0/examples/models/ex_model_Ar_P_Morse_07C/ex_model_Ar_P_Morse_07C.c File Reference

```
#include <stdlib.h>
#include <stdio.h>
#include <string.h>
#include <math.h>
#include "KIM_ModelHeaders.h"
#include "KIM_ModelComputeLogMacros.h"
#include "KIM_ModelCreateLogMacros.h"
#include "KIM_ModelRefreshLogMacros.h"
#include "KIM_ModelDestroyLogMacros.h"
#include "KIM_ModelComputeArgumentsCreateLogMacros.h"
#include "KIM_ModelComputeArgumentsDestroyLogMacros.h"
```

Macros

- #define TRUE 1
- #define FALSE 0
- #define DIM 3 /* dimensionality of space */
- #define SPECCODE 1 /* internal species code */
- #define CUTOFF 8.15 /* Angstroms */
- #define EPSILON -0.0134783698072604 /* eV */
- #define PARAM_C 1.545 /* 1/Angstroms */
- #define RZERO 3.786 /* Angstroms */

Typedefs

- typedef struct buffer buffer

Functions

- int model_create (KIM_ModelCreate *const modelCreate, KIM_LengthUnit const requestedLengthUnit, KIM_EnergyUnit const requestedEnergyUnit, KIM_ChargeUnit const requestedChargeUnit, KIM_TemperatureUnit const requestedTemperatureUnit, KIM_TimeUnit const requestedTimeUnit)
- static int compute (KIM_ModelCompute const *const modelCompute, KIM_ModelComputeArguments const *const modelComputeArguments)
- static int compute_arguments_create (KIM_ModelCompute const *const modelCompute, KIM_ModelComputeArgumentsCreate *const modelComputeArgumentsCreate)
- static int compute_arguments_destroy (KIM_ModelCompute const *const modelCompute, KIM_ModelComputeArgumentsDestroy *const modelComputeArgumentsDestroy)
- static int model_refresh (KIM_ModelRefresh *const modelRefresh)
- static int model_destroy (KIM_ModelDestroy *const modelDestroy)
- static void calc_phi (double *epsilon, double *C, double *Rzero, double *shift, double *cutoff, double r, double *phi)
- static void calc_phi_dphi (double *epsilon, double *C, double *Rzero, double *shift, double *cutoff, double r, double *phi, double *dphi)
- static void calc_phi_d2phi (double *epsilon, double *C, double *Rzero, double *shift, double *cutoff, double r, double *phi, double *dphi, double *d2phi)

12.153.1 Macro Definition Documentation

12.153.1.1 CUTOFF

```
#define CUTOFF 8.15 /* Angstroms */
```

Definition at line 57 of file `ex_model_Ar_P_Morse_07C.c`.

12.153.1.2 DIM

```
#define DIM 3 /* dimensionality of space */
```

Definition at line 55 of file `ex_model_Ar_P_Morse_07C.c`.

12.153.1.3 EPSILON

```
#define EPSILON -0.0134783698072604 /* eV */
```

Definition at line 58 of file `ex_model_Ar_P_Morse_07C.c`.

12.153.1.4 FALSE

```
#define FALSE 0
```

Definition at line 50 of file `ex_model_Ar_P_Morse_07C.c`.

12.153.1.5 PARAM_C

```
#define PARAM_C 1.545 /* 1/Angstroms */
```

Definition at line 59 of file `ex_model_Ar_P_Morse_07C.c`.

12.153.1.6 RZERO

```
#define RZERO 3.786 /* Angstroms */
```

Definition at line 60 of file ex_model_Ar_P_Morse_07C.c.

12.153.1.7 SPECCODE

```
#define SPECCODE 1 /* internal species code */
```

Definition at line 56 of file ex_model_Ar_P_Morse_07C.c.

12.153.1.8 TRUE

```
#define TRUE 1
```

Definition at line 49 of file ex_model_Ar_P_Morse_07C.c.

12.153.2 Typedef Documentation

12.153.2.1 buffer

```
typedef struct buffer buffer
```

Definition at line 68 of file ex_model_Ar_P_Morse_07C.c.

12.153.3 Function Documentation

12.153.3.1 calc_phi()

```
static void calc_phi (  
    double * epsilon,  
    double * C,  
    double * Rzero,  
    double * shift,  
    double * cutoff,  
    double r,  
    double * phi ) [static]
```

Definition at line 112 of file ex_model_Ar_P_Morse_07C.c.

12.153.3.2 calc_phi_d2phi()

```
static void calc_phi_d2phi (
    double * epsilon,
    double * C,
    double * Rzero,
    double * shift,
    double * cutoff,
    double r,
    double * phi,
    double * dphi,
    double * d2phi ) [static]
```

Definition at line 157 of file `ex_model_Ar_P_Morse_07C.c`.

12.153.3.3 calc_phi_dphi()

```
static void calc_phi_dphi (
    double * epsilon,
    double * C,
    double * Rzero,
    double * shift,
    double * cutoff,
    double r,
    double * phi,
    double * dphi ) [static]
```

Definition at line 133 of file `ex_model_Ar_P_Morse_07C.c`.

12.153.3.4 compute()

```
static int compute (
    KIM_ModelCompute const *const modelCompute,
    KIM_ModelComputeArguments const *const modelComputeArguments ) [static]
```

Definition at line 184 of file `ex_model_Ar_P_Morse_07C.c`.

12.153.3.5 compute_arguments_create()

```
static int compute_arguments_create (
    KIM_ModelCompute const *const modelCompute,
    KIM_ModelComputeArgumentsCreate *const modelComputeArgumentsCreate ) [static]
```

Definition at line 554 of file `ex_model_Ar_P_Morse_07C.c`.

12.153.3.6 compute_arguments_destroy()

```
static int compute_arguments_destroy (
    KIM_ModelCompute const *const modelCompute,
    KIM_ModelComputeArgumentsDestroy *const modelComputeArgumentsDestroy ) [static]
```

Definition at line 599 of file ex_model_Ar_P_Morse_07C.c.

12.153.3.7 model_create()

```
int model_create (
    KIM_ModelCreate *const modelCreate,
    KIM_LengthUnit const requestedLengthUnit,
    KIM_EnergyUnit const requestedEnergyUnit,
    KIM_ChargeUnit const requestedChargeUnit,
    KIM_TemperatureUnit const requestedTemperatureUnit,
    KIM_TimeUnit const requestedTimeUnit )
```

Definition at line 428 of file ex_model_Ar_P_Morse_07C.c.

12.153.3.8 model_destroy()

```
int model_destroy (
    KIM_ModelDestroy *const modelDestroy ) [static]
```

Definition at line 541 of file ex_model_Ar_P_Morse_07C.c.

12.153.3.9 model_refresh()

```
static int model_refresh (
    KIM_ModelRefresh *const modelRefresh ) [static]
```

Definition at line 520 of file ex_model_Ar_P_Morse_07C.c.

12.154 kim-api-v2.0.0-beta.0/docs/porting-content-from-v1-to-v2-examples/simulators/step0/ex_test_Ar_fcc_cluster/ex_test_Ar_fcc_cluster.c File Reference

```
#include <stdlib.h>
#include <stdio.h>
#include <math.h>
#include "KIM_API_C.h"
#include "KIM_API_status.h"
```

Macros

- `#define NAMESTRLEN 128`
- `#define FCCSPACING 5.260`
- `#define DIM 3`
- `#define NCELLSPERSIDE 2`
- `#define NCLUSTERPARTS`
- `#define REPORT_ERROR(LN, FL, MSG, STAT)`

Functions

- `void fcc_cluster_neighborlist` (int half, int numberOfParticles, double *coords, double cutoff, NeighList *nl)
- `int get_cluster_neigh` (void *kimmdl, int *mode, int *request, int *part, int *numnei, int **nei1part, double **Rij)
- `void create_FCC_cluster` (double FCCspacing, int nCellsPerSide, double *coords)
- `int main` ()

12.154.1 Macro Definition Documentation

12.154.1.1 DIM

```
#define DIM 3
```

Definition at line 42 of file `ex_test_Ar_fcc_cluster.c`.

12.154.1.2 FCCSPACING

```
#define FCCSPACING 5.260
```

Definition at line 41 of file `ex_test_Ar_fcc_cluster.c`.

12.154.1.3 NAMESTRLEN

```
#define NAMESTRLEN 128
```

Definition at line 39 of file `ex_test_Ar_fcc_cluster.c`.

12.154.1.4 NCELLSPERSIDE

```
#define NCELLSPERSIDE 2
```

Definition at line 43 of file ex_test_Ar_fcc_cluster.c.

12.154.1.5 NCLUSTERPARTS

```
#define NCLUSTERPARTS
```

Value:

```
(4*(NCELLSPERSIDE*NCELLSPERSIDE*NCELLSPERSIDE) + \
                                     6*(NCELLSPERSIDE*NCELLSPERSIDE) \
                                     + 3*(NCELLSPERSIDE) + 1)
```

Definition at line 44 of file ex_test_Ar_fcc_cluster.c.

12.154.1.6 REPORT_ERROR

```
#define REPORT_ERROR(  
    LN,  
    FL,  
    MSG,  
    STAT )
```

Value:

```
{  
    \ KIM_API_report_error(LN, FL, MSG, STAT); \  
    exit(STAT); \  
}
```

Definition at line 48 of file ex_test_Ar_fcc_cluster.c.

12.154.2 Function Documentation

12.154.2.1 create_FCC_cluster()

```
void create_FCC_cluster (  
    double FCCspacing,  
    int nCellsPerSide,  
    double * coords )
```

Definition at line 206 of file ex_test_Ar_fcc_cluster.c.

12.154.2.2 fcc_cluster_neighborlist()

```
void fcc_cluster_neighborlist (
    int half,
    int numberOfParticles,
    double * coords,
    double cutoff,
    NeighList * nl )
```

Definition at line 324 of file `ex_test_Ar_fcc_cluster.c`.

12.154.2.3 get_cluster_neigh()

```
int get_cluster_neigh (
    void * kimmcl,
    int * mode,
    int * request,
    int * part,
    int * numnei,
    int ** neilpart,
    double ** Rij )
```

Definition at line 368 of file `ex_test_Ar_fcc_cluster.c`.

12.154.2.4 main()

```
int main ( )
```

Definition at line 72 of file `ex_test_Ar_fcc_cluster.c`.

12.155 [kim-api-v2.0.0-beta.0/docs/porting-content-from-v1-to-v2-examples/simulators/step1/ex_test_Ar_fcc_cluster/ex_test_Ar_fcc_cluster.c](#) File Reference

```
#include <stdlib.h>
#include <stdio.h>
#include <math.h>
#include "KIM_API_C.h"
#include "KIM_API_status.h"
```

Macros

- `#define NAMESTRLEN` 128
- `#define FCCSPACING` 5.260
- `#define DIM` 3
- `#define NCELLSPERSIDE` 2
- `#define NCLUSTERPARTS`
- `#define REPORT_ERROR`(LN, FL, MSG, STAT)

- void [fcc_cluster_neighborlist](#) (int half, int numberOfParticles, double *coords, double cutoff, NeighList *nl)
- int [get_cluster_neigh](#) (void *kimmdl, int *mode, int *request, int *part, int *numnei, int **nei1part, double **Rij)
- void [create_FCC_cluster](#) (double FCCspacing, int nCellsPerSide, double *coords)
- int [main](#) ()

12.155.1 Macro Definition Documentation

12.155.1.1 DIM

```
#define DIM 3
```

Definition at line 42 of file ex_test_Ar_fcc_cluster.c.

12.155.1.2 FCCSPACING

```
#define FCCSPACING 5.260
```

Definition at line 41 of file ex_test_Ar_fcc_cluster.c.

12.155.1.3 NAMESTRLEN

```
#define NAMESTRLEN 128
```

Definition at line 39 of file ex_test_Ar_fcc_cluster.c.

12.155.1.4 NCELLSPERSIDE

```
#define NCELLSPERSIDE 2
```

Definition at line 43 of file ex_test_Ar_fcc_cluster.c.

12.155.1.5 NCLUSTERPARTS

```
#define NCLUSTERPARTS
```

Value:

```
(4*(NCELLSPERSIDE*NCELLSPERSIDE*NCELLSPERSIDE) + \
      6*(NCELLSPERSIDE*NCELLSPERSIDE)           \
      + 3*(NCELLSPERSIDE) + 1)
```

Definition at line 44 of file `ex_test_Ar_fcc_cluster.c`.

