

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 atomic 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" interface which facilitates and simplifies (as much as possible) the exchange of memory pointers between the simulator and model.

This documentaion is organized into the following components:

1. [Features of the KIM API package](#)
2. [Theory](#)
3. [Implementation](#)
4. [Summary of Differences Between kim-api-v1 and kim-api-v2](#)
5. 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](#)).
6. Example stand-alone models written in C ([ex_model_Ar_P_Morse_07C.c](#)) and Fortran ([ex_model_Ar_P_MLJ_F03.F03](#))
7. Example model drivers written in C++ ([LennardJones612Implementation.hpp](#)), C ([ex_model_driver_P_Morse.c](#)), and Fortran ([ex_model_driver_P_LJ.F90](#)).
8. Example parameterized models ([ex_model_Ar_P_LJ.params](#), [ex_model_Ar_P_Morse.params](#), [LennardJones612_Universal.pa](#)

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 77, Fortran 90/95, Fortran 2003.
- **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, ArgumentName, CallbackName, 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* 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.
- **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". At the conceptual level, 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.

At the conceptual level, 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 a predetermined 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 $\mathbf{r}^{(j,i)} \equiv \mathbf{r}^{(j)} - \mathbf{r}^{(i)}$ for the relative position vector from particle i to particle j , and the notation $r^{(j,i)}$ for the magnitude of the vector $\mathbf{r}^{(j,i)}$. Note that $r^{(j,i)} = r^{(i,j)}$ and these are simply two different notations for the same quantity. However, when taken as a function of particle position vectors, $r^{(j,i)} = \bar{r}^{(j,i)}(\mathbf{r}^{(j)}, \mathbf{r}^{(i)}) \equiv \|\mathbf{r}^{(j)} - \mathbf{r}^{(i)}\|$, there is a difference. In particular,

$$\frac{\partial \bar{r}^{(j,i)}}{\partial \mathbf{r}^{(j)}} = -\frac{\partial \bar{r}^{(i,j)}}{\partial \mathbf{r}^{(j)}}.$$

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,

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

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, use 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,

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

Second, the configuration's "Partial Force" on particle j , $\mathbf{f}^{\mathcal{C}(j)}$, 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.

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

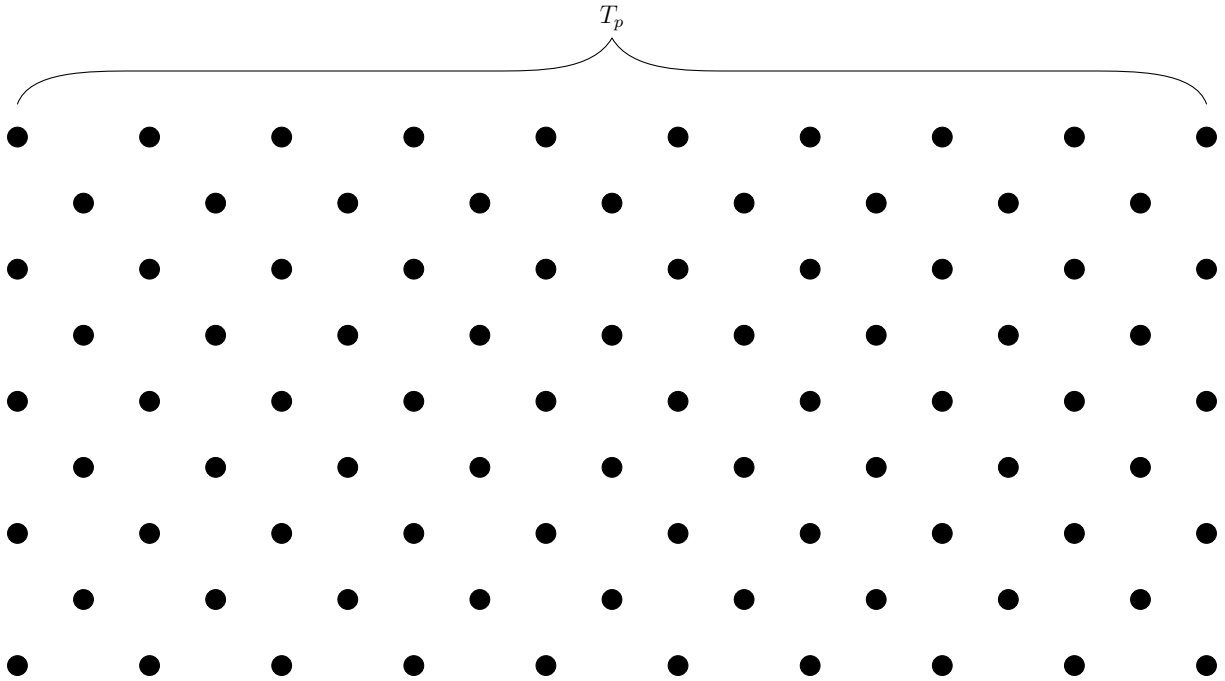
Note that an equivalent expression for the partial virial tensor is given by

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

Domain Decomposition

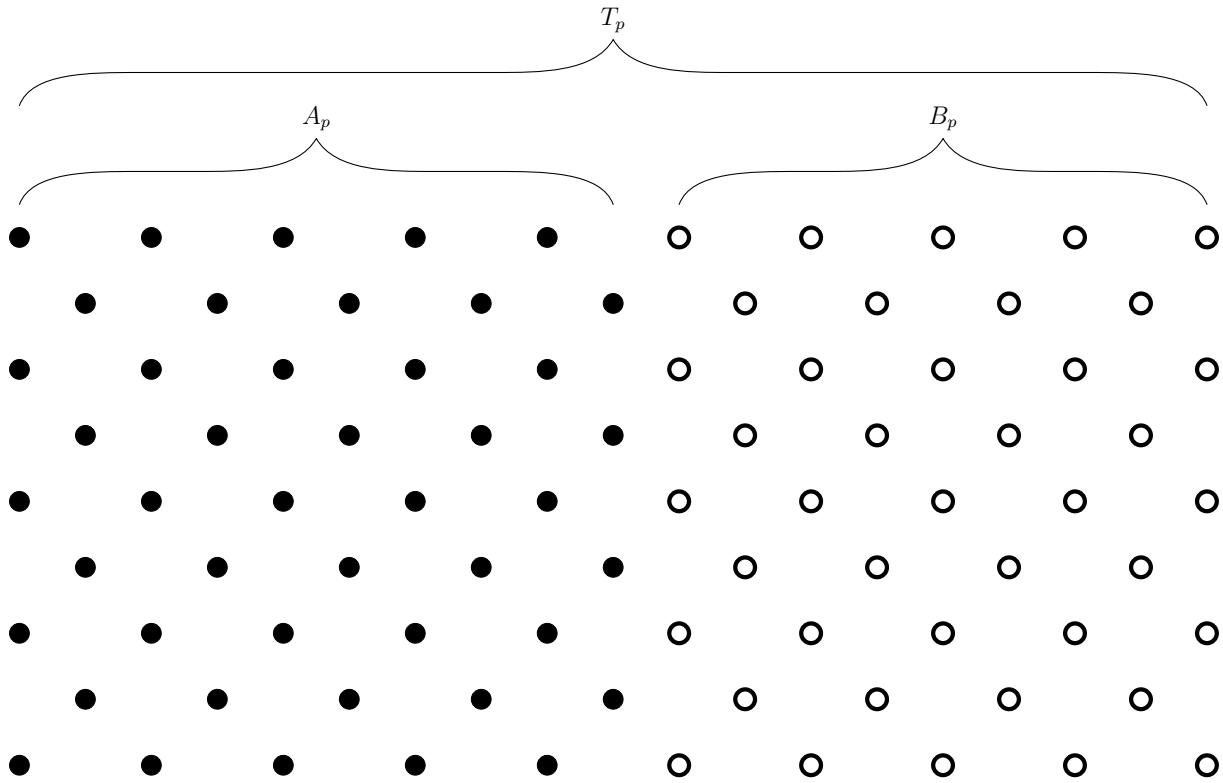
The definitions of a configuration's partial energy, forces, and virial are designed to allow for easy (and low communication) parallel computation via domain decomposition. This section presents a simple example that illustrates how this works.