12.155.1.6 REPORT_ERROR

```
#define REPORT_ERROR(
    LN,
    FL,
    MSG,
    STAT )
```

Value:

```
{
    \
    KIM_API_report_error(LN, FL, MSG, STAT); \
    exit(STAT);
}
```

Definition at line 48 of file `ex_test_Ar_fcc_cluster.c`.

12.155.2 Function Documentation

12.155.2.1 create_FCC_cluster()

```
void create_FCC_cluster (
    double FCCspacing,
    int nCellsPerSide,
    double * coords )
```

Definition at line 205 of file `ex_test_Ar_fcc_cluster.c`.

12.155.2.2 fcc_cluster_neighborlist()

```
void fcc_cluster_neighborlist (
    int half,
    int numberOfParticles,
    double * coords,
    double cutoff,
    NeighList * nl )
```

Definition at line 323 of file ex_test_Ar_fcc_cluster.c.

12.155.2.3 get_cluster_neigh()

```
int get_cluster_neigh (
    void * kimmdl,
    int * mode,
    int * request,
    int * part,
    int * numnei,
    int ** neilpart,
    double ** Rij )
```

Definition at line 367 of file ex_test_Ar_fcc_cluster.c.

12.155.2.4 main()

```
int main ( )
```

Definition at line 71 of file ex_test_Ar_fcc_cluster.c.

12.156 kim-api-v2.0.0-beta.0/docs/porting-content-from-v1-to-v2-examples/simulators/step3/ex_test_Ar_fcc_cluster/ex_test_Ar_fcc_cluster.c File Reference

```
#include <stdlib.h>
#include <stdio.h>
#include <math.h>
#include "KIM_SimulatorHeaders.h"
```

Macros

- #define TRUE 1
- #define FALSE 0
- #define NAMESTRLEN 128
- #define FCCSPACING 5.260
- #define DIM 3
- #define NCELLSPERSIDE 2
- #define NCLUSTERPARTS
- #define MY_ERROR(message)
- #define MY_WARNING(message)

Functions

- void [fcc_cluster_neighborlist](#) (int half, int numberOfParticles, double *coords, double cutoff, NeighList *nl)
- int [get_cluster_neigh](#) (void const *const dataObject, int const numberOfCutoffs, double const *const cutoffs, int const neighborListIndex, int const particleNumber, int *const numberOfNeighbors, int const **const neighborsOfParticle)
- void [create_FCC_cluster](#) (double FCCspacing, int nCellsPerSide, double *coords)
- int [main](#) ()

12.156.1 Macro Definition Documentation

12.156.1.1 DIM

```
#define DIM 3
```

Definition at line 44 of file `ex_test_Ar_fcc_cluster.c`.

12.156.1.2 FALSE

```
#define FALSE 0
```

Definition at line 39 of file `ex_test_Ar_fcc_cluster.c`.

12.156.1.3 FCCSPACING

```
#define FCCSPACING 5.260
```

Definition at line 43 of file `ex_test_Ar_fcc_cluster.c`.

12.156.1.4 MY_ERROR

```
#define MY_ERROR(  
    message )
```

Value:

```
{  
    printf("* Error : \"%s\" %d:%s\n", message,  
        __LINE__, __FILE__);  
    exit(1);  
}
```

```
\\  
\\  
\\
```

Definition at line 51 of file `ex_test_Ar_fcc_cluster.c`.

12.156.1.5 MY_WARNING

```
#define MY_WARNING(  
    message )
```

Value:

```
{  
    printf("* Error : \"%s\" %d:%s\n", message,  
        __LINE__, __FILE__);  
}
```

Definition at line 58 of file ex_test_Ar_fcc_cluster.c.

12.156.1.6 NAMESTRLEN

```
#define NAMESTRLEN 128
```

Definition at line 41 of file ex_test_Ar_fcc_cluster.c.

12.156.1.7 NCELLSPERSIDE

```
#define NCELLSPERSIDE 2
```

Definition at line 45 of file ex_test_Ar_fcc_cluster.c.

12.156.1.8 NCLUSTERPARTS

```
#define NCLUSTERPARTS
```

Value:

```
(4 * (NCELLSPERSIDE * NCELLSPERSIDE * NCELLSPERSIDE) + \br/>    6 * (NCELLSPERSIDE * NCELLSPERSIDE) + \br/>    3 * (NCELLSPERSIDE) + 1)
```

Definition at line 46 of file ex_test_Ar_fcc_cluster.c.

12.156.1.9 TRUE

```
#define TRUE 1
```

Definition at line 38 of file ex_test_Ar_fcc_cluster.c.

12.156.2 Function Documentation

12.156.2.1 create_FCC_cluster()

```
void create_FCC_cluster (
    double FCCspacing,
    int nCellsPerSide,
    double * coords )
```

Definition at line 222 of file `ex_test_Ar_fcc_cluster.c`.

12.156.2.2 fcc_cluster_neighborlist()

```
void fcc_cluster_neighborlist (
    int half,
    int numberOfParticles,
    double * coords,
    double cutoff,
    NeighList * nl )
```

Definition at line 340 of file `ex_test_Ar_fcc_cluster.c`.

12.156.2.3 get_cluster_neigh()

```
int get_cluster_neigh (
    void const *const dataObject,
    int const numberOfCutoffs,
    double const *const cutoffs,
    int const neighborListIndex,
    int const particleNumber,
    int *const numberOfNeighbors,
    int const **const neighborsOfParticle )
```

Definition at line 386 of file `ex_test_Ar_fcc_cluster.c`.

12.156.2.4 main()

```
int main ( )
```

Definition at line 88 of file `ex_test_Ar_fcc_cluster.c`.

```
#include <stdlib.h>
#include <stdio.h>
#include <math.h>
#include "KIM_SimulatorHeaders.h"
```

Macros

- #define [TRUE](#) 1
- #define [FALSE](#) 0
- #define [NAMESTRLEN](#) 128
- #define [FCCSPACING](#) 5.260
- #define [DIM](#) 3
- #define [NCELLSPERSIDE](#) 2
- #define [NCLUSTERPARTS](#)
- #define [MY_ERROR](#)(message)
- #define [MY_WARNING](#)(message)

Functions

- void [fcc_cluster_neighborlist](#) (int half, int numberOfParticles, double *coords, double cutoff, NeighList *nl)
- int [get_cluster_neigh](#) (void const *const dataObject, int const numberOfCutoffs, double const *const cutoffs, int const neighborListIndex, int const particleNumber, int *const numberOfNeighbors, int const **const neighborsOfParticle)
- void [create_FCC_cluster](#) (double FCCspacing, int nCellsPerSide, double *coords)
- int [main](#) ()

12.157.1 Macro Definition Documentation

12.157.1.1 DIM

```
#define DIM 3
```

Definition at line 44 of file ex_test_Ar_fcc_cluster.c.

12.157.1.2 FALSE

```
#define FALSE 0
```

Definition at line 39 of file ex_test_Ar_fcc_cluster.c.

12.157.1.3 FCCSPACING

```
#define FCCSPACING 5.260
```

Definition at line 43 of file `ex_test_Ar_fcc_cluster.c`.

12.157.1.4 MY_ERROR

```
#define MY_ERROR(  
    message )
```

Value:

```
{  
    printf("* Error : \"%s\" %d:%s\n", message,  
           __LINE__, __FILE__);  
    exit(1);  
}
```

\\
\\
\\

Definition at line 51 of file `ex_test_Ar_fcc_cluster.c`.

12.157.1.5 MY_WARNING

```
#define MY_WARNING(  
    message )
```

Value:

```
{  
    printf("* Error : \"%s\" %d:%s\n", message,  
           __LINE__, __FILE__);  
}
```

\\
\\
\\

Definition at line 58 of file `ex_test_Ar_fcc_cluster.c`.

12.157.1.6 NAMESTRLEN

```
#define NAMESTRLEN 128
```

Definition at line 41 of file `ex_test_Ar_fcc_cluster.c`.

12.157.1.7 NCELLSPERSIDE

```
#define NCELLSPERSIDE 2
```

Definition at line 45 of file ex_test_Ar_fcc_cluster.c.

12.157.1.8 NCLUSTERPARTS

```
#define NCLUSTERPARTS
```

Value:

```
(4*(NCELLSPERSIDE*NCELLSPERSIDE*NCELLSPERSIDE) + \
      6*(NCELLSPERSIDE*NCELLSPERSIDE) + \
      + 3*(NCELLSPERSIDE) + 1)
```

Definition at line 46 of file ex_test_Ar_fcc_cluster.c.

12.157.1.9 TRUE

```
#define TRUE 1
```

Definition at line 38 of file ex_test_Ar_fcc_cluster.c.

12.157.2 Function Documentation

12.157.2.1 create_FCC_cluster()

```
void create_FCC_cluster (
    double FCCspacing,
    int nCellsPerSide,
    double * coords )
```

Definition at line 297 of file ex_test_Ar_fcc_cluster.c.

12.157.2.2 fcc_cluster_neighborlist()

```
void fcc_cluster_neighborlist (
    int half,
    int numberOfParticles,
    double * coords,
    double cutoff,
    NeighList * nl )
```

Definition at line 415 of file `ex_test_Ar_fcc_cluster.c`.

12.157.2.3 get_cluster_neigh()

```
int get_cluster_neigh (
    void const *const dataObject,
    int const numberOfCutoffs,
    double const *const cutoffs,
    int const neighborListIndex,
    int const particleNumber,
    int *const numberOfNeighbors,
    int const **const neighborsOfParticle )
```

Definition at line 461 of file `ex_test_Ar_fcc_cluster.c`.

12.157.2.4 main()

```
int main ( )
```

Definition at line 88 of file `ex_test_Ar_fcc_cluster.c`.

12.158 kim-api-v2.0.0-beta.0/docs/porting-content-from-v1-to-v2-examples/simulators/step5/ex_test_Ar_fcc_cluster/ex_test_Ar_fcc_cluster.c File Reference

```
#include <stdlib.h>
#include <stdio.h>
#include <math.h>
#include "KIM_SimulatorHeaders.h"
```

Macros

- `#define TRUE 1`
- `#define FALSE 0`
- `#define NAMESTRLEN 128`
- `#define FCCSPACING 5.260`
- `#define DIM 3`
- `#define NCELLSPERSIDE 2`
- `#define NCLUSTERPARTS`
- `#define MY_ERROR(message)`
- `#define MY_WARNING(message)`

- void [fcc_cluster_neighborlist](#) (int half, int numberOfParticles, double *coords, double cutoff, NeighList *nl)
- int [get_cluster_neigh](#) (void const *const dataObject, int const numberOfCutoffs, double const *const cutoffs, int const neighborListIndex, int const particleNumber, int *const numberOfNeighbors, int const **const neighborsOfParticle)
- void [create_FCC_cluster](#) (double FCCspacing, int nCellsPerSide, double *coords)
- int [main](#) ()

12.158.1 Macro Definition Documentation

12.158.1.1 DIM

```
#define DIM 3
```

Definition at line 44 of file ex_test_Ar_fcc_cluster.c.

12.158.1.2 FALSE

```
#define FALSE 0
```

Definition at line 39 of file ex_test_Ar_fcc_cluster.c.

12.158.1.3 FCCSPACING

```
#define FCCSPACING 5.260
```

Definition at line 43 of file ex_test_Ar_fcc_cluster.c.

12.158.1.4 MY_ERROR

```
#define MY_ERROR(  
    message )
```

Value:

```
{  
    printf("* Error : \"%s\" %d:%s\n", message,  
        __LINE__, __FILE__);  
    exit(1);  
}
```

Definition at line 51 of file ex_test_Ar_fcc_cluster.c.

12.158.1.5 MY_WARNING

```
#define MY_WARNING(  
    message )
```

Value:

```
{  
    printf("* Error : \"%s\" %d:%s\n", message,  
        __LINE__, __FILE__);  
}
```

Definition at line 58 of file ex_test_Ar_fcc_cluster.c.

12.158.1.6 NAMESTRLEN

```
#define NAMESTRLEN 128
```

Definition at line 41 of file ex_test_Ar_fcc_cluster.c.

12.158.1.7 NCELLSPERSIDE

```
#define NCELLSPERSIDE 2
```

Definition at line 45 of file ex_test_Ar_fcc_cluster.c.

12.158.1.8 NCLUSTERPARTS

```
#define NCLUSTERPARTS
```

Value:

```
(4 * (NCELLSPERSIDE * NCELLSPERSIDE * NCELLSPERSIDE) + \
    6 * (NCELLSPERSIDE * NCELLSPERSIDE) + \
    3 * (NCELLSPERSIDE) + 1)
```

Definition at line 46 of file ex_test_Ar_fcc_cluster.c.

12.158.1.9 TRUE

```
#define TRUE 1
```

Definition at line 38 of file ex_test_Ar_fcc_cluster.c.

12.158.2.1 create_FCC_cluster()

```
void create_FCC_cluster (
    double FCCspacing,
    int nCellsPerSide,
    double * coords )
```

Definition at line 349 of file ex_test_Ar_fcc_cluster.c.

12.158.2.2 fcc_cluster_neighborlist()

```
void fcc_cluster_neighborlist (
    int half,
    int numberOfParticles,
    double * coords,
    double cutoff,
    NeighList * nl )
```

Definition at line 467 of file ex_test_Ar_fcc_cluster.c.

12.158.2.3 get_cluster_neigh()

```
int get_cluster_neigh (
    void const *const dataObject,
    int const numberOfCutoffs,
    double const *const cutoffs,
    int const neighborListIndex,
    int const particleNumber,
    int *const numberOfNeighbors,
    int const **const neighborsOfParticle )
```

Definition at line 513 of file ex_test_Ar_fcc_cluster.c.

12.158.2.4 main()

```
int main ( )
```

Definition at line 88 of file ex_test_Ar_fcc_cluster.c.

12.159 kim-api-v2.0.0-beta.0/examples/simulators/ex_test_Ar_fcc_cluster/ex_test_Ar_fcc_cluster.c File Reference

```
#include <stdlib.h>
#include <stdio.h>
#include <math.h>
#include "KIM_SimulatorHeaders.h"
```

Macros

- `#define TRUE 1`
- `#define FALSE 0`
- `#define NAMESTRLEN 128`
- `#define FCCSPACING 5.260`
- `#define DIM 3`
- `#define NCELLSPERSIDE 2`
- `#define NCLUSTERPARTS`
- `#define MY_ERROR(message)`
- `#define MY_WARNING(message)`

Functions

- void `fcc_cluster_neighborlist` (int half, int numberOfParticles, double *coords, double cutoff, NeighList *nl)
- int `get_cluster_neigh` (void const *const dataObject, int const numberOfCutoffs, double const *const cutoffs, int const neighborListIndex, int const particleNumber, int *const numberOfNeighbors, int const **const neighborsOfParticle)
- void `create_FCC_cluster` (double FCCspacing, int nCellsPerSide, double *coords)
- int `main` ()

12.159.1 Macro Definition Documentation

12.159.1.1 DIM

```
#define DIM 3
```

Definition at line 44 of file `ex_test_Ar_fcc_cluster.c`.

12.159.1.2 FALSE

```
#define FALSE 0
```

Definition at line 39 of file `ex_test_Ar_fcc_cluster.c`.

12.159.1.3 FCCSPACING

```
#define FCCSPACING 5.260
```

Definition at line 43 of file ex_test_Ar_fcc_cluster.c.

12.159.1.4 MY_ERROR

```
#define MY_ERROR(  
    message )
```

Value:

```
{  
    printf("* Error : \"%s\" %d:%s\n", message,  
        __LINE__, __FILE__);  
    exit(1);  
}
```

\\
\\
\\

Definition at line 51 of file ex_test_Ar_fcc_cluster.c.

12.159.1.5 MY_WARNING

```
#define MY_WARNING(  
    message )
```

Value:

```
{  
    printf("* Error : \"%s\" %d:%s\n", message,  
        __LINE__, __FILE__);  
}
```

\\
\\
\\

Definition at line 58 of file ex_test_Ar_fcc_cluster.c.

12.159.1.6 NAMESTRLEN

```
#define NAMESTRLEN 128
```

Definition at line 41 of file ex_test_Ar_fcc_cluster.c.

12.159.1.7 NCELLSPERSIDE

```
#define NCELLSPERSIDE 2
```

Definition at line 45 of file `ex_test_Ar_fcc_cluster.c`.

12.159.1.8 NCLUSTERPARTS

```
#define NCLUSTERPARTS
```

Value:

```
(4*(NCELLSPERSIDE*NCELLSPERSIDE*NCELLSPERSIDE) + \
      6*(NCELLSPERSIDE*NCELLSPERSIDE) + \
      + 3*(NCELLSPERSIDE) + 1)
```

Definition at line 46 of file `ex_test_Ar_fcc_cluster.c`.

12.159.1.9 TRUE

```
#define TRUE 1
```

Definition at line 38 of file `ex_test_Ar_fcc_cluster.c`.

12.159.2 Function Documentation

12.159.2.1 create_FCC_cluster()

```
void create_FCC_cluster (
    double FCCspacing,
    int nCellsPerSide,
    double * coords )
```

Definition at line 349 of file `ex_test_Ar_fcc_cluster.c`.

12.159.2.2 fcc_cluster_neighborlist()

```
void fcc_cluster_neighborlist (
    int half,
    int numberOfParticles,
    double * coords,
    double cutoff,
    NeighList * nl )
```

Definition at line 467 of file ex_test_Ar_fcc_cluster.c.

12.159.2.3 get_cluster_neigh()

```
int get_cluster_neigh (
    void const *const dataObject,
    int const numberOfCutoffs,
    double const *const cutoffs,
    int const neighborListIndex,
    int const particleNumber,
    int *const numberOfNeighbors,
    int const **const neighborsOfParticle )
```

Definition at line 513 of file ex_test_Ar_fcc_cluster.c.

12.159.2.4 main()

```
int main ( )
```

Definition at line 88 of file ex_test_Ar_fcc_cluster.c.

12.160 kim-api-v2.0.0-beta.0/docs/porting-content-from-v1-to-v2-examples/simulators/step0/ex_↵
_test_Ar_fcc_cluster_cpp/ex_test_Ar_fcc_cluster_cpp.cpp File Reference

```
#include <stdlib.h>
#include <iomanip>
#include <string>
#include <cmath>
#include "KIM_API.h"
#include "KIM_API_status.h"
```

Macros

- #define NAMESTRLEN 128
- #define FCCSPACING 5.260
- #define DIM 3
- #define NCELLSPERSIDE 2
- #define NCLUSTERPARTS
- #define REPORT_ERROR(LN, FL, MSG, STAT)

Functions

- char const *const [descriptor](#) ()
- void [fcc_cluster_neighborlist](#) (int half, int numberOfParticles, double *coords, double cutoff, NeighList *nl)
- int [get_cluster_neigh](#) (void *kimmdl, int *mode, int *request, int *part, int *numnei, int **nei1part, double **Rij)
- void [create_FCC_cluster](#) (double FCCspacing, int nCellsPerSide, double *coords)
- int [main](#) ()

12.160.1 Macro Definition Documentation

12.160.1.1 DIM

```
#define DIM 3
```

Definition at line 43 of file `ex_test_Ar_fcc_cluster_cpp.cpp`.

12.160.1.2 FCCSPACING

```
#define FCCSPACING 5.260
```

Definition at line 42 of file `ex_test_Ar_fcc_cluster_cpp.cpp`.

12.160.1.3 NAMESTRLEN

```
#define NAMESTRLEN 128
```

Definition at line 40 of file `ex_test_Ar_fcc_cluster_cpp.cpp`.

12.160.1.4 NCELLSPERSIDE

```
#define NCELLSPERSIDE 2
```

Definition at line 44 of file `ex_test_Ar_fcc_cluster_cpp.cpp`.

12.160.1.5 NCLUSTERPARTS

```
#define NCLUSTERPARTS
```

Value:

```
(4*(NCELLSPERSIDE*NCELLSPERSIDE*NCELLSPERSIDE) + \
      6*(NCELLSPERSIDE*NCELLSPERSIDE) \
      + 3*(NCELLSPERSIDE) + 1)
```

Definition at line 45 of file ex_test_Ar_fcc_cluster_cpp.cpp.

12.160.1.6 REPORT_ERROR

```
#define REPORT_ERROR(
    LN,
    FL,
    MSG,
    STAT )
```

Value:

```
{
    kim_cluster_model.report_error(LN, FL, MSG, STAT); \
    exit(STAT); \
}
```

Definition at line 49 of file ex_test_Ar_fcc_cluster_cpp.cpp.

12.160.2 Function Documentation

12.160.2.1 create_FCC_cluster()

```
void create_FCC_cluster (
    double FCCspacing,
    int nCellsPerSide,
    double * coords )
```

Definition at line 192 of file ex_test_Ar_fcc_cluster_cpp.cpp.

12.160.2.2 descriptor()

```
char const *const descriptor ( )
```

Definition at line 441 of file ex_test_Ar_fcc_cluster_cpp.cpp.

12.160.2.3 fcc_cluster_neighborlist()

```
void fcc_cluster_neighborlist (
    int half,
    int numberOfParticles,
    double * coords,
    double cutoff,
    NeighList * nl )
```

Definition at line 310 of file `ex_test_Ar_fcc_cluster_cpp.cpp`.

12.160.2.4 get_cluster_neigh()

```
int get_cluster_neigh (
    void * kimmdl,
    int * mode,
    int * request,
    int * part,
    int * numnei,
    int ** neilpart,
    double ** Rij )
```

Definition at line 354 of file `ex_test_Ar_fcc_cluster_cpp.cpp`.

12.160.2.5 main()

```
int main ( )
```

Definition at line 74 of file `ex_test_Ar_fcc_cluster_cpp.cpp`.

12.161 [kim-api-v2.0.0-beta.0/docs/porting-content-from-v1-to-v2-examples/simulators/step1/ex_test_Ar_fcc_cluster_cpp/ex_test_Ar_fcc_cluster_cpp.cpp](#) File Reference

```
#include <stdlib.h>
#include <iomanip>
#include <string>
#include <cmath>
#include "KIM_API.h"
#include "KIM_API_status.h"
```

Macros

- `#define NAMESTRLEN` 128
- `#define FCCSPACING` 5.260
- `#define DIM` 3
- `#define NCELLSPERSIDE` 2
- `#define NCLUSTERPARTS`
- `#define REPORT_ERROR`(LN, FL, MSG, STAT)

- char const *const [descriptor](#) ()
- void [fcc_cluster_neighborlist](#) (int half, int numberOfParticles, double *coords, double cutoff, NeighList *nl)
- int [get_cluster_neigh](#) (void *kimmdl, int *mode, int *request, int *part, int *numnei, int **nei1part, double **Rij)
- void [create_FCC_cluster](#) (double FCCspacing, int nCellsPerSide, double *coords)
- int [main](#) ()

12.161.1 Macro Definition Documentation

12.161.1.1 DIM

```
#define DIM 3
```

Definition at line 43 of file ex_test_Ar_fcc_cluster_cpp.cpp.

12.161.1.2 FCCSPACING

```
#define FCCSPACING 5.260
```

Definition at line 42 of file ex_test_Ar_fcc_cluster_cpp.cpp.

12.161.1.3 NAMESTRLEN

```
#define NAMESTRLEN 128
```

Definition at line 40 of file ex_test_Ar_fcc_cluster_cpp.cpp.

12.161.1.4 NCELLSPERSIDE

```
#define NCELLSPERSIDE 2
```

Definition at line 44 of file ex_test_Ar_fcc_cluster_cpp.cpp.

12.161.1.5 NCLUSTERPARTS

```
#define NCLUSTERPARTS
```

Value:

```
(4*(NCELLSPERSIDE*NCELLSPERSIDE*NCELLSPERSIDE) + \
      6*(NCELLSPERSIDE*NCELLSPERSIDE)           \
      + 3*(NCELLSPERSIDE) + 1)
```

Definition at line 45 of file `ex_test_Ar_fcc_cluster_cpp.cpp`.

12.161.1.6 REPORT_ERROR

```
#define REPORT_ERROR(
    LN,
    FL,
    MSG,
    STAT )
```

Value:

```
{
    kim_cluster_model.report_error(LN, FL, MSG, STAT); \
    exit(STAT);
}
```

Definition at line 49 of file `ex_test_Ar_fcc_cluster_cpp.cpp`.

12.161.2 Function Documentation

12.161.2.1 create_FCC_cluster()

```
void create_FCC_cluster (
    double FCCspacing,
    int nCellsPerSide,
    double * coords )
```

Definition at line 191 of file `ex_test_Ar_fcc_cluster_cpp.cpp`.

12.161.2.2 descriptor()

```
char const* const descriptor ( )
```

Definition at line 415 of file `ex_test_Ar_fcc_cluster_cpp.cpp`.