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 $T_{np} = \emptyset$. 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 $A_p \cup B_p = T_p$.



Then 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 four routines which perform specific tasks. The first is the *ModelCreate* (or *ModelDriverCreate*) routine, which performs all necessary initialization tasks. The second is the *ModelCompute* routine, which performs the core computational tasks. The third is the *ModelRefresh* routine, which performs any necessary updates after a simulator makes changes to the model's parameters (if this is supported). The fourth is the *ModelDestroy* routine, which performs all necessary finalization tasks.

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 provides a set of "Arguments" to the model's *ModelCompute* function. There are input arguments that include the various components that make up a configuration (number of particles, particle position vectors, etc.). And, there are output arguments that include the quantities (like partial energy and partial forces), defined in Section [Theory](#), associated with the configuration. There are also "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 arguments and callbacks defined as part of the official API. Each 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 for every argument defined by the KIM API. It is the responsibility of the simulator to use the model object interface to determine the support status of each argument and to use this information to determine if the model is capable of performing the desired computation.

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

Input argument table:

Argument Name	Unit	Data Type	Extent	Memory Layout	Valid Support Statuses (bold – default)
numberOfParticles	N/A	double	1		requiredByAPI
particleSpecies \leftrightarrow Codes	N/A	integer	numberOfParticles	$sc^{(0)}, sc^{(1)}, \dots$	requiredByAPI
particle \leftrightarrow 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 argument table:

Argument Name	Unit	Data Type	Extent	Memory Layout	Valid Support Statuses (bold – default)
<code>partialEnergy</code>	energy	double	1		required, optional, notSupported
<code>partialForces</code>	force	double	<code>numberOfParticles</code> * 3	$f_1^{C(0)}, f_2^{C(0)}, f_3^{C(0)}, f_1^{C(1)}, f_2^{C(1)}, f_3^{C(1)}$	required, optional, notSupported
<code>partialParticle↔Energy</code>	energy	double	<code>numberOfParticles</code>	$E^{C(0)}, E^{C(1)}, E^{C(2)}$	required, optional, notSupported
<code>partialVirial</code>	energy	double	6	$V_{11}^C, V_{22}^C, V_{33}^C, V_{23}^C, V_{32}^C, V_{12}^C$	required, optional, notSupported
<code>partialParticleVirial</code>	energy	double	<code>numberOfParticles</code> * 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, $\mathbf{V}^{C(i)}$.

Callback table:

Callback Name	Valid Support Statuses (bold – default)
<code>GetNeighborList</code>	requiredByAPI
<code>ProcessDEDrTerm</code>	required, optional, notSupported
<code>ProcessD2EDr2Term</code>	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↔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. In particular, the model must, in principle, be able to independently construct its own equivalent neighbor list using just the particle coordinates.

- 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.

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

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

- 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.
- **KIM Descriptor Files Have Been Eliminated:** kim-api-v2 does not use *KIM descriptor files*. Instead, kim-api-v2 models register their units, conventions, species, arguments, and parameters in their *ModelCreate* 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 (which also executes the model initialization), 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 bigger 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 processing 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 arguments communicated between the simulator and the model. 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 binding 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 (or are currently being) 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::SetCallbackPointer` becomes `KIM_Model_SetCallbackPointer`.
- C++ → Fortran: Replace "::" with "_". Where camel-case is used in C++, convert to snake-case. Convert to all lower-case. For example, `KIM::Model::SetCallbackPointer` becomes `kim_model_set_callback_pointer`.

Identifier Name translation table:

kim-api-v1	kim-api-v2 C++ Binding
KIM_API_file_init	N/A
KIM_API_string_init	KIM::Model::Create
KIM_API_get_version	KIM::SEM_VER::GetSemVer
KIM_API_get_version_major	N/A
KIM_API_get_version_minor	N/A
KIM_API_get_version_prerelease	N/A
KIM_API_get_version_build_metadata	N/A
N/A	KIM::SEM_VER::ParseSemVer
KIM_API_version_newer	KIM::SEM_VER::IsLessThan
KIM_API_model_info	N/A
KIM_API_allocate	N/A
KIM_API_c_free	N/A
KIM_API_free	KIM::Model::Destroy
KIM_API_print	KIM::Model::String , KIM::ModelCreate::String , KIM::ModelCompute::String , KIM::ModelRefresh::String , KIM::ModelDestroy::String
KIM_API_model_compute	KIM::Model::Compute
KIM_API_model_destroy	N/A
KIM_API_get_model_index_shift	N/A
N/A	KIM::ModelCreate::SetModelNumbering , KIM::ModelDriverCreate::SetModelNumbering
KIM_API_set_model_buffer	KIM::ModelCreate::SetModelBufferPointer , KIM::ModelDriverCreate::SetModelBufferPointer
KIM_API_set_sim_buffer	KIM::Model::SetSimulatorBufferPointer
KIM_API_get_model_buffer	KIM::ModelCompute::GetModelBufferPointer , KIM::ModelDestroy::GetModelBufferPointer , KIM::ModelRefresh::GetModelBufferPointer
KIM_API_get_sim_buffer	KIM::Model::GetSimulatorBufferPointer
KIM_API_is_half_neighbors	N/A
KIM_API_set_data	KIM::Model::SetArgumentPointer
N/A	KIM::ModelCreate::SetArgumentSupportStatus , KIM::ModelDriverCreate::SetArgumentSupportStatus
N/A	KIM::ModelCreate::SetCallbackSupportStatus , KIM::ModelDriverCreate::SetCallbackSupportStatus
KIM_API_set_method	KIM::Model::SetCallbackPointer
KIM_API_get_data	KIM::ModelCompute::GetArgumentPointer
KIM_API_get_method	N/A
N/A	KIM::ModelCompute::IsCallbackPresent
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

kim-api-v1	kim-api-v2 C++ Binding
N/A	KIM::ModelCreate::SetNeighborListCutoffsPointer, KIM::ModelDriverCreate::SetNeighborListCutoffsPointer, KIM::ModelRefresh::SetNeighborListCutoffsPointer
N/A	KIM::Model::GetArgumentSupportStatus
N/A	KIM::Model::GetCallbackSupportStatus
N/A	KIM::ModelCreate::SetRefreshPointer, KIM::ModelDriverCreate::SetRefreshPointer
N/A	KIM::ModelCreate::SetDestroyPointer, KIM::ModelDriverCreate::SetDestroyPointer
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
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::ModelCompute::GetNeighborList
KIM_API_process_dEdr	KIM::ModelCompute::ProcessDEDrTerm
KIM_API_process_d2Edr2	KIM::ModelCompute::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
N/A	KIM::Model::SetLogID
N/A	KIM::Model::PushLogVerbosity
N/A	KIM::Model::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-v1	kim-api-v2 C++ Binding
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
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KIM_API_setm_compute_by_index	N/A
KIM_API_getm_data	N/A
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KIM_API_setm_method	N/A
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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

Next Section: [Browse files](#).

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6.1 Namespace List

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Chapter 9

Namespace Documentation

9.1 error Module Reference

Functions/Subroutines

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

9.1.1 Function/Subroutine Documentation

9.1.1.1 [my_error\(\)](#)

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

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

9.1.1.2 [my_warning\(\)](#)

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

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

9.2 ex_model_ar_p_ml_j_f03 Module Reference

Functions/Subroutines

- subroutine, public [compute_energy_forces](#) (model_compute_handle, ierr)
- subroutine, public [model_destroy_func](#) (model_destroy_handle, ierr)
- subroutine, public [model_refresh_func](#) (model_refresh_handle, ierr)

Variables

- integer(c_int), parameter, public [speccode](#) = 1
- real(c_double), parameter, public [model_cutoff](#) = 8.15_cd

9.2.1 Function/Subroutine Documentation

9.2.1.1 compute_energy_forces()

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

Definition at line 166 of file ex_model_Ar_P_MLJ_F03.F03.