12.161.2.3 fcc_cluster_neighborlist()

```
void fcc_cluster_neighborlist (
    int half,
    int numberOfParticles,
    double * coords,
    double cutoff,
    NeighList * nl )
```

Definition at line 309 of file ex_test_Ar_fcc_cluster_cpp.cpp.

12.161.2.4 get_cluster_neigh()

```
int get_cluster_neigh (
    void * kimmDL,
    int * mode,
    int * request,
    int * part,
    int * numnei,
    int ** neilpart,
    double ** Rij )
```

Definition at line 353 of file ex_test_Ar_fcc_cluster_cpp.cpp.

12.161.2.5 main()

```
int main ( )
```

Definition at line 73 of file ex_test_Ar_fcc_cluster_cpp.cpp.

12.162 kim-api-v2.0.0-beta.0/docs/porting-content-from-v1-to-v2-examples/simulators/step3/ex_↵
_test_Ar_fcc_cluster_cpp/ex_test_Ar_fcc_cluster_cpp.cpp File Reference

```
#include <stdlib.h>
#include <iostream>
#include <iomanip>
#include <string>
#include <cmath>
#include "KIM_LogVerbosity.hpp"
#include "KIM_LanguageName.hpp"
#include "KIM_DataType.hpp"
#include "KIM_SpeciesName.hpp"
#include "KIM_Numbering.hpp"
#include "KIM_Model.hpp"
#include "KIM_ArgumentName.hpp"
#include "KIM_CallbackName.hpp"
#include "KIM_SupportStatus.hpp"
#include "KIM_UnitSystem.hpp"
```

Macros

- `#define NAMESTRLEN 128`
- `#define FCCSPACING 5.260`
- `#define DIM 3`
- `#define NCELLSPERSIDE 2`
- `#define NCLUSTERPARTS`
- `#define MY_ERROR(message)`
- `#define MY_WARNING(message)`

Functions

- `char const *const descriptor ()`
- `void fcc_cluster_neighborlist (int half, int numberOfParticles, double *coords, double cutoff, NeighList *nl)`
- `int get_cluster_neigh (void const *const dataObject, int const numberOfCutoffs, double const *const cutoffs, int const neighborListIndex, int const particleNumber, int *const numberOfNeighbors, int const **const neighborsOfParticle)`
- `void create_FCC_cluster (double FCCspacing, int nCellsPerSide, double *coords)`
- `int main ()`

12.162.1 Macro Definition Documentation

12.162.1.1 DIM

```
#define DIM 3
```

Definition at line 52 of file `ex_test_Ar_fcc_cluster_cpp.cpp`.

12.162.1.2 FCCSPACING

```
#define FCCSPACING 5.260
```

Definition at line 51 of file `ex_test_Ar_fcc_cluster_cpp.cpp`.

12.162.1.3 MY_ERROR

```
#define MY_ERROR(  
    message )
```

Value:

```
{  
    std::cout << "* Error : \"" << message << "\" : "  
                << __LINE__ << " : " << __FILE__ << std::endl;  
    exit(1);  
}
```

Definition at line 58 of file `ex_test_Ar_fcc_cluster_cpp.cpp`.

12.162.1.4 MY_WARNING

```
#define MY_WARNING(  
    message )
```

Value:

```
{  
    std::cout << "* Error : \"" << message << "\" : "  
    << __LINE__ << " : " << __FILE__ << std::endl;  
}
```

Definition at line 65 of file ex_test_Ar_fcc_cluster_cpp.cpp.

12.162.1.5 NAMESTRLEN

```
#define NAMESTRLEN 128
```

Definition at line 49 of file ex_test_Ar_fcc_cluster_cpp.cpp.

12.162.1.6 NCELLSPERSIDE

```
#define NCELLSPERSIDE 2
```

Definition at line 53 of file ex_test_Ar_fcc_cluster_cpp.cpp.

12.162.1.7 NCLUSTERPARTS

```
#define NCLUSTERPARTS
```

Value:

```
(4*(NCELLSPERSIDE*NCELLSPERSIDE*NCELLSPERSIDE) + \  
    6*(NCELLSPERSIDE*NCELLSPERSIDE) \  
    + 3*(NCELLSPERSIDE) + 1)
```

Definition at line 54 of file ex_test_Ar_fcc_cluster_cpp.cpp.

12.162.2 Function Documentation

12.162.2.1 create_FCC_cluster()

```
void create_FCC_cluster (
    double FCCspacing,
    int nCellsPerSide,
    double * coords )
```

Definition at line 215 of file `ex_test_Ar_fcc_cluster_cpp.cpp`.

12.162.2.2 descriptor()

```
char const* const descriptor ( )
```

Definition at line 412 of file `ex_test_Ar_fcc_cluster_cpp.cpp`.

12.162.2.3 fcc_cluster_neighborlist()

```
void fcc_cluster_neighborlist (
    int half,
    int numberOfParticles,
    double * coords,
    double cutoff,
    NeighList * nl )
```

Definition at line 333 of file `ex_test_Ar_fcc_cluster_cpp.cpp`.

12.162.2.4 get_cluster_neigh()

```
int get_cluster_neigh (
    void const *const dataObject,
    int const numberOfCutoffs,
    double const *const cutoffs,
    int const neighborListIndex,
    int const particleNumber,
    int *const numberOfNeighbors,
    int const **const neighborsOfParticle )
```

Definition at line 379 of file `ex_test_Ar_fcc_cluster_cpp.cpp`.

12.162.2.5 main()

```
int main ( )
```

Definition at line 96 of file `ex_test_Ar_fcc_cluster_cpp.cpp`.


```
#include <stdlib.h>
#include <iostream>
#include <iomanip>
#include <string>
#include <cmath>
#include "KIM_LogVerbosity.hpp"
#include "KIM_LanguageName.hpp"
#include "KIM_DataType.hpp"
#include "KIM_SpeciesName.hpp"
#include "KIM_Numbering.hpp"
#include "KIM_Model.hpp"
#include "KIM_ArgumentName.hpp"
#include "KIM_CallbackName.hpp"
#include "KIM_SupportStatus.hpp"
#include "KIM_UnitSystem.hpp"
```

Macros

- #define NAMESTRLEN 128
- #define FCCSPACING 5.260
- #define DIM 3
- #define NCELLSPERSIDE 2
- #define NCLUSTERPARTS
- #define MY_ERROR(message)
- #define MY_WARNING(message)

Functions

- void fcc_cluster_neighborlist (int half, int numberOfParticles, double *coords, double cutoff, NeighList *nl)
- int get_cluster_neigh (void const *const dataObject, int const numberOfCutoffs, double const *const cutoffs, int const neighborListIndex, int const particleNumber, int *const numberOfNeighbors, int const **const neighborsOfParticle)
- void create_FCC_cluster (double FCCspacing, int nCellsPerSide, double *coords)
- int main ()

12.163.1 Macro Definition Documentation

12.163.1.1 DIM

```
#define DIM 3
```

Definition at line 52 of file ex_test_Ar_fcc_cluster_cpp.cpp.

12.163.1.2 FCCSPACING

```
#define FCCSPACING 5.260
```

Definition at line 51 of file `ex_test_Ar_fcc_cluster_cpp.cpp`.

12.163.1.3 MY_ERROR

```
#define MY_ERROR(  
    message )
```

Value:

```
{  
    std::cout << "* Error : \"" << message << "\" : "  
        << __LINE__ << " : " << __FILE__ << std::endl;  
    exit(1);  
}
```

Definition at line 58 of file `ex_test_Ar_fcc_cluster_cpp.cpp`.

12.163.1.4 MY_WARNING

```
#define MY_WARNING(  
    message )
```

Value:

```
{  
    std::cout << "* Error : \"" << message << "\" : "  
        << __LINE__ << " : " << __FILE__ << std::endl;  
}
```

Definition at line 65 of file `ex_test_Ar_fcc_cluster_cpp.cpp`.

12.163.1.5 NAMESTRLEN

```
#define NAMESTRLEN 128
```

Definition at line 49 of file `ex_test_Ar_fcc_cluster_cpp.cpp`.

12.163.1.6 NCELLSPERSIDE

```
#define NCELLSPERSIDE 2
```

Definition at line 53 of file ex_test_Ar_fcc_cluster_cpp.cpp.

12.163.1.7 NCLUSTERPARTS

```
#define NCLUSTERPARTS
```

Value:

```
(4*(NCELLSPERSIDE*NCELLSPERSIDE*NCELLSPERSIDE) + \
    6*(NCELLSPERSIDE*NCELLSPERSIDE) + \
    + 3*(NCELLSPERSIDE) + 1)
```

Definition at line 54 of file ex_test_Ar_fcc_cluster_cpp.cpp.

12.163.2 Function Documentation

12.163.2.1 create_FCC_cluster()

```
void create_FCC_cluster (
    double FCCspacing,
    int nCellsPerSide,
    double * coords )
```

Definition at line 342 of file ex_test_Ar_fcc_cluster_cpp.cpp.

12.163.2.2 fcc_cluster_neighborlist()

```
void fcc_cluster_neighborlist (
    int half,
    int numberOfParticles,
    double * coords,
    double cutoff,
    NeighList * nl )
```

Definition at line 460 of file ex_test_Ar_fcc_cluster_cpp.cpp.

12.163.2.3 `get_cluster_neigh()`

```
int get_cluster_neigh (
    void const *const dataObject,
    int const numberOfCutoffs,
    double const *const cutoffs,
    int const neighborListIndex,
    int const particleNumber,
    int *const numberOfNeighbors,
    int const **const neighborsOfParticle )
```

Definition at line 506 of file `ex_test_Ar_fcc_cluster_cpp.cpp`.

12.163.2.4 `main()`

```
int main ( )
```

Definition at line 95 of file `ex_test_Ar_fcc_cluster_cpp.cpp`.

12.164 kim-api-v2.0.0-beta.0/docs/porting-content-from-v1-to-v2-examples/simulators/step5/ex_test_Ar_fcc_cluster_cpp/ex_test_Ar_fcc_cluster_cpp File Reference

```
#include <stdlib.h>
#include <stdio.h>
#include <iostream>
#include <iomanip>
#include <string>
#include <cmath>
#include "KIM_SimulatorHeaders.hpp"
```

Macros

- `#define NAMESTRLEN` 128
- `#define FCCSPACING` 5.260
- `#define DIM` 3
- `#define NCELLSPERSIDE` 2
- `#define NCLUSTERPARTS`
- `#define MY_ERROR(message)`
- `#define MY_WARNING(message)`

Functions

- void `fcc_cluster_neighborlist` (int half, int numberOfParticles, double *coords, double cutoff, NeighList *nl)
- int `get_cluster_neigh` (void const *const dataObject, int const numberOfCutoffs, double const *const cutoffs, int const neighborListIndex, int const particleNumber, int *const numberOfNeighbors, int const **const neighborsOfParticle)
- void `create_FCC_cluster` (double FCCspacing, int nCellsPerSide, double *coords)
- int `main` ()

12.164.1 Macro Definition Documentation

12.164.1.1 DIM

```
#define DIM 3
```

Definition at line 44 of file ex_test_Ar_fcc_cluster_cpp.cpp.

12.164.1.2 FCCSPACING

```
#define FCCSPACING 5.260
```

Definition at line 43 of file ex_test_Ar_fcc_cluster_cpp.cpp.

12.164.1.3 MY_ERROR

```
#define MY_ERROR(  
    message )
```

Value:

```
{  
    std::cout << "* Error : \"" << message << "\" : "  
    << __LINE__ << " : " << __FILE__ << std::endl;  
    exit(1);  
}
```

Definition at line 50 of file ex_test_Ar_fcc_cluster_cpp.cpp.

12.164.1.4 MY_WARNING

```
#define MY_WARNING(  
    message )
```

Value:

```
{  
    std::cout << "* Error : \"" << message << "\" : "  
    << __LINE__ << " : " << __FILE__ << std::endl;  
}
```

Definition at line 57 of file ex_test_Ar_fcc_cluster_cpp.cpp.

12.164.1.5 NAMESTRLEN

```
#define NAMESTRLEN 128
```

Definition at line 41 of file `ex_test_Ar_fcc_cluster_cpp.cpp`.

12.164.1.6 NCELLSPERSIDE

```
#define NCELLSPERSIDE 2
```

Definition at line 45 of file `ex_test_Ar_fcc_cluster_cpp.cpp`.

12.164.1.7 NCLUSTERPARTS

```
#define NCLUSTERPARTS
```

Value:

```
(4*(NCELLSPERSIDE*NCELLSPERSIDE*NCELLSPERSIDE) + \
      6*(NCELLSPERSIDE*NCELLSPERSIDE) + \
      3*(NCELLSPERSIDE) + 1)
```

Definition at line 46 of file `ex_test_Ar_fcc_cluster_cpp.cpp`.

12.164.2 Function Documentation**12.164.2.1 create_FCC_cluster()**

```
void create_FCC_cluster (
    double FCCspacing,
    int nCellsPerSide,
    double * coords )
```

Definition at line 374 of file `ex_test_Ar_fcc_cluster_cpp.cpp`.

12.164.2.2 fcc_cluster_neighborlist()

```
void fcc_cluster_neighborlist (
    int half,
    int numberOfParticles,
    double * coords,
    double cutoff,
    NeighList * nl )
```

Definition at line 492 of file ex_test_Ar_fcc_cluster_cpp.cpp.

12.164.2.3 get_cluster_neigh()

```
int get_cluster_neigh (
    void const *const dataObject,
    int const numberOfCutoffs,
    double const *const cutoffs,
    int const neighborListIndex,
    int const particleNumber,
    int *const numberOfNeighbors,
    int const **const neighborsOfParticle )
```

Definition at line 538 of file ex_test_Ar_fcc_cluster_cpp.cpp.

12.164.2.4 main()

```
int main ( )
```

Definition at line 87 of file ex_test_Ar_fcc_cluster_cpp.cpp.

12.165 kim-api-v2.0.0-beta.0/examples/simulators/ex_test_Ar_fcc_cluster_cpp/ex_test_Ar_fcc_cluster_cpp.cpp File Reference

```
#include <stdlib.h>
#include <stdio.h>
#include <iostream>
#include <iomanip>
#include <string>
#include <cmath>
#include "KIM_SimulatorHeaders.hpp"
```

Macros

- `#define NAMESTRLEN 128`
- `#define FCCSPACING 5.260`
- `#define DIM 3`
- `#define NCELLSPERSIDE 2`
- `#define NCLUSTERPARTS`
- `#define MY_ERROR(message)`
- `#define MY_WARNING(message)`

Functions

- `void fcc_cluster_neighborlist` (int half, int numberOfParticles, double *coords, double cutoff, NeighList *nl)
- `int get_cluster_neigh` (void const *const dataObject, int const numberOfCutoffs, double const *const cutoffs, int const neighborListIndex, int const particleNumber, int *const numberOfNeighbors, int const **const neighborsOfParticle)
- `void create_FCC_cluster` (double FCCspacing, int nCellsPerSide, double *coords)
- `int main` ()

12.165.1 Macro Definition Documentation

12.165.1.1 DIM

```
#define DIM 3
```

Definition at line 44 of file `ex_test_Ar_fcc_cluster_cpp.cpp`.

12.165.1.2 FCCSPACING

```
#define FCCSPACING 5.260
```

Definition at line 43 of file `ex_test_Ar_fcc_cluster_cpp.cpp`.

12.165.1.3 MY_ERROR

```
#define MY_ERROR(  
    message )
```

Value:

```
{  
    std::cout << " * Error : \"" << message << "\" : "  
    << __LINE__ << " : " << __FILE__ << std::endl;  
    exit(1);  
}
```

Definition at line 50 of file `ex_test_Ar_fcc_cluster_cpp.cpp`.

12.165.1.4 MY_WARNING

```
#define MY_WARNING(
    message )
```

Value:

```
{
    std::cout << "* Error : \"" << message << "\" : "
               << __LINE__ << " : " << __FILE__ << std::endl;
}
```

Definition at line 57 of file ex_test_Ar_fcc_cluster_cpp.cpp.

12.165.1.5 NAMESTRLEN

```
#define NAMESTRLEN 128
```

Definition at line 41 of file ex_test_Ar_fcc_cluster_cpp.cpp.

12.165.1.6 NCELLSPERSIDE

```
#define NCELLSPERSIDE 2
```

Definition at line 45 of file ex_test_Ar_fcc_cluster_cpp.cpp.

12.165.1.7 NCLUSTERPARTS

```
#define NCLUSTERPARTS
```

Value:

```
(4*(NCELLSPERSIDE*NCELLSPERSIDE*NCELLSPERSIDE) + \
  6*(NCELLSPERSIDE*NCELLSPERSIDE) + 3*(NCELLSPERSIDE) + 1)
```

Definition at line 46 of file ex_test_Ar_fcc_cluster_cpp.cpp.

12.165.2 Function Documentation

12.165.2.1 create_FCC_cluster()

```
void create_FCC_cluster (
    double FCCspacing,
    int nCellsPerSide,
    double * coords )
```

Definition at line 374 of file `ex_test_Ar_fcc_cluster_cpp.cpp`.

12.165.2.2 fcc_cluster_neighborlist()

```
void fcc_cluster_neighborlist (
    int half,
    int numberOfParticles,
    double * coords,
    double cutoff,
    NeighList * nl )
```

Definition at line 492 of file `ex_test_Ar_fcc_cluster_cpp.cpp`.

12.165.2.3 get_cluster_neigh()

```
int get_cluster_neigh (
    void const *const dataObject,
    int const numberOfCutoffs,
    double const *const cutoffs,
    int const neighborListIndex,
    int const particleNumber,
    int *const numberOfNeighbors,
    int const **const neighborsOfParticle )
```

Definition at line 538 of file `ex_test_Ar_fcc_cluster_cpp.cpp`.

12.165.2.4 main()

```
int main ( )
```

Definition at line 87 of file `ex_test_Ar_fcc_cluster_cpp.cpp`.

12.166 kim-api-v2.0.0-beta.0/docs/porting-content-from-v1-to-v2-examples/simulators/step0/ex_test_Ar_fcc_cluster_fortran/ex_test_Ar_fcc_cluster_fortran.F90 File Reference

```
#include "KIM_API_status.h"
```

- type [mod_neighborlist::neighobject_type](#)

Modules

- module [mod_neighborlist](#)
- module [mod_utility](#)

Macros

- `#define THIS_FILE_NAME __FILE__`
- `#define TRUEFALSE(TRUTH) merge(1,0,(TRUTH))`

Functions/Subroutines

- integer(c_int) function, public [mod_neighborlist::get_neigh](#) (pkim, mode, request, part, numnei, pnei1part, pRij)
- subroutine [mod_utility::mi_opbc_cluster_neighborlist](#) (half, numberOfParticles, coords, rcut, boxSideLengths, neighObject)
- subroutine [mod_utility::neigh_pure_cluster_neighborlist](#) (half, numberOfParticles, coords, cutoff, neigh↔Object)
- subroutine [mod_utility::neigh_rvec_cluster_neighborlist](#) (half, numberOfParticles, coords, cutoff, neighObject)
- subroutine [mod_utility::create_fcc_configuration](#) (FCCspacing, nCellsPerSide, periodic, coords, MiddlePart↔Id)
- program [ex_test_ar_fcc_cluster_fortran](#)

12.166.1 Macro Definition Documentation

12.166.1.1 THIS_FILE_NAME

```
#define THIS_FILE_NAME __FILE__
```

12.166.1.2 TRUEFALSE

```
#define TRUEFALSE(  
    TRUTH ) merge(1,0,(TRUTH))
```

12.166.2 Function/Subroutine Documentation

12.166.2.1 `ex_test_ar_fcc_cluster_fortran()`

```
program ex_test_ar_fcc_cluster_fortran ( )
```

Definition at line 461 of file `ex_test_Ar_fcc_cluster_fortran.F90`.

12.167 `kim-api-v2.0.0-beta.0/docs/porting-content-from-v1-to-v2-examples/simulators/step1/ex_test_Ar_fcc_cluster_fortran/ex_test_Ar_fcc_cluster_fortran.F90` File Reference

```
#include "KIM_API_status.h"
```

Data Types

- type `mod_neighborlist::neighobject_type`

Modules

- module `mod_neighborlist`
- module `mod_utility`

Macros

- `#define THIS_FILE_NAME __FILE__`
- `#define TRUEFALSE(TRUTH) merge(1,0,(TRUTH))`

Functions/Subroutines

- integer(`c_int`) function, public `mod_neighborlist::get_neigh` (`pkim`, `mode`, `request`, `part`, `numnei`, `pnei1part`, `pRij`)
- subroutine `mod_utility::neigh_pure_cluster_neighborlist` (`half`, `numberOfParticles`, `coords`, `cutoff`, `neighObject`)
- subroutine `mod_utility::create_fcc_configuration` (`FCCspacing`, `nCellsPerSide`, `periodic`, `coords`, `MiddlePartId`)
- program `ex_test_ar_fcc_cluster_fortran`

12.167.1 Macro Definition Documentation

12.167.1.1 `THIS_FILE_NAME`

```
#define THIS_FILE_NAME __FILE__
```

```
#define TRUEFALSE(  
    TRUTH ) merge(1,0,(TRUTH))
```

12.167.2 Function/Subroutine Documentation

12.167.2.1 ex_test_ar_fcc_cluster_fortran()

```
program ex_test_ar_fcc_cluster_fortran ( )
```

Definition at line 327 of file ex_test_Ar_fcc_cluster_fortran.F90.

12.168 kim-api-v2.0.0-beta.0/docs/porting-content-from-v1-to-v2-examples/simulators/step3/ex_test_Ar_fcc_cluster_fortran/ex_test_Ar_fcc_cluster_fortran.F90 File Reference

Data Types

- type [mod_neighborlist::neighobject_type](#)

Modules

- module [error](#)
- module [mod_neighborlist](#)
- module [mod_utility](#)

Functions/Subroutines

- subroutine [error::my_error](#) (message, line, file)
- subroutine [error::my_warning](#) (message, line, file)
- subroutine, public [mod_neighborlist::get_neigh](#) (data_object, number_of_cutoffs, cutoffs, neighbor_list_index, request, numnei, pnei1part, ierr)
- subroutine [mod_utility::neigh_pure_cluster_neighborlist](#) (half, numberOfParticles, coords, cutoff, neighObject)
- subroutine [mod_utility::create_fcc_configuration](#) (FCCspacing, nCellsPerSide, periodic, coords, MiddlePartId)
- program [ex_test_ar_fcc_cluster_fortran](#)

12.168.1 Function/Subroutine Documentation

12.168.1.1 `ex_test_ar_fcc_cluster_fortran()`

```
program ex_test_ar_fcc_cluster_fortran ( )
```

Definition at line 338 of file `ex_test_Ar_fcc_cluster_fortran.F90`.

12.169 kim-api-v2.0.0-beta.0/docs/porting-content-from-v1-to-v2-examples/simulators/step4/ex_test_Ar_fcc_cluster_fortran/ex_test_Ar_fcc_cluster_fortran.F90 File Reference

Data Types

- type [mod_neighborlist::neighobject_type](#)

Modules

- module [error](#)
- module [mod_neighborlist](#)
- module [mod_utility](#)

Functions/Subroutines

- subroutine [error::my_error](#) (message, line, file)
- subroutine [error::my_warning](#) (message, line, file)
- subroutine, public [mod_neighborlist::get_neigh](#) (data_object, number_of_cutoffs, cutoffs, neighbor_list_index, request, numnei, pnei1part, ierr)
- subroutine [mod_utility::neigh_pure_cluster_neighborlist](#) (half, numberOfParticles, coords, cutoff, neighObject)
- subroutine [mod_utility::create_fcc_configuration](#) (FCCspacing, nCellsPerSide, periodic, coords, MiddlePartId)
- program [ex_test_ar_fcc_cluster_fortran](#)

12.169.1 Function/Subroutine Documentation

12.169.1.1 `ex_test_ar_fcc_cluster_fortran()`

```
program ex_test_ar_fcc_cluster_fortran ( )
```

Definition at line 338 of file `ex_test_Ar_fcc_cluster_fortran.F90`.

12.170 kim-api-v2.0.0-beta.0/docs/porting-content-from-v1-to-v2-examples/simulators/step5/ex_test_Ar_fcc_cluster_fortran/ex_test_Ar_fcc_cluster_fortran.F90 File Reference

Data Types

- type [mod_neighborlist::neighobject_type](#)

Modules

- module [error](#)
- module [mod_neighborlist](#)
- module [mod_utility](#)

Functions/Subroutines

- subroutine [error::my_error](#) (message, line, file)
- subroutine [error::my_warning](#) (message, line, file)
- subroutine, public [mod_neighborlist::get_neigh](#) (data_object, number_of_cutoffs, cutoffs, neighbor_list_index, request, numnei, pnei1part, ierr)
- subroutine [mod_utility::neigh_pure_cluster_neighborlist](#) (half, numberOfParticles, coords, cutoff, neighborlist)
- subroutine [mod_utility::create_fcc_configuration](#) (FCCspacing, nCellsPerSide, periodic, coords, MiddleParticle)
- program [ex_test_ar_fcc_cluster_fortran](#)

12.170.1 Function/Subroutine Documentation

12.170.1.1 [ex_test_ar_fcc_cluster_fortran\(\)](#)

```
program ex_test_ar_fcc_cluster_fortran ( )
```

Definition at line 339 of file [ex_test_Ar_fcc_cluster_fortran.F90](#).