9.2.1.2 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 362 of file ex_model_Ar_P_MLJ_F03.F03.

9.2.1.3 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 390 of file ex_model_Ar_P_MLJ_F03.F03.

9.2.2 Variable Documentation

9.2.2.1 model_cutoff

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

Definition at line 63 of file ex_model_Ar_P_MLJ_F03.F03.

9.2.2.2 speccode

```
integer(c_int), parameter, public ex_model_ar_p_ml_j_f03::speccode = 1
```

Definition at line 62 of file ex_model_Ar_P_MLJ_F03.F03.

9.3 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, ierr)
- subroutine, public [refresh](#) (model_refresh_handle, ierr)
- subroutine, public [destroy](#) (model_destroy_handle, ierr)

Variables

- integer(c_int), parameter, public [speccode](#) = 1

9.3.1 Function/Subroutine Documentation

9.3.1.1 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 93 of file ex_model_driver_P_LJ.F90.

9.3.1.2 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 129 of file ex_model_driver_P_LJ.F90.

9.3.1.3 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 167 of file ex_model_driver_P_LJ.F90.

9.3.1.4 compute_energy_forces()

```
subroutine, public ex_model_driver_p_lj::compute_energy_forces (
    type(kim_model_compute_handle_type), intent(in) model_compute_handle,
    integer(c_int), intent(out) ierr )
```

Definition at line 205 of file ex_model_driver_P_LJ.F90.

9.3.1.5 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 519 of file ex_model_driver_P_LJ.F90.

9.3.1.6 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 476 of file `ex_model_driver_P_LJ.F90`.

9.3.2 Variable Documentation

9.3.2.1 speccode

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

Definition at line 65 of file `ex_model_driver_P_LJ.F90`.

9.4 KIM Namespace Reference

Namespaces

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

Classes

- class [ArgumentName](#)
- class [CallbackName](#)
- class [ChargeUnit](#)
- class [DataType](#)
- class [EnergyUnit](#)
- class [LanguageName](#)
- class [LengthUnit](#)
- class [Log](#)
- class [LogVerbosity](#)
- class [Model](#)
- class [ModelCompute](#)
- class [ModelCreate](#)
- class [ModelDestroy](#)
- class [ModelDriverCreate](#)
- class [ModelRefresh](#)
- class [Numbering](#)
- class [SpeciesName](#)
- class [SupportStatus](#)
- class [TemperatureUnit](#)
- class [TimeUnit](#)

Typedefs

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

9.4.1 Typedef Documentation

9.4.1.1 func

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

Definition at line 40 of file KIM_func.hpp.

9.5 KIM::ARGUMENT_NAME Namespace Reference

Classes

- struct [Comparator](#)

Functions

- void [GetNumberOfArguments](#) (int *const numberOfArguments)
- int [GetArgumentName](#) (int const index, [ArgumentName](#) *const argumentName)
- int [GetArgumentDataType](#) ([ArgumentName](#) const argumentName, [DataType](#) *const dataType)

Variables

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

9.5.1 Function Documentation

9.5.1.1 GetArgumentDataType()

```
int KIM::ARGUMENT_NAME::GetArgumentDataType (
    ArgumentName const argumentName,
    DataType *const dataType )
```

9.5.1.2 GetArgumentName()

```
int KIM::ARGUMENT_NAME::GetArgumentName (
    int const index,
    ArgumentName *const argumentName )
```

9.5.1.3 GetNumberOfArguments()

```
void KIM::ARGUMENT_NAME::GetNumberOfArguments (
    int *const numberOfArguments )
```

9.5.2 Variable Documentation

9.5.2.1 coordinates

[ArgumentName](#) const KIM::ARGUMENT_NAME::coordinates

9.5.2.2 numberOfParticles

`ArgumentName` const KIM::ARGUMENT_NAME::numberOfParticles

9.5.2.3 partialEnergy

`ArgumentName` const KIM::ARGUMENT_NAME::partialEnergy

9.5.2.4 partialForces

`ArgumentName` const KIM::ARGUMENT_NAME::partialForces

9.5.2.5 partialParticleEnergy

`ArgumentName` const KIM::ARGUMENT_NAME::partialParticleEnergy

9.5.2.6 partialParticleVirial

`ArgumentName` const KIM::ARGUMENT_NAME::partialParticleVirial

9.5.2.7 partialVirial

`ArgumentName` const KIM::ARGUMENT_NAME::partialVirial

9.5.2.8 particleContributing

`ArgumentName` const KIM::ARGUMENT_NAME::particleContributing

9.5.2.9 particleSpeciesCodes

`ArgumentName` const KIM::ARGUMENT_NAME::particleSpeciesCodes

9.6 KIM::CALLBACK_NAME Namespace Reference

Classes

- struct [Comparator](#)

Functions

- void [GetNumberOfCallbacks](#) (int *const numberOfCallbacks)
- int [GetCallbackName](#) (int const index, [CallbackName](#) *const callbackName)

Variables

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

9.6.1 Function Documentation

9.6.1.1 GetCallbackName()

```
int KIM::CALLBACK_NAME::GetCallbackName (
    int const index,
    CallbackName *const callbackName )
```

9.6.1.2 GetNumberOfCallbacks()

```
void KIM::CALLBACK_NAME::GetNumberOfCallbacks (
    int *const numberOfCallbacks )
```

9.6.2 Variable Documentation

9.6.2.1 GetNeighborList

```
CallbackName const KIM::CALLBACK_NAME::GetNeighborList
```


9.6.2.2 ProcessD2EDr2Term

`CallbackName` const KIM::CALLBACK_NAME::ProcessD2EDr2Term

9.6.2.3 ProcessDEDrTerm

`CallbackName` const KIM::CALLBACK_NAME::ProcessDEDrTerm

9.7 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](#)

9.7.1 Function Documentation

9.7.1.1 GetChargeUnit()

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

9.7.1.2 GetNumberOfChargeUnits()

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


9.7.2 Variable Documentation

9.7.2.1 C

`ChargeUnit` const KIM::CHARGE_UNIT::C

9.7.2.2 e

`ChargeUnit` const KIM::CHARGE_UNIT::e

9.7.2.3 statC

`ChargeUnit` const KIM::CHARGE_UNIT::statC

9.7.2.4 unused

`ChargeUnit` const KIM::CHARGE_UNIT::unused

9.8 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`

9.8.1 Function Documentation

9.8.1.1 GetDataType()

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

9.8.1.2 GetNumberOfDataTypes()

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

9.8.2 Variable Documentation

9.8.2.1 Double

```
DataType const KIM::DATA_TYPE::Double
```

9.8.2.2 Integer

```
DataType const KIM::DATA_TYPE::Integer
```

9.9 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](#)

9.9.1 Function Documentation

9.9.1.1 GetEnergyUnit()

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

9.9.1.2 GetNumberOfEnergyUnits()

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

9.9.2 Variable Documentation

9.9.2.1 amu_A2_per_ps2

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

9.9.2.2 erg

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


9.9.2.3 eV

`EnergyUnit` const KIM::ENERGY_UNIT::eV

9.9.2.4 Hartree

`EnergyUnit` const KIM::ENERGY_UNIT::Hartree

9.9.2.5 J

`EnergyUnit` const KIM::ENERGY_UNIT::J

9.9.2.6 kcal_mol

`EnergyUnit` const KIM::ENERGY_UNIT::kcal_mol

9.9.2.7 unused

`EnergyUnit` const KIM::ENERGY_UNIT::unused

9.10 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`

9.10.1 Function Documentation

9.10.1.1 GetLanguageName()

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

9.10.1.2 GetNumberOfLanguageNames()

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

9.10.2 Variable Documentation

9.10.2.1 `c`

```
LanguageName const KIM::LANGUAGE_NAME::c
```

9.10.2.2 `cpp`

```
LanguageName const KIM::LANGUAGE_NAME::cpp
```

9.10.2.3 `fortran`

```
LanguageName const KIM::LANGUAGE_NAME::fortran
```

9.11 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](#)