12.171 kim-api-v2.0.0-beta.0/examples/simulators/ex_test_Ar_fcc_cluster_fortran/ex_test_Ar_fcc_cluster_fortran.F90 File Reference

Data Types

- type [mod_neighborlist::neighobject_type](#)

Modules

- module [error](#)
- module [mod_neighborlist](#)
- module [mod_utility](#)

Functions/Subroutines

- subroutine [error::my_error](#) (message, line, file)
- subroutine [error::my_warning](#) (message, line, file)
- subroutine, public [mod_neighborlist::get_neigh](#) (data_object, number_of_cutoffs, cutoffs, neighbor_list↔ index, request, numnei, pnei1part, ierr)
- subroutine [mod_utility::neigh_pure_cluster_neighborlist](#) (half, numberOfParticles, coords, cutoff, neigh↔ Object)
- subroutine [mod_utility::create_fcc_configuration](#) (FCCspacing, nCellsPerSide, periodic, coords, MiddlePart↔ Id)
- program [ex_test_ar_fcc_cluster_fortran](#)

12.171.1 Function/Subroutine Documentation

12.171.1.1 [ex_test_ar_fcc_cluster_fortran\(\)](#)

```
program ex_test_ar_fcc_cluster_fortran ( )
```

Definition at line 339 of file [ex_test_Ar_fcc_cluster_fortran.F90](#).

12.172 [kim-api-v2.0.0-beta.0/docs/src/features.txt](#) File Reference

12.173 [kim-api-v2.0.0-beta.0/docs/src/implementation.txt](#) File Reference

12.174 [kim-api-v2.0.0-beta.0/docs/src/introduction.txt](#) File Reference

12.175 [kim-api-v2.0.0-beta.0/docs/src/porting-content-from-v1-to-v2.txt](#) File Reference

12.176 [kim-api-v2.0.0-beta.0/docs/src/theory.txt](#) File Reference

12.177 [kim-api-v2.0.0-beta.0/docs/src/version2-differences.txt](#) File Reference

12.178 [kim-api-v2.0.0-beta.0/examples/model_drivers/ex_model_driver_P_LJ/ex_model↔_driver_P_LJ.F90](#) File Reference

```
#include "kim_model_compute_log_macros.fd"
#include "kim_model_compute_arguments_create_log_macros.fd"
#include "kim_model_compute_arguments_destroy_log_macros.fd"
#include "kim_model_driver_create_log_macros.fd"
```


Modules

- module [ex_model_driver_p_lj](#)

Functions/Subroutines

- subroutine, public [ex_model_driver_p_lj::calc_phi](#) (model_epsilon, model_sigma, model_shift, model_cutoff, r, phi)
- subroutine, public [ex_model_driver_p_lj::calc_phi_dphi](#) (model_epsilon, model_sigma, model_shift, model_↵_cutoff, r, phi, dphi)
- subroutine, public [ex_model_driver_p_lj::calc_phi_dphi_d2phi](#) (model_epsilon, model_sigma, model_shift, model_cutoff, r, phi, dphi, d2phi)
- subroutine, public [ex_model_driver_p_lj::compute_energy_forces](#) (model_compute_handle, model_↵_compute_arguments_handle, ierr)
- subroutine, public [ex_model_driver_p_lj::refresh](#) (model_refresh_handle, ierr)
- subroutine, public [ex_model_driver_p_lj::destroy](#) (model_destroy_handle, ierr)
- subroutine, public [ex_model_driver_p_lj::compute_arguments_create](#) (model_compute_handle, model_↵_compute_arguments_create_handle, ierr)
- subroutine, public [ex_model_driver_p_lj::compute_arguments_destroy](#) (model_compute_handle, model_↵_compute_arguments_destroy_handle, ierr)
- subroutine [model_driver_create_routine](#) (model_driver_create_handle, requested_length_unit, requested_↵_energy_unit, requested_charge_unit, requested_temperature_unit, requested_time_unit, ierr)

Variables

- integer(c_int), parameter, public [ex_model_driver_p_lj::speccode](#) = 1

12.178.1 Function/Subroutine Documentation

12.178.1.1 model_driver_create_routine()

```
subroutine model_driver_create_routine (
    type(kim_model_driver_create_handle_type), intent(inout) model_driver_create_↵
handle,
    type(kim_length_unit_type), intent(in), value requested_length_unit,
    type(kim_energy_unit_type), intent(in), value requested_energy_unit,
    type(kim_charge_unit_type), intent(in), value requested_charge_unit,
    type(kim_temperature_unit_type), intent(in), value requested_temperature_unit,
    type(kim_time_unit_type), intent(in), value requested_time_unit,
    integer(c_int), intent(out) ierr )
```

Definition at line 648 of file [ex_model_driver_P_LJ.F90](#).

- 12.179 [kim-api-v2.0.0-beta.0/examples/model_drivers/ex_model_driver_P_LJ/README](#)
File Reference
- 12.180 [kim-api-v2.0.0-beta.0/examples/model_drivers/ex_model_driver_P_Morse/README](#)
DME File Reference
- 12.181 [kim-api-v2.0.0-beta.0/examples/model_drivers/LennardJones612__MD_414112407348__003/README](#)
File Reference
- 12.182 [kim-api-v2.0.0-beta.0/examples/models/ex_model_Ar_P_LJ/README](#) File Reference
- 12.183 [kim-api-v2.0.0-beta.0/examples/models/ex_model_Ar_P_MLJ_F03/README](#) File Reference
- 12.184 [kim-api-v2.0.0-beta.0/examples/models/ex_model_Ar_P_Morse/README](#) File Reference
- 12.185 [kim-api-v2.0.0-beta.0/examples/models/ex_model_Ar_P_Morse_07C/README](#)
File Reference
- 12.186 [kim-api-v2.0.0-beta.0/examples/models/LennardJones612_UniversalShifted__MO_959249795837_003/README](#)
File Reference
- 12.187 [kim-api-v2.0.0-beta.0/examples/simulators/utility_forces_numer_deriv/README](#)
File Reference
- 12.188 [kim-api-v2.0.0-beta.0/examples/model_drivers/ex_model_driver_P_Morse/ex_model_driver_P_Morse.c](#) File Reference

```
#include <stdlib.h>
#include <stdio.h>
#include <string.h>
#include <math.h>
#include "KIM_ModelDriverHeaders.h"
#include "KIM_ModelComputeLogMacros.h"
#include "KIM_ModelDriverCreateLogMacros.h"
#include "KIM_ModelComputeArgumentsCreateLogMacros.h"
#include "KIM_ModelComputeArgumentsDestroyLogMacros.h"
```

Macros

- `#define TRUE 1`
- `#define FALSE 0`
- `#define DIM 3 /* dimensionality of space */`
- `#define SPECCODE 1 /* internal species code */`

Functions

- `int model_driver_create (KIM_ModelDriverCreate *const modelDriverCreate, KIM_LengthUnit const requestedLengthUnit, KIM_EnergyUnit const requestedEnergyUnit, KIM_ChargeUnit const requestedChargeUnit, KIM_TemperatureUnit const requestedTemperatureUnit, KIM_TimeUnit const requestedTimeUnit)`
- `static int destroy (KIM_ModelDestroy *const modelDestroy)`
- `static int compute (KIM_ModelCompute const *const modelCompute, KIM_ModelComputeArguments const *const modelComputeArguments)`
- `static int compute_arguments_create (KIM_ModelCompute const *const modelCompute, KIM_ModelComputeArgumentsCreate *const modelComputeArgumentsCreate)`
- `static int compute_arguments_destroy (KIM_ModelCompute const *const modelCompute, KIM_ModelComputeArgumentsDestroy *const modelComputeArgumentsDestroy)`
- `static int refresh (KIM_ModelRefresh *const modelRefresh)`
- `static void calc_phi (double const *epsilon, double const *C, double const *Rzero, double const *shift, double const cutoff, double const r, double *phi)`
- `static void calc_phi_dphi (double const *epsilon, double const *C, double const *Rzero, double const *shift, double const cutoff, double const r, double *phi, double *dphi)`

12.188.1 Macro Definition Documentation**12.188.1.1 DIM**

```
#define DIM 3 /* dimensionality of space */
```

Definition at line 55 of file `ex_model_driver_P_Morse.c`.

12.188.1.2 FALSE

```
#define FALSE 0
```

Definition at line 50 of file `ex_model_driver_P_Morse.c`.

12.188.1.3 SPECCODE

```
#define SPECCODE 1 /* internal species code */
```

Definition at line 56 of file `ex_model_driver_P_Morse.c`.

12.188.1.4 TRUE

```
#define TRUE 1
```

Definition at line 49 of file `ex_model_driver_P_Morse.c`.

12.188.2 Function Documentation

12.188.2.1 `calc_phi()`

```
static void calc_phi (  
    double const * epsilon,  
    double const * C,  
    double const * Rzero,  
    double const * shift,  
    double const cutoff,  
    double const r,  
    double * phi ) [static]
```

Definition at line 113 of file `ex_model_driver_P_Morse.c`.

12.188.2.2 `calc_phi_dphi()`

```
static void calc_phi_dphi (  
    double const * epsilon,  
    double const * C,  
    double const * Rzero,  
    double const * shift,  
    double const cutoff,  
    double const r,  
    double * phi,  
    double * dphi ) [static]
```

Definition at line 140 of file `ex_model_driver_P_Morse.c`.

12.188.2.3 compute()

```
static int compute (
    KIM_ModelCompute const *const modelCompute,
    KIM_ModelComputeArguments const *const modelComputeArguments ) [static]
```

Definition at line 171 of file ex_model_driver_P_Morse.c.

12.188.2.4 compute_arguments_create()

```
static int compute_arguments_create (
    KIM_ModelCompute const *const modelCompute,
    KIM_ModelComputeArgumentsCreate *const modelComputeArgumentsCreate ) [static]
```

Definition at line 593 of file ex_model_driver_P_Morse.c.

12.188.2.5 compute_arguments_destroy()

```
static int compute_arguments_destroy (
    KIM_ModelCompute const *const modelCompute,
    KIM_ModelComputeArgumentsDestroy *const modelComputeArgumentsDestroy ) [static]
```

Definition at line 626 of file ex_model_driver_P_Morse.c.

12.188.2.6 destroy()

```
static int destroy (
    KIM_ModelDestroy *const modelDestroy ) [static]
```

Definition at line 575 of file ex_model_driver_P_Morse.c.

12.188.2.7 model_driver_create()

```
int model_driver_create (
    KIM_ModelDriverCreate *const modelDriverCreate,
    KIM_LengthUnit const requestedLengthUnit,
    KIM_EnergyUnit const requestedEnergyUnit,
    KIM_ChargeUnit const requestedChargeUnit,
    KIM_TemperatureUnit const requestedTemperatureUnit,
    KIM_TimeUnit const requestedTimeUnit )
```

Definition at line 392 of file ex_model_driver_P_Morse.c.

12.188.2.8 refresh()

```
static int refresh (
    KIM_ModelRefresh *const modelRefresh ) [static]
```

Definition at line 558 of file `ex_model_driver_P_Morse.c`.

12.189 kim-api-v2.0.0-beta.0/examples/model_drivers/LennardJones612__MD_414112407348__003/CreateDispatch.sh File Reference**12.190 kim-api-v2.0.0-beta.0/examples/model_drivers/LennardJones612__MD_414112407348__003/LennardJones612.cpp File Reference**

```
#include <cmath>
#include <cstdlib>
#include <cstring>
#include <fstream>
#include <iostream>
#include "LennardJones612.hpp"
#include "LennardJones612Implementation.hpp"
```

Functions

- int `model_driver_create` (KIM::ModelDriverCreate *const modelDriverCreate, KIM::LengthUnit const requestedLengthUnit, KIM::EnergyUnit const requestedEnergyUnit, KIM::ChargeUnit const requestedChargeUnit, KIM::TemperatureUnit const requestedTemperatureUnit, KIM::TimeUnit const requestedTimeUnit)

12.190.1 Function Documentation**12.190.1.1 model_driver_create()**

```
int model_driver_create (
    KIM::ModelDriverCreate *const modelDriverCreate,
    KIM::LengthUnit const requestedLengthUnit,
    KIM::EnergyUnit const requestedEnergyUnit,
    KIM::ChargeUnit const requestedChargeUnit,
    KIM::TemperatureUnit const requestedTemperatureUnit,
    KIM::TimeUnit const requestedTimeUnit )
```

Definition at line 50 of file `LennardJones612.cpp`.