9.11.1 Function Documentation

9.11.1.1 [GetLengthUnit\(\)](#)

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

9.11.1.2 [GetNumberOfLengthUnits\(\)](#)

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

9.11.2 Variable Documentation

9.11.2.1 [A](#)

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

9.11.2.2 [Bohr](#)

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


9.11.2.3 cm

`LengthUnit` const KIM::LENGTH_UNIT::cm

9.11.2.4 m

`LengthUnit` const KIM::LENGTH_UNIT::m

9.11.2.5 nm

`LengthUnit` const KIM::LENGTH_UNIT::nm

9.11.2.6 unused

`LengthUnit` const KIM::LENGTH_UNIT::unused

9.12 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](#)

9.12.1 Function Documentation

9.12.1.1 GetLogVerbosity()

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

9.12.1.2 GetNumberOfLogVerbosities()

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

9.12.2 Variable Documentation

9.12.2.1 debug

```
LogVerbosity const KIM::LOG_VERBOSITY::debug
```

9.12.2.2 error

```
LogVerbosity const KIM::LOG_VERBOSITY::error
```

9.12.2.3 fatal

```
LogVerbosity const KIM::LOG_VERBOSITY::fatal
```

9.12.2.4 information

```
LogVerbosity const KIM::LOG_VERBOSITY::information
```

9.12.2.5 silent

```
LogVerbosity const KIM::LOG_VERBOSITY::silent
```


9.12.2.6 warning

```
LogVerbosity const KIM::LOG_VERBOSITY::warning
```

9.13 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](#)

9.13.1 Function Documentation

9.13.1.1 GetNumbering()

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

9.13.1.2 GetNumberOfNumberings()

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

9.13.2 Variable Documentation

9.13.2.1 oneBased

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

9.13.2.2 zeroBased

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

9.14 KIM::SEM_VER Namespace Reference

Functions

- void [GetSemVer](#) (std::string *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)

9.14.1 Function Documentation

9.14.1.1 GetSemVer()

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

9.14.1.2 IsLessThan()

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

9.14.1.3 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 )
```


9.15 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](#)

9.15.1 Function Documentation

9.15.1.1 GetNumberOfSpeciesNames()

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

9.15.1.2 GetSpeciesName()

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

9.15.2 Variable Documentation

9.15.2.1 Ac

```
SpeciesName const KIM::SPECIES_NAME::Ac
```

9.15.2.2 Ag

```
SpeciesName const KIM::SPECIES_NAME::Ag
```

9.15.2.3 Al

```
SpeciesName const KIM::SPECIES_NAME::Al
```

9.15.2.4 Am

```
SpeciesName const KIM::SPECIES_NAME::Am
```

9.15.2.5 Ar

```
SpeciesName const KIM::SPECIES_NAME::Ar
```


9.15.2.6 As

`SpeciesName` const KIM::SPECIES_NAME::As

9.15.2.7 At

`SpeciesName` const KIM::SPECIES_NAME::At

9.15.2.8 Au

`SpeciesName` const KIM::SPECIES_NAME::Au

9.15.2.9 B

`SpeciesName` const KIM::SPECIES_NAME::B

9.15.2.10 Ba

`SpeciesName` const KIM::SPECIES_NAME::Ba

9.15.2.11 Be

`SpeciesName` const KIM::SPECIES_NAME::Be

9.15.2.12 Bh

`SpeciesName` const KIM::SPECIES_NAME::Bh

9.15.2.13 Bi

`SpeciesName` const KIM::SPECIES_NAME::Bi

9.15.2.14 Bk

`SpeciesName` const KIM::SPECIES_NAME::Bk

9.15.2.15 Br

`SpeciesName` const KIM::SPECIES_NAME::Br

9.15.2.16 C

`SpeciesName` const KIM::SPECIES_NAME::C

9.15.2.17 Ca

`SpeciesName` const KIM::SPECIES_NAME::Ca

9.15.2.18 Cd

`SpeciesName` const KIM::SPECIES_NAME::Cd

9.15.2.19 Ce

`SpeciesName` const KIM::SPECIES_NAME::Ce

9.15.2.20 Cf

`SpeciesName` const KIM::SPECIES_NAME::Cf

9.15.2.21 Cl

`SpeciesName` const KIM::SPECIES_NAME::Cl

9.15.2.22 Cm

`SpeciesName` const KIM::SPECIES_NAME::Cm

9.15.2.23 Cn

`SpeciesName` const KIM::SPECIES_NAME::Cn

9.15.2.24 Co

`SpeciesName` const KIM::SPECIES_NAME::Co

9.15.2.25 Cr

`SpeciesName` const KIM::SPECIES_NAME::Cr

9.15.2.26 Cs

`SpeciesName` const KIM::SPECIES_NAME::Cs

9.15.2.27 Cu

`SpeciesName` const KIM::SPECIES_NAME::Cu

9.15.2.28 Db

`SpeciesName` const KIM::SPECIES_NAME::Db

9.15.2.29 Ds

`SpeciesName` const KIM::SPECIES_NAME::Ds

9.15.2.30 Dy

`SpeciesName` const KIM::SPECIES_NAME::Dy

9.15.2.31 electron

`SpeciesName` const KIM::SPECIES_NAME::electron

9.15.2.32 Er

`SpeciesName` const KIM::SPECIES_NAME::Er

9.15.2.33 Es

`SpeciesName` const KIM::SPECIES_NAME::Es

9.15.2.34 Eu

`SpeciesName` const KIM::SPECIES_NAME::Eu

9.15.2.35 F

`SpeciesName` const KIM::SPECIES_NAME::F

9.15.2.36 Fe

`SpeciesName` const KIM::SPECIES_NAME::Fe

9.15.2.37 Fl

`SpeciesName` const KIM::SPECIES_NAME::Fl

9.15.2.38 Fm

`SpeciesName` const KIM::SPECIES_NAME::Fm

9.15.2.39 Fr

`SpeciesName` const KIM::SPECIES_NAME::Fr

9.15.2.40 Ga

`SpeciesName` const KIM::SPECIES_NAME::Ga

9.15.2.41 Gd

`SpeciesName` const KIM::SPECIES_NAME::Gd

9.15.2.42 Ge

`SpeciesName` const KIM::SPECIES_NAME::Ge

9.15.2.43 H

`SpeciesName` const KIM::SPECIES_NAME::H

9.15.2.44 He

`SpeciesName` const KIM::SPECIES_NAME::He

9.15.2.45 Hf

`SpeciesName` const KIM::SPECIES_NAME::Hf

9.15.2.46 Hg

`SpeciesName` const KIM::SPECIES_NAME::Hg

9.15.2.47 Ho

`SpeciesName` const KIM::SPECIES_NAME::Ho

9.15.2.48 Hs

`SpeciesName` const KIM::SPECIES_NAME::Hs

9.15.2.49 I

`SpeciesName` const KIM::SPECIES_NAME::I

9.15.2.50 In

`SpeciesName` const KIM::SPECIES_NAME::In

9.15.2.51 Ir

`SpeciesName` const KIM::SPECIES_NAME::Ir

9.15.2.52 K

`SpeciesName` const KIM::SPECIES_NAME::K

9.15.2.53 Kr

`SpeciesName` const KIM::SPECIES_NAME::Kr

9.15.2.54 La

`SpeciesName` const KIM::SPECIES_NAME::La

9.15.2.55 Li

`SpeciesName` const KIM::SPECIES_NAME::Li

9.15.2.56 Lr

`SpeciesName` const KIM::SPECIES_NAME::Lr

9.15.2.57 Lu

`SpeciesName` const KIM::SPECIES_NAME::Lu

9.15.2.58 Lv

`SpeciesName` const KIM::SPECIES_NAME::Lv

9.15.2.59 Md

`SpeciesName` const KIM::SPECIES_NAME::Md

9.15.2.60 Mg

`SpeciesName` const KIM::SPECIES_NAME::Mg

9.15.2.61 Mn

`SpeciesName` const KIM::SPECIES_NAME::Mn

9.15.2.62 Mo

`SpeciesName` const KIM::SPECIES_NAME::Mo

9.15.2.63 Mt

`SpeciesName` const KIM::SPECIES_NAME::Mt

9.15.2.64 N

`SpeciesName` const KIM::SPECIES_NAME::N

9.15.2.65 Na

`SpeciesName` const KIM::SPECIES_NAME::Na

9.15.2.66 Nb

`SpeciesName` const KIM::SPECIES_NAME::Nb

9.15.2.67 Nd

`SpeciesName` const KIM::SPECIES_NAME::Nd

9.15.2.68 Ne

`SpeciesName` const KIM::SPECIES_NAME::Ne

9.15.2.69 Ni

`SpeciesName` const KIM::SPECIES_NAME::Ni

9.15.2.70 No

`SpeciesName` const KIM::SPECIES_NAME::No

9.15.2.71 Np

`SpeciesName` const KIM::SPECIES_NAME::Np

9.15.2.72 O

`SpeciesName` const KIM::SPECIES_NAME::O

9.15.2.73 Os

`SpeciesName` const KIM::SPECIES_NAME::Os

9.15.2.74 P

`SpeciesName` const KIM::SPECIES_NAME::P

9.15.2.75 Pa

`SpeciesName` const KIM::SPECIES_NAME::Pa

9.15.2.76 Pb

`SpeciesName` const KIM::SPECIES_NAME::Pb

9.15.2.77 Pd

`SpeciesName` const KIM::SPECIES_NAME::Pd

9.15.2.78 Pm

`SpeciesName` const KIM::SPECIES_NAME::Pm

9.15.2.79 Po

`SpeciesName` const KIM::SPECIES_NAME::Po

9.15.2.80 Pr

`SpeciesName` const KIM::SPECIES_NAME::Pr

9.15.2.81 Pt

`SpeciesName` const KIM::SPECIES_NAME::Pt

9.15.2.82 Pu

`SpeciesName` const KIM::SPECIES_NAME::Pu

9.15.2.83 Ra

`SpeciesName` const KIM::SPECIES_NAME::Ra

9.15.2.84 Rb

`SpeciesName` const KIM::SPECIES_NAME::Rb

9.15.2.85 Re

`SpeciesName` const KIM::SPECIES_NAME::Re

9.15.2.86 Rf

`SpeciesName` const KIM::SPECIES_NAME::Rf

9.15.2.87 Rg

`SpeciesName` const KIM::SPECIES_NAME::Rg

9.15.2.88 Rh

`SpeciesName` const KIM::SPECIES_NAME::Rh

9.15.2.89 Rn

`SpeciesName` const KIM::SPECIES_NAME::Rn

9.15.2.90 Ru

`SpeciesName` const KIM::SPECIES_NAME::Ru

9.15.2.91 S

`SpeciesName` const KIM::SPECIES_NAME::S

9.15.2.92 Sb

`SpeciesName` const KIM::SPECIES_NAME::Sb

9.15.2.93 Sc

`SpeciesName` const KIM::SPECIES_NAME::Sc

9.15.2.94 Se

`SpeciesName` const KIM::SPECIES_NAME::Se

9.15.2.95 Sg

`SpeciesName` const KIM::SPECIES_NAME::Sg

9.15.2.96 Si

`SpeciesName` const KIM::SPECIES_NAME::Si

9.15.2.97 Sm

`SpeciesName` const KIM::SPECIES_NAME::Sm

9.15.2.98 Sn

`SpeciesName` const KIM::SPECIES_NAME::Sn

9.15.2.99 Sr

`SpeciesName` const KIM::SPECIES_NAME::Sr

9.15.2.100 Ta

`SpeciesName` const KIM::SPECIES_NAME::Ta

9.15.2.101 Tb

`SpeciesName` const KIM::SPECIES_NAME::Tb

9.15.2.102 Tc

`SpeciesName` const KIM::SPECIES_NAME::Tc

9.15.2.103 Te

`SpeciesName` const KIM::SPECIES_NAME::Te

9.15.2.104 Th

`SpeciesName` const KIM::SPECIES_NAME::Th

9.15.2.105 Ti

`SpeciesName` const KIM::SPECIES_NAME::Ti

9.15.2.106 Tl

`SpeciesName` const KIM::SPECIES_NAME::Tl

9.15.2.107 Tm

`SpeciesName` const KIM::SPECIES_NAME::Tm

9.15.2.108 U

`SpeciesName` const KIM::SPECIES_NAME::U

9.15.2.109 user01

`SpeciesName` const KIM::SPECIES_NAME::user01

9.15.2.110 user02

`SpeciesName` const KIM::SPECIES_NAME::user02

9.15.2.111 user03

`SpeciesName` const KIM::SPECIES_NAME::user03

9.15.2.112 user04

`SpeciesName` const KIM::SPECIES_NAME::user04

9.15.2.113 user05

`SpeciesName` const KIM::SPECIES_NAME::user05

9.15.2.114 user06

`SpeciesName` const KIM::SPECIES_NAME::user06

9.15.2.115 user07

`SpeciesName` const KIM::SPECIES_NAME::user07

9.15.2.116 user08

`SpeciesName` const KIM::SPECIES_NAME::user08

9.15.2.117 user09

`SpeciesName` const KIM::SPECIES_NAME::user09

9.15.2.118 user10

`SpeciesName` const KIM::SPECIES_NAME::user10

9.15.2.119 user11

`SpeciesName` const KIM::SPECIES_NAME::user11

9.15.2.120 user12

`SpeciesName` const KIM::SPECIES_NAME::user12

9.15.2.121 user13

`SpeciesName` const KIM::SPECIES_NAME::user13

9.15.2.122 user14

`SpeciesName` const KIM::SPECIES_NAME::user14

9.15.2.123 user15

`SpeciesName` const KIM::SPECIES_NAME::user15

9.15.2.124 user16

`SpeciesName` const KIM::SPECIES_NAME::user16

9.15.2.125 user17

`SpeciesName` const KIM::SPECIES_NAME::user17

9.15.2.126 user18

`SpeciesName` const KIM::SPECIES_NAME::user18

9.15.2.127 user19

`SpeciesName` const KIM::SPECIES_NAME::user19

9.15.2.128 user20

`SpeciesName` const KIM::SPECIES_NAME::user20

9.15.2.129 Uuo

`SpeciesName` const KIM::SPECIES_NAME::Uuo

9.15.2.130 Uup

`SpeciesName` const KIM::SPECIES_NAME::Uup

9.15.2.131 Uus

`SpeciesName` const KIM::SPECIES_NAME::Uus

9.15.2.132 Uut

`SpeciesName` const KIM::SPECIES_NAME::Uut

9.15.2.133 V

`SpeciesName` const KIM::SPECIES_NAME::V

9.15.2.134 W

`SpeciesName` const KIM::SPECIES_NAME::W

9.15.2.135 Xe

`SpeciesName` const KIM::SPECIES_NAME::Xe

9.15.2.136 Y

`SpeciesName` const KIM::SPECIES_NAME::Y

9.15.2.137 Yb

`SpeciesName` const KIM::SPECIES_NAME::Yb

9.15.2.138 Zn

`SpeciesName` const KIM::SPECIES_NAME::Zn

9.15.2.139 Zr

`SpeciesName` const KIM::SPECIES_NAME::Zr

9.16 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](#)

9.16.1 Function Documentation

9.16.1.1 GetNumberOfSupportStatuses()

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

9.16.1.2 GetSupportStatus()

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

9.16.2 Variable Documentation

9.16.2.1 notSupported

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

9.16.2.2 optional

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

9.16.2.3 required

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


9.16.2.4 requiredByAPI

[SupportStatus](#) const KIM::SUPPORT_STATUS::requiredByAPI

9.17 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](#)

9.17.1 Function Documentation

9.17.1.1 GetNumberOfTemperatureUnits()

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

9.17.1.2 GetTemperatureUnit()

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

9.17.2 Variable Documentation

9.17.2.1 K

`TemperatureUnit` const KIM::TEMPERATURE_UNIT::K

9.17.2.2 unused

`TemperatureUnit` const KIM::TEMPERATURE_UNIT::unused

9.18 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`

9.18.1 Function Documentation

9.18.1.1 GetNumberOfTimeUnits()

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

9.18.1.2 GetTimeUnit()

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


9.18.2 Variable Documentation

9.18.2.1 fs

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

9.18.2.2 ns