12.191 kim-api-v2.0.0-beta.0/examples/model_drivers/LennardJones612__MD_414112407348_003/↵
LennardJones612.hpp File

Reference 487
12.191 kim-api-v2.0.0-beta.0/examples/model_drivers/LennardJones612__MD_414112407348_003/LennardJones612.hpp File Reference

```
#include "KIM_ModelDriverHeaders.hpp"
```

Classes

- class [LennardJones612](#)

Functions

- int [model_driver_create](#) ([KIM::ModelDriverCreate](#) *const modelDriverCreate, [KIM::LengthUnit](#) const requestedLengthUnit, [KIM::EnergyUnit](#) const requestedEnergyUnit, [KIM::ChargeUnit](#) const requestedChargeUnit, [KIM::TemperatureUnit](#) const requestedTemperatureUnit, [KIM::TimeUnit](#) const requestedTimeUnit)

12.191.1 Function Documentation

12.191.1.1 model_driver_create()

```
int model_driver_create (  
    KIM::ModelDriverCreate *const modelDriverCreate,  
    KIM::LengthUnit const requestedLengthUnit,  
    KIM::EnergyUnit const requestedEnergyUnit,  
    KIM::ChargeUnit const requestedChargeUnit,  
    KIM::TemperatureUnit const requestedTemperatureUnit,  
    KIM::TimeUnit const requestedTimeUnit )
```

Definition at line 50 of file LennardJones612.cpp.

12.192 kim-api-v2.0.0-beta.0/examples/model_drivers/LennardJones612__MD_414112407348_003/LennardJones612Implementation.cpp File Reference

```
#include <cmath>  
#include <cstdlib>  
#include <cstring>  
#include <fstream>  
#include <iostream>  
#include <map>  
#include "LennardJones612Implementation.hpp"  
#include "KIM_ModelDriverHeaders.hpp"  
#include "KIM_ModelDriverCreateLogMacros.hpp"  
#include "KIM_ModelRefreshLogMacros.hpp"  
#include "LennardJones612ImplementationComputeDispatch.cpp"  
#include "KIM_ModelComputeArgumentsCreateLogMacros.hpp"  
#include "KIM_ModelComputeArgumentsLogMacros.hpp"  
#include "KIM_ModelComputeLogMacros.hpp"
```

Macros

- `#define MAXLINE 1024`
- `#define IGNORE_RESULT(fn) if(fn){}`

Functions

- void `AllocateAndInitialize2DArray` (double **&arrayPtr, int const extentZero, int const extentOne)
- void `Deallocate2DArray` (double **&arrayPtr)

12.192.1 Macro Definition Documentation

12.192.1.1 IGNORE_RESULT

```
#define IGNORE_RESULT(  
    fn ) if(fn){}
```

Definition at line 43 of file LennardJones612Implementation.cpp.

12.192.1.2 MAXLINE

```
#define MAXLINE 1024
```

Definition at line 42 of file LennardJones612Implementation.cpp.

12.192.2 Function Documentation

12.192.2.1 AllocateAndInitialize2DArray()

```
void AllocateAndInitialize2DArray (  
    double **& arrayPtr,  
    int const extentZero,  
    int const extentOne )
```

Definition at line 1001 of file LennardJones612Implementation.cpp.

12.192.2.2 Deallocate2DArray()

```
void Deallocate2DArray (
    double **& arrayPtr )
```

Definition at line 1022 of file LennardJones612Implementation.cpp.

12.193 kim-api-v2.0.0-beta.0/examples/model_drivers/LennardJones612__MD_414112407348_003/LennardJones612Implementation.hpp File Reference

```
#include <vector>
#include <cmath>
#include "KIM_LogVerbosity.hpp"
#include "LennardJones612.hpp"
#include "KIM_ModelComputeLogMacros.hpp"
```

Classes

- class [LennardJones612Implementation](#)

Macros

- #define [DIMENSION](#) 3
- #define [ONE](#) 1.0
- #define [HALF](#) 0.5
- #define [MAX_PARAMETER_FILES](#) 1
- #define [PARAM_SHIFT_INDEX](#) 0
- #define [PARAM_CUTOFFS_INDEX](#) 1
- #define [PARAM_EPSILONS_INDEX](#) 2
- #define [PARAM_SIGMAS_INDEX](#) 3
- #define [LENNARD_JONES_PHI](#)(exshift)

Typedefs

- typedef int() [GetNeighborFunction](#)(void const *const, int const, int *const, int const **const)
- typedef double [VectorOfSizeDIM](#)[[DIMENSION](#)]
- typedef double [VectorOfSizeSix](#)[6]

Functions

- void [AllocateAndInitialize2DArray](#) (double **&arrayPtr, int const extentZero, int const extentOne)
- void [Deallocate2DArray](#) (double **&arrayPtr)

12.193.1 Macro Definition Documentation

12.193.1.1 DIMENSION

```
#define DIMENSION 3
```

Definition at line 39 of file LennardJones612Implementation.hpp.

12.193.1.2 HALF

```
#define HALF 0.5
```

Definition at line 41 of file LennardJones612Implementation.hpp.

12.193.1.3 LENNARD_JONES_PHI

```
#define LENNARD_JONES_PHI(  
    exshift )
```

Value:

```
phi = r6iv * (constFourEpsSig12_2D[iSpecies][jSpecies]*r6iv -  
             constFourEpsSig6_2D[iSpecies][jSpecies]) exshift; \
```

Definition at line 272 of file LennardJones612Implementation.hpp.

12.193.1.4 MAX_PARAMETER_FILES

```
#define MAX_PARAMETER_FILES 1
```

Definition at line 43 of file LennardJones612Implementation.hpp.

12.193.1.5 ONE

```
#define ONE 1.0
```

Definition at line 40 of file LennardJones612Implementation.hpp.

12.193.1.6 PARAM_CUTOFFS_INDEX

```
#define PARAM_CUTOFFS_INDEX 1
```

Definition at line 46 of file LennardJones612Implementation.hpp.

12.193.1.7 PARAM_EPSILONS_INDEX

```
#define PARAM_EPSILONS_INDEX 2
```

Definition at line 47 of file LennardJones612Implementation.hpp.

12.193.1.8 PARAM_SHIFT_INDEX

```
#define PARAM_SHIFT_INDEX 0
```

Definition at line 45 of file LennardJones612Implementation.hpp.

12.193.1.9 PARAM_SIGMAS_INDEX

```
#define PARAM_SIGMAS_INDEX 3
```

Definition at line 48 of file LennardJones612Implementation.hpp.

12.193.2 Typedef Documentation

12.193.2.1 GetNeighborFunction

```
typedef int() GetNeighborFunction(void const *const, int const, int *const, int const **const)
```

Definition at line 58 of file LennardJones612Implementation.hpp.

12.193.2.2 VectorOfSizeDIM

```
typedef double VectorOfSizeDIM[DIMENSION]
```

Definition at line 61 of file LennardJones612Implementation.hpp.

12.193.2.3 VectorOfSizeSix

```
typedef double VectorOfSizeSix[6]
```

Definition at line 62 of file LennardJones612Implementation.hpp.

12.193.3 Function Documentation

12.193.3.1 AllocateAndInitialize2DArray()

```
void AllocateAndInitialize2DArray (
    double **& arrayPtr,
    int const extentZero,
    int const extentOne )
```

Definition at line 1001 of file LennardJones612Implementation.cpp.

12.193.3.2 Deallocate2DArray()

```
void Deallocate2DArray (
    double **& arrayPtr )
```

Definition at line 1022 of file LennardJones612Implementation.cpp.

12.194 kim-api-v2.0.0-beta.0/examples/models/ex_model_Ar_P_LJ/ex_model_Ar_P_LJ.params File Reference

12.195 kim-api-v2.0.0-beta.0/examples/models/ex_model_Ar_P_Morse/ex_model_Ar_P_Morse.params File Reference

12.196 kim-api-v2.0.0-beta.0/examples/models/LennardJones612_UniversalShifted__MO_959249795837_003/LennardJones612_UniversalShifted.params File Reference

12.197 kim-api-v2.0.0-beta.0/examples/simulators/utility_forces_numer_deriv/utility_forces_numer_deriv.F03 File Reference

Data Types

- type [mod_neighborlist::neighobject_type](#)

Modules

- module [error](#)
- module [mod_neighborlist](#)
- module [mod_utilities](#)

Functions/Subroutines

- subroutine [error::my_error](#) (message, line, file)
- subroutine [error::my_warning](#) (message, line, file)
- subroutine, public [mod_neighborlist::get_neigh](#) (data_object, number_of_cutoffs, cutoffs, neighbor_list↔ index, request, numnei, pnei1part, ierr)
- subroutine [mod_utilities::check_model_compatibility](#) (compute_arguments_handle, forces_optional, model↔ _is_compatible, ierr)
- subroutine [mod_utilities::get_model_supported_species](#) (model_handle, max_species, model_species, num_species, ier)
- subroutine [mod_utilities::update_neighborlist](#) (DIM, N, coords, cutoff, cutpad, do_update_list, coordsave, neighObject, ierr)
- subroutine [mod_utilities::neigh_pure_cluster_neighborlist](#) (half, numberOfParticles, coords, cutoff, neigh↔ Object)
- subroutine [mod_utilities::create_fcc_configuration](#) (FCCspacing, nCellsPerSide, periodic, coords, Middle↔ PartId)
- subroutine [mod_utilities::compute_numer_deriv](#) (partnum, dir, model_handle, compute_arguments_handle, DIM, N, coords, cutoff, cutpad, energy, do_update_list, coordsave, neighObject, deriv, deriv_err, ierr)
- real(c_double) function [dfridr](#) (h, err)
- program [vc_forces_numer_deriv](#)

12.197.1 Function/Subroutine Documentation

12.197.1.1 [dfridr\(\)](#)

```
real(c_double) function compute_numer_deriv::dfridr (
    real(c_double), intent(inout) h,
    real(c_double), intent(out) err )
```

Definition at line 655 of file `utility_forces_numer_deriv.F03`.

12.197.1.2 [vc_forces_numer_deriv\(\)](#)

```
program vc_forces_numer_deriv ( )
```

Definition at line 774 of file `utility_forces_numer_deriv.F03`.