```
TimeUnit const KIM::TIME_UNIT::ns
```

9.18.2.3 ps

```
TimeUnit const KIM::TIME_UNIT::ps
```

9.18.2.4 s

```
TimeUnit const KIM::TIME_UNIT::s
```

9.18.2.5 unused

```
TimeUnit const KIM::TIME_UNIT::unused
```

9.19 kim_argument_name_module Module Reference

Variables

- type(kim_argument_name_type), public, protected [kim_argument_name_number_of_particles](#)
- type(kim_argument_name_type), public, protected [kim_argument_name_particle_species_codes](#)
- type(kim_argument_name_type), public, protected [kim_argument_name_particle_contributing](#)
- type(kim_argument_name_type), public, protected [kim_argument_name_coordinates](#)
- type(kim_argument_name_type), public, protected [kim_argument_name_partial_energy](#)
- type(kim_argument_name_type), public, protected [kim_argument_name_partial_forces](#)
- type(kim_argument_name_type), public, protected [kim_argument_name_partial_particle_energy](#)
- type(kim_argument_name_type), public, protected [kim_argument_name_partial_virial](#)
- type(kim_argument_name_type), public, protected [kim_argument_name_partial_particle_virial](#)

9.19.1 Variable Documentation

9.19.1.1 kim_argument_name_coordinates

```
type(kim_argument_name_type), public, protected kim_argument_name_module::kim_argument_name_↵  
coordinates
```

Definition at line 73 of file kim_argument_name_module.f90.

9.19.1.2 kim_argument_name_number_of_particles

```
type(kim_argument_name_type), public, protected kim_argument_name_module::kim_argument_name_↵  
number_of_particles
```

Definition at line 64 of file kim_argument_name_module.f90.

9.19.1.3 kim_argument_name_partial_energy

```
type(kim_argument_name_type), public, protected kim_argument_name_module::kim_argument_name_↵  
partial_energy
```

Definition at line 76 of file kim_argument_name_module.f90.

9.19.1.4 kim_argument_name_partial_forces

```
type(kim_argument_name_type), public, protected kim_argument_name_module::kim_argument_name_↵  
partial_forces
```

Definition at line 79 of file kim_argument_name_module.f90.

9.19.1.5 kim_argument_name_partial_particle_energy

```
type(kim_argument_name_type), public, protected kim_argument_name_module::kim_argument_name_↵  
partial_particle_energy
```

Definition at line 82 of file kim_argument_name_module.f90.

9.19.1.6 kim_argument_name_partial_particle_virial

```
type(kim_argument_name_type), public, protected kim_argument_name_module::kim_argument_name_↵  
partial_particle_virial
```

Definition at line 88 of file kim_argument_name_module.f90.

9.19.1.7 kim_argument_name_partial_virial

```
type(kim_argument_name_type), public, protected kim_argument_name_module::kim_argument_name_↵  
partial_virial
```

Definition at line 85 of file kim_argument_name_module.f90.

9.19.1.8 kim_argument_name_particle_contributing

```
type(kim_argument_name_type), public, protected kim_argument_name_module::kim_argument_name_↵  
particle_contributing
```

Definition at line 70 of file kim_argument_name_module.f90.

9.19.1.9 kim_argument_name_particle_species_codes

```
type(kim_argument_name_type), public, protected kim_argument_name_module::kim_argument_name_↵  
particle_species_codes
```

Definition at line 67 of file kim_argument_name_module.f90.

9.20 kim_callback_name_module Module Reference

Variables

- type(kim_callback_name_type), public, protected [kim_callback_name_get_neighbor_list](#)
- type(kim_callback_name_type), public, protected [kim_callback_name_process_dedr_term](#)
- type(kim_callback_name_type), public, protected [kim_callback_name_process_d2edr2_term](#)

9.20.1 Variable Documentation

9.20.1.1 kim_callback_name_get_neighbor_list

```
type(kim_callback_name_type), public, protected kim_callback_name_module::kim_callback_name_↵  
get_neighbor_list
```

Definition at line 57 of file kim_callback_name_module.f90.

9.20.1.2 kim_callback_name_process_d2edr2_term

```
type(kim_callback_name_type), public, protected kim_callback_name_module::kim_callback_name_↵  
process_d2edr2_term
```

Definition at line 63 of file kim_callback_name_module.f90.

9.20.1.3 kim_callback_name_process_dedr_term

```
type(kim_callback_name_type), public, protected kim_callback_name_module::kim_callback_name_↵  
process_dedr_term
```

Definition at line 60 of file kim_callback_name_module.f90.

9.21 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](#)

9.21.1 Variable Documentation

9.21.1.1 kim_charge_unit_c

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

Definition at line 58 of file kim_charge_unit_module.f90.

9.21.1.2 kim_charge_unit_e

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

Definition at line 61 of file kim_charge_unit_module.f90.

9.21.1.3 kim_charge_unit_statc

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

Definition at line 64 of file kim_charge_unit_module.f90.

9.21.1.4 kim_charge_unit_unused

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

Definition at line 55 of file kim_charge_unit_module.f90.

9.22 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](#)

9.22.1 Variable Documentation

9.22.1.1 kim_data_type_double

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

Definition at line 56 of file kim_data_type_module.f90.

9.22.1.2 kim_data_type_integer

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

Definition at line 53 of file kim_data_type_module.f90.

9.23 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](#)

9.23.1 Variable Documentation

9.23.1.1 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 61 of file kim_energy_unit_module.f90.

9.23.1.2 kim_energy_unit_erg

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

Definition at line 64 of file kim_energy_unit_module.f90.

9.23.1.3 kim_energy_unit_ev

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

Definition at line 67 of file kim_energy_unit_module.f90.

9.23.1.4 kim_energy_unit_hartree

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

Definition at line 70 of file kim_energy_unit_module.f90.

9.23.1.5 kim_energy_unit_j

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

Definition at line 73 of file kim_energy_unit_module.f90.

9.23.1.6 kim_energy_unit_kcal_mol

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

Definition at line 76 of file kim_energy_unit_module.f90.

9.23.1.7 kim_energy_unit_unused

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

Definition at line 58 of file kim_energy_unit_module.f90.

9.24 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](#)

9.24.1 Variable Documentation

9.24.1.1 kim_language_name_c

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

Definition at line 57 of file kim_language_name_module.f90.

9.24.1.2 kim_language_name_cpp

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

Definition at line 54 of file kim_language_name_module.f90.

9.24.1.3 kim_language_name_fortran

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

Definition at line 60 of file kim_language_name_module.f90.

9.25 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](#)

9.25.1 Variable Documentation

9.25.1.1 kim_length_unit_a

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

Definition at line 60 of file kim_length_unit_module.f90.

9.25.1.2 kim_length_unit_bohr

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

Definition at line 63 of file kim_length_unit_module.f90.

9.25.1.3 kim_length_unit_cm

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

Definition at line 66 of file kim_length_unit_module.f90.

9.25.1.4 kim_length_unit_m

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

Definition at line 69 of file kim_length_unit_module.f90.

9.25.1.5 kim_length_unit_nm

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

Definition at line 72 of file kim_length_unit_module.f90.

9.25.1.6 kim_length_unit_unused

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

Definition at line 57 of file kim_length_unit_module.f90.

9.26 kim_log_module Module Reference

Data Types

- interface [kim_log_pop_verbosity](#)

Variables

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

9.26.1 Variable Documentation

9.26.1.1 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.

9.27 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), public [kim_log_file](#)
- character(len=65536), public [kim_log_message](#)

9.27.1 Variable Documentation

9.27.1.1 kim_log_file

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

Definition at line 159 of file kim_log_verbosity_module.f90.

9.27.1.2 kim_log_message

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

Definition at line 160 of file kim_log_verbosity_module.f90.

9.27.1.3 kim_log_verbosity_debug

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

Definition at line 79 of file kim_log_verbosity_module.f90.

9.27.1.4 kim_log_verbosity_error

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

Definition at line 70 of file kim_log_verbosity_module.f90.

9.27.1.5 kim_log_verbosity_fatal

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

Definition at line 67 of file kim_log_verbosity_module.f90.

9.27.1.6 kim_log_verbosity_information

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

Definition at line 76 of file kim_log_verbosity_module.f90.

9.27.1.7 kim_log_verbosity_silent

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

Definition at line 64 of file kim_log_verbosity_module.f90.

9.27.1.8 kim_log_verbosity_warning

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

Definition at line 73 of file kim_log_verbosity_module.f90.

9.28 kim_model_compute_module Module Reference

Data Types

- interface [kim_model_compute_get_model_buffer_pointer](#)
- interface [kim_model_compute_get_neighbor_list](#)
- interface [kim_model_compute_string](#)

Variables

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

9.28.1 Variable Documentation

9.28.1.1 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 57 of file kim_model_compute_module.f90.

9.29 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_argument_support_status](#)
- interface [kim_model_create_set_callback_support_status](#)
- 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](#)

9.29.1 Variable Documentation

9.29.1.1 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.

9.30 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](#)

9.30.1 Variable Documentation

9.30.1.1 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.

9.31 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_argument_support_status](#)
- interface [kim_model_driver_create_set_callback_support_status](#)
- 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](#)

9.31.1 Variable Documentation

9.31.1.1 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.

9.32 kim_model_module Module Reference

Data Types

- interface [kim_model_compute](#)
- interface [kim_model_create](#)
- interface [kim_model_destroy](#)
- interface [kim_model_get_callback_support_status](#)
- interface [kim_model_get_number_of_parameters](#)
- interface [kim_model_get_units](#)
- interface [kim_model_pop_log_verbosity](#)
- interface [kim_model_set_callback_pointer](#)
- interface [kim_model_set_simulator_buffer_pointer](#)

Variables

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

9.32.1 Variable Documentation

9.32.1.1 kim_model_null_handle

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

Definition at line 73 of file kim_model_module.f90.

9.33 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](#)

9.33.1 Variable Documentation

9.33.1.1 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.

9.34 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](#)

9.34.1 Variable Documentation

9.34.1.1 kim_numbering_one_based

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

Definition at line 56 of file kim_numbering_module.f90.

9.34.1.2 kim_numbering_zero_based

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

Definition at line 53 of file kim_numbering_module.f90.

9.35 kim_sem_ver_module Module Reference

9.36 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](#)
- type(kim_species_name_type), public, protected [kim_species_name_ru](#)
- type(kim_species_name_type), public, protected [kim_species_name_rh](#)
- type(kim_species_name_type), public, protected [kim_species_name_pd](#)

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- `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](#)

9.36.1 Variable Documentation

9.36.1.1 `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`.

9.36.1.2 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.

9.36.1.3 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.

9.36.1.4 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.

9.36.1.5 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.

9.36.1.6 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.

9.36.1.7 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.

9.36.1.8 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.

9.36.1.9 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.

9.36.1.10 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.

9.36.1.11 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.

9.36.1.12 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.

9.36.1.13 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.

9.36.1.14 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.

9.36.1.15 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.

9.36.1.16 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.

9.36.1.17 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.

9.36.1.18 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.

9.36.1.19 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.

9.36.1.20 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.

9.36.1.21 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.

9.36.1.22 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.

9.36.1.23 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.

9.36.1.24 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.

9.36.1.25 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.

9.36.1.26 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.

9.36.1.27 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.

9.36.1.28 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.

9.36.1.29 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.

9.36.1.30 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.

9.36.1.31 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.

9.36.1.32 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.

9.36.1.33 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.

9.36.1.34 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.

9.36.1.35 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.

9.36.1.36 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.

9.36.1.37 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.

9.36.1.38 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.

9.36.1.39 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.

9.36.1.40 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.

9.36.1.41 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.

9.36.1.42 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.

9.36.1.43 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.

9.36.1.44 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.

9.36.1.45 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.

9.36.1.46 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.

9.36.1.47 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.

9.36.1.48 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.

9.36.1.49 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.

9.36.1.50 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.

9.36.1.51 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.

9.36.1.52 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.

9.36.1.53 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.

9.36.1.54 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.

9.36.1.55 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.

9.36.1.56 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.

9.36.1.57 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.

9.36.1.58 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.

9.36.1.59 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.

9.36.1.60 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.

9.36.1.61 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.

9.36.1.62 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.

9.36.1.63 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.

9.36.1.64 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.

9.36.1.65 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.

9.36.1.66 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.

9.36.1.67 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.

9.36.1.68 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.

9.36.1.69 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.

9.36.1.70 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.

9.36.1.71 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.

9.36.1.72 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.

9.36.1.73 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.

9.36.1.74 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.

9.36.1.75 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.

9.36.1.76 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.

9.36.1.77 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.

9.36.1.78 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.

9.36.1.79 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.

9.36.1.80 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.

9.36.1.81 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.

9.36.1.82 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.

9.36.1.83 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.

9.36.1.84 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.

9.36.1.85 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.

9.36.1.86 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.

9.36.1.87 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.

9.36.1.88 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.

9.36.1.89 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.

9.36.1.90 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.

9.36.1.91 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.

9.36.1.92 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.

9.36.1.93 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.

9.36.1.94 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.

9.36.1.95 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.

9.36.1.96 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.

9.36.1.97 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.

9.36.1.98 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.

9.36.1.99 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.

9.36.1.100 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.

9.36.1.101 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.

9.36.1.102 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.

9.36.1.103 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.

9.36.1.104 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.

9.36.1.105 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.

9.36.1.106 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.

9.36.1.107 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.

9.36.1.108 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.

9.36.1.109 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.

9.36.1.110 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.

9.36.1.111 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.

9.36.1.112 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.

9.36.1.113 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.

9.36.1.114 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.

9.36.1.115 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.

9.36.1.116 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.

9.36.1.117 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.

9.36.1.118 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.

9.36.1.119 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.

9.36.1.120 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.

9.36.1.121 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.

9.36.1.122 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.

9.36.1.123 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.

9.36.1.124 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.

9.36.1.125 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.

9.36.1.126 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.

9.36.1.127 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.

9.36.1.128 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.

9.36.1.129 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.

9.36.1.130 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.

9.36.1.131 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.

9.36.1.132 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.

9.36.1.133 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.

9.36.1.134 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.

9.36.1.135 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.

9.36.1.136 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.

9.36.1.137 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.

9.36.1.138 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.

9.36.1.139 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.

9.37 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](#)

9.37.1 Variable Documentation

9.37.1.1 kim_support_status_not_supported

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

Definition at line 58 of file kim_support_status_module.f90.

9.37.1.2 kim_support_status_optional

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

Definition at line 64 of file kim_support_status_module.f90.

9.37.1.3 kim_support_status_required

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

Definition at line 61 of file kim_support_status_module.f90.

9.37.1.4 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 55 of file kim_support_status_module.f90.

9.38 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](#)

9.38.1 Variable Documentation

9.38.1.1 kim_temperature_unit_k

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

Definition at line 56 of file kim_temperature_unit_module.f90.

9.38.1.2 kim_temperature_unit_unused

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

Definition at line 53 of file kim_temperature_unit_module.f90.

9.39 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](#)

9.39.1 Variable Documentation

9.39.1.1 kim_time_unit_fs

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

Definition at line 58 of file kim_time_unit_module.f90.

9.39.1.2 kim_time_unit_ns

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

Definition at line 62 of file kim_time_unit_module.f90.

9.39.1.3 kim_time_unit_ps

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

Definition at line 60 of file kim_time_unit_module.f90.

9.39.1.4 kim_time_unit_s

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

Definition at line 64 of file kim_time_unit_module.f90.

9.39.1.5 kim_time_unit_unused

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

Definition at line 56 of file kim_time_unit_module.f90.

9.40 kim_unit_system_module Module Reference

9.41 mod_neighborlist Module Reference

Data Types

- type [neighobject_type](#)

Functions/Subroutines

- subroutine, public [get_neigh](#) (data_object, neighbor_list_index, request, numnei, pnei1part, ierr)

9.41.1 Function/Subroutine Documentation

9.41.1.1 get_neigh()