Variables

- type(kim_compute_arguments_handle_type), public, protected [kim_compute_arguments_module::kim_compute_arguments_n](#)

12.201 kim-api-v2.0.0-beta.0/fortran/include/kim_compute_callback_name_module.f90 File Reference

Modules

- module [kim_compute_callback_name_module](#)

Variables

- type(kim_compute_callback_name_type), public, protected [kim_compute_callback_name_module::kim_compute_callback_nar](#)
- type(kim_compute_callback_name_type), public, protected [kim_compute_callback_name_module::kim_compute_callback_nar](#)
- type(kim_compute_callback_name_type), public, protected [kim_compute_callback_name_module::kim_compute_callback_nar](#)

12.202 kim-api-v2.0.0-beta.0/fortran/include/kim_data_type_module.f90 File Reference

Modules

- module [kim_data_type_module](#)

Variables

- type(kim_data_type_type), public, protected [kim_data_type_module::kim_data_type_integer](#)
- type(kim_data_type_type), public, protected [kim_data_type_module::kim_data_type_double](#)

12.203 kim-api-v2.0.0-beta.0/fortran/include/kim_energy_unit_module.f90 File Reference

Modules

- module [kim_energy_unit_module](#)

Variables

- type(kim_energy_unit_type), public, protected [kim_energy_unit_module::kim_energy_unit_unused](#)
- type(kim_energy_unit_type), public, protected [kim_energy_unit_module::kim_energy_unit_amu_a2_per_ps2](#)
- type(kim_energy_unit_type), public, protected [kim_energy_unit_module::kim_energy_unit_erg](#)
- type(kim_energy_unit_type), public, protected [kim_energy_unit_module::kim_energy_unit_ev](#)
- type(kim_energy_unit_type), public, protected [kim_energy_unit_module::kim_energy_unit_hartree](#)
- type(kim_energy_unit_type), public, protected [kim_energy_unit_module::kim_energy_unit_j](#)
- type(kim_energy_unit_type), public, protected [kim_energy_unit_module::kim_energy_unit_kcal_mol](#)

12.204 kim-api-v2.0.0-beta.0/fortran/include/kim_language_name_module.f90 File Reference

Modules

- module [kim_language_name_module](#)

Variables

- type(kim_language_name_type), public, protected [kim_language_name_module::kim_language_name_cpp](#)
- type(kim_language_name_type), public, protected [kim_language_name_module::kim_language_name_c](#)
- type(kim_language_name_type), public, protected [kim_language_name_module::kim_language_name_fortran](#)

12.205 kim-api-v2.0.0-beta.0/fortran/include/kim_length_unit_module.f90 File Reference

Modules

- module [kim_length_unit_module](#)

Variables

- type(kim_length_unit_type), public, protected [kim_length_unit_module::kim_length_unit_unused](#)
- type(kim_length_unit_type), public, protected [kim_length_unit_module::kim_length_unit_a](#)
- type(kim_length_unit_type), public, protected [kim_length_unit_module::kim_length_unit_bohr](#)
- type(kim_length_unit_type), public, protected [kim_length_unit_module::kim_length_unit_cm](#)
- type(kim_length_unit_type), public, protected [kim_length_unit_module::kim_length_unit_m](#)
- type(kim_length_unit_type), public, protected [kim_length_unit_module::kim_length_unit_nm](#)

12.206 kim-api-v2.0.0-beta.0/fortran/include/kim_log_module.f90 File Reference

Data Types

- interface [kim_log_module::kim_log_pop_verbosity](#)

Modules

- module [kim_log_module](#)

Variables

- type(kim_log_handle_type), public, protected [kim_log_module::kim_log_null_handle](#)

12.207 kim-api-v2.0.0-beta.0/fortran/include/kim_log_verbosity_module.f90 File Reference

Modules

- module [kim_log_verbosity_module](#)

Variables

- type(kim_log_verbosity_type), public, protected [kim_log_verbosity_module::kim_log_verbosity_silent](#)
- type(kim_log_verbosity_type), public, protected [kim_log_verbosity_module::kim_log_verbosity_fatal](#)
- type(kim_log_verbosity_type), public, protected [kim_log_verbosity_module::kim_log_verbosity_error](#)
- type(kim_log_verbosity_type), public, protected [kim_log_verbosity_module::kim_log_verbosity_warning](#)
- type(kim_log_verbosity_type), public, protected [kim_log_verbosity_module::kim_log_verbosity_information](#)
- type(kim_log_verbosity_type), public, protected [kim_log_verbosity_module::kim_log_verbosity_debug](#)
- character(len=4096, kind=c_char), public [kim_log_verbosity_module::kim_log_file](#)
- character(len=65536, kind=c_char), public [kim_log_verbosity_module::kim_log_message](#)

12.208 kim-api-v2.0.0-beta.0/fortran/include/kim_model_compute_arguments_create_log_macros.fd File Reference

12.209 kim-api-v2.0.0-beta.0/fortran/include/kim_model_compute_arguments_create_module.f90 File Reference

Data Types

- interface [kim_model_compute_arguments_create_module::kim_model_compute_arguments_create_set_callback_support_sta](#)
- interface [kim_model_compute_arguments_create_module::kim_model_compute_arguments_create_set_model_buffer_pointer](#)
- interface [kim_model_compute_arguments_create_module::kim_model_compute_arguments_create_string](#)

Modules

- module [kim_model_compute_arguments_create_module](#)

Variables

- type(kim_model_compute_arguments_create_handle_type), public, protected [kim_model_compute_arguments_create_module](#)

12.210 kim-api-v2.0.0-beta.0/fortran/include/kim_model_compute_arguments_destroy_log_macros.fd File Reference

12.211 kim-api-v2.0.0-beta.0/fortran/include/kim_model_compute_arguments_destroy_module.f90 File Reference

Data Types

- interface [kim_model_compute_arguments_destroy_module::kim_model_compute_arguments_destroy_string](#)

Modules

- module [kim_model_compute_arguments_destroy_module](#)

Variables

- type(kim_model_compute_arguments_destroy_handle_type), public, protected [kim_model_compute_arguments_destroy_mod](#)

12.212 [kim-api-v2.0.0-beta.0/fortran/include/kim_model_compute_arguments_log_macros.fd](#) File Reference ↩

12.213 [kim-api-v2.0.0-beta.0/fortran/include/kim_model_compute_arguments_module.f90](#) File Reference

Data Types

- interface [kim_model_compute_arguments_module::kim_model_compute_arguments_get_neighbor_list](#)
- interface [kim_model_compute_arguments_module::kim_model_compute_arguments_set_model_buffer_pointer](#)
- interface [kim_model_compute_arguments_module::kim_model_compute_arguments_string](#)

Modules

- module [kim_model_compute_arguments_module](#)

Variables

- type(kim_model_compute_arguments_handle_type), public, protected [kim_model_compute_arguments_module::kim_model_c](#)

12.214 [kim-api-v2.0.0-beta.0/fortran/include/kim_model_compute_log_macros.fd](#) File Reference

12.215 [kim-api-v2.0.0-beta.0/fortran/include/kim_model_compute_module.f90](#) File Reference

Data Types

- interface [kim_model_compute_module::kim_model_compute_string](#)

Modules

- module [kim_model_compute_module](#)

Variables

- type(kim_model_compute_handle_type), public, protected [kim_model_compute_module::kim_model_compute_null_handle](#)

12.216 kim-api-v2.0.0-beta.0/fortran/include/kim_model_create_log_macros.fd File Reference

12.217 kim-api-v2.0.0-beta.0/fortran/include/kim_model_create_module.f90 File Reference

Data Types

- interface [kim_model_create_module::kim_model_create_set_influence_distance_pointer](#)
- interface [kim_model_create_module::kim_model_create_set_destroy_pointer](#)
- interface [kim_model_create_module::kim_model_create_set_compute_arguments_create_pointer](#)
- interface [kim_model_create_module::kim_model_create_set_compute_arguments_destroy_pointer](#)
- interface [kim_model_create_module::kim_model_create_set_compute_pointer](#)
- interface [kim_model_create_module::kim_model_create_set_species_code](#)
- interface [kim_model_create_module::kim_model_create_set_model_buffer_pointer](#)
- interface [kim_model_create_module::kim_model_create_convert_unit](#)
- interface [kim_model_create_module::kim_model_create_log_entry](#)
- interface [kim_model_create_module::kim_model_create_string](#)

Modules

- module [kim_model_create_module](#)

Variables

- type(kim_model_create_handle_type), public, protected [kim_model_create_module::kim_model_create_null_handle](#)

12.218 kim-api-v2.0.0-beta.0/fortran/include/kim_model_destroy_log_macros.fd File Reference

12.219 kim-api-v2.0.0-beta.0/fortran/include/kim_model_destroy_module.f90 File Reference

Data Types

- interface [kim_model_destroy_module::kim_model_destroy_string](#)

Modules

- module [kim_model_destroy_module](#)

Variables

- type(kim_model_destroy_handle_type), public, protected [kim_model_destroy_module::kim_model_destroy_null_handle](#)

12.220 kim-api-v2.0.0-beta.0/fortran/include/kim_model_driver_create_log_macros.fd File Reference

12.221 kim-api-v2.0.0-beta.0/fortran/include/kim_model_driver_create_module.f90 File Reference

Data Types

- interface [kim_model_driver_create_module::kim_model_driver_create_set_influence_distance_pointer](#)
- interface [kim_model_driver_create_module::kim_model_driver_create_set_destroy_pointer](#)
- interface [kim_model_driver_create_module::kim_model_driver_create_set_compute_arguments_create_pointer](#)
- interface [kim_model_driver_create_module::kim_model_driver_create_set_compute_arguments_destroy_pointer](#)
- interface [kim_model_driver_create_module::kim_model_driver_create_set_compute_pointer](#)
- interface [kim_model_driver_create_module::kim_model_driver_create_set_species_code](#)
- interface [kim_model_driver_create_module::kim_model_driver_create_set_model_buffer_pointer](#)
- interface [kim_model_driver_create_module::kim_model_driver_create_convert_unit](#)
- interface [kim_model_driver_create_module::kim_model_driver_create_log_entry](#)
- interface [kim_model_driver_create_module::kim_model_driver_create_string](#)

Modules

- module [kim_model_driver_create_module](#)

Variables

- type(kim_model_driver_create_handle_type), public, protected [kim_model_driver_create_module::kim_model_driver_create_n](#)

12.222 kim-api-v2.0.0-beta.0/fortran/include/kim_model_driver_headers_module.f90 File Reference

Modules

- module [kim_model_driver_headers_module](#)

12.223 kim-api-v2.0.0-beta.0/fortran/include/kim_model_headers_module.f90 File Refer- ence

Modules

- module [kim_model_headers_module](#)

12.224 kim-api-v2.0.0-beta.0/fortran/include/kim_model_module.f90 File Reference

Data Types

- interface [kim_model_module::kim_model_destroy](#)
- interface [kim_model_module::kim_model_compute_arguments_create](#)
- interface [kim_model_module::kim_model_compute_arguments_destroy](#)
- interface [kim_model_module::kim_model_compute](#)
- interface [kim_model_module::kim_model_clear_influence_dist_and_cutoffs_then_refresh_model](#)
- interface [kim_model_module::kim_model_get_number_of_parameters](#)
- interface [kim_model_module::kim_model_set_simulator_buffer_pointer](#)
- interface [kim_model_module::kim_model_pop_log_verbosity](#)

Modules

- module [kim_model_module](#)

Variables

- type([kim_model_handle_type](#)), public, protected [kim_model_module::kim_model_null_handle](#)

12.225 kim-api-v2.0.0-beta.0/fortran/include/kim_model_refresh_log_macros.fd File Reference

12.226 kim-api-v2.0.0-beta.0/fortran/include/kim_model_refresh_module.f90 File Reference

Data Types

- interface [kim_model_refresh_module::kim_model_refresh_string](#)

Modules

- module [kim_model_refresh_module](#)

Variables

- type([kim_model_refresh_handle_type](#)), public, protected [kim_model_refresh_module::kim_model_refresh_null_handle](#)

12.227 kim-api-v2.0.0-beta.0/fortran/include/kim_numbering_module.f90 File Reference

Modules

- module [kim_numbering_module](#)

Variables

- type(kim_numbering_type), public, protected [kim_numbering_module::kim_numbering_zero_based](#)
- type(kim_numbering_type), public, protected [kim_numbering_module::kim_numbering_one_based](#)

12.228 kim-api-v2.0.0-beta.0/fortran/include/kim_sem_ver_module.f90 File Reference

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- module [kim_sem_ver_module](#)

12.229 kim-api-v2.0.0-beta.0/fortran/include/kim_simulator_headers_module.f90 File Reference

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- module [kim_simulator_headers_module](#)

12.230 kim-api-v2.0.0-beta.0/fortran/include/kim_species_name_module.f90 File Reference

Modules

- module [kim_species_name_module](#)

Variables

- type(kim_species_name_type), public, protected [kim_species_name_module::kim_species_name_electron](#)
- type(kim_species_name_type), public, protected [kim_species_name_module::kim_species_name_h](#)
- type(kim_species_name_type), public, protected [kim_species_name_module::kim_species_name_he](#)
- type(kim_species_name_type), public, protected [kim_species_name_module::kim_species_name_li](#)
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- type(kim_species_name_type), public, protected [kim_species_name_module::kim_species_name_p](#)
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- type(kim_species_name_type), public, protected [kim_species_name_module::kim_species_name_ar](#)

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- type(kim_species_name_type), public, protected [kim_species_name_module::kim_species_name_user11](#)
- type(kim_species_name_type), public, protected [kim_species_name_module::kim_species_name_user12](#)
- type(kim_species_name_type), public, protected [kim_species_name_module::kim_species_name_user13](#)
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Modules

- module [kim_support_status_module](#)

Variables

- type(kim_support_status_type), public, protected [kim_support_status_module::kim_support_status_required_by_api](#)
- type(kim_support_status_type), public, protected [kim_support_status_module::kim_support_status_not_supported](#)
- type(kim_support_status_type), public, protected [kim_support_status_module::kim_support_status_required](#)
- type(kim_support_status_type), public, protected [kim_support_status_module::kim_support_status_optional](#)

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Variables

- type(kim_temperature_unit_type), public, protected [kim_temperature_unit_module::kim_temperature_unit_unused](#)
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- module [kim_unit_system_module](#)

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