```
subroutine public mod_neighborlist::get_neigh (
    type(c_ptr), intent(in), value data_object,
    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) pnei1part,
    integer(c_int), intent(out) ierr )
```

Definition at line 89 of file ex_test_Ar_fcc_cluster_fortran.F90.

Chapter 10

Class Documentation

10.1 KIM::ArgumentName Class Reference

```
#include <KIM_ArgumentName.hpp>
```

Public Member Functions

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

Public Attributes

- int [argumentNameID](#)

10.1.1 Detailed Description

Definition at line 44 of file KIM_ArgumentName.hpp.

10.1.2 Constructor & Destructor Documentation

10.1.2.1 [ArgumentName](#)() [1/3]

```
KIM::ArgumentName::ArgumentName ( )
```


10.1.2.2 `ArgumentName()` [2/3]

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

10.1.2.3 `ArgumentName()` [3/3]

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

10.1.3 Member Function Documentation

10.1.3.1 `operator!=()`

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

10.1.3.2 `operator==()`

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

10.1.3.3 `String()`

```
std::string KIM::ArgumentName::String ( ) const
```

10.1.4 Member Data Documentation

10.1.4.1 `argumentNameID`

```
int KIM::ArgumentName::argumentNameID
```

Definition at line 47 of file `KIM_ArgumentName.hpp`.

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

- `kim-api-v2.0.0-alpha.0/cpp/include/KIM_ArgumentName.hpp`

10.2 KIM::CallbackName Class Reference

```
#include <KIM_CallbackName.hpp>
```

Public Member Functions

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

Public Attributes

- int [callbackNameID](#)

10.2.1 Detailed Description

Definition at line 42 of file KIM_CallbackName.hpp.

10.2.2 Constructor & Destructor Documentation

10.2.2.1 [CallbackName\(\)](#) [1/3]

```
KIM::CallbackName::CallbackName ( )
```

10.2.2.2 [CallbackName\(\)](#) [2/3]

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

10.2.2.3 [CallbackName\(\)](#) [3/3]

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


10.2.3 Member Function Documentation

10.2.3.1 operator"!=()

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

10.2.3.2 operator==(

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

10.2.3.3 String()

```
std::string KIM::CallbackName::String ( ) const
```

10.2.4 Member Data Documentation

10.2.4.1 callbackNameID

```
int KIM::CallbackName::callbackNameID
```

Definition at line 45 of file KIM_CallbackName.hpp.

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

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

10.3 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 [String](#) () const

Public Attributes

- int [chargeUnitID](#)

10.3.1 Detailed Description

Definition at line 42 of file KIM_ChargeUnit.hpp.

10.3.2 Constructor & Destructor Documentation

10.3.2.1 [ChargeUnit\(\)](#) [1/3]

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

10.3.2.2 [ChargeUnit\(\)](#) [2/3]

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

10.3.2.3 [ChargeUnit\(\)](#) [3/3]

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

10.3.3 Member Function Documentation

10.3.3.1 operator!=(())

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

10.3.3.2 operator==(())

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

10.3.3.3 String()

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

10.3.4 Member Data Documentation

10.3.4.1 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-alpha.0/cpp/include/[KIM_ChargeUnit.hpp](#)

10.4 KIM::CALLBACK_NAME::Comparator Struct Reference

```
#include <KIM_CallbackName.hpp>
```

Public Member Functions

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

10.4.1 Detailed Description

Definition at line 64 of file KIM_CallbackName.hpp.

10.4.2 Member Function Documentation

10.4.2.1 operator()()

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

Definition at line 66 of file KIM_CallbackName.hpp.

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

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

10.5 KIM::DATA_TYPE::Comparator Struct Reference

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

Public Member Functions

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

10.5.1 Detailed Description

Definition at line 63 of file KIM_DataType.hpp.

10.5.2 Member Function Documentation

10.5.2.1 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-alpha.0/cpp/include/[KIM_DataType.hpp](#)

10.6 KIM::TIME_UNIT::Comparator Struct Reference

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

Public Member Functions

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

10.6.1 Detailed Description

Definition at line 66 of file `KIM_TimeUnit.hpp`.

10.6.2 Member Function Documentation

10.6.2.1 [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-alpha.0/cpp/include/KIM_TimeUnit.hpp`

10.7 KIM::LOG_VERBOSITY::Comparator Struct Reference

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

Public Member Functions

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

10.7.1 Detailed Description

Definition at line 75 of file `KIM_LogVerbosity.hpp`.

10.7.2 Member Function Documentation

10.7.2.1 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-alpha.0/cpp/include/KIM_LogVerbosity.hpp

10.8 KIM::ARGUMENT_NAME::Comparator Struct Reference

```
#include <KIM_ArgumentName.hpp>
```

Public Member Functions

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

10.8.1 Detailed Description

Definition at line 75 of file KIM_ArgumentName.hpp.

10.8.2 Member Function Documentation

10.8.2.1 operator()

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

Definition at line 77 of file KIM_ArgumentName.hpp.

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

- kim-api-v2.0.0-alpha.0/cpp/include/KIM_ArgumentName.hpp

10.9 KIM::ENERGY_UNIT::Comparator Struct Reference

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


Public Member Functions

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

10.9.1 Detailed Description

Definition at line 68 of file [KIM_EnergyUnit.hpp](#).

10.9.2 Member Function Documentation

10.9.2.1 [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-alpha.0/cpp/include/KIM_EnergyUnit.hpp](#)

10.10 KIM::CHARGE_UNIT::Comparator Struct Reference

```
#include <KIM\_ChargeUnit.hpp>
```

Public Member Functions

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

10.10.1 Detailed Description

Definition at line 65 of file [KIM_ChargeUnit.hpp](#).

10.10.2 Member Function Documentation

10.10.2.1 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-alpha.0/cpp/include/KIM_ChargeUnit.hpp

10.11 KIM::LANGUAGE_NAME::Comparator Struct Reference

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

Public Member Functions

- bool operator() (LanguageName const &a, LanguageName const &b) const

10.11.1 Detailed Description

Definition at line 63 of file KIM_LanguageName.hpp.

10.11.2 Member Function Documentation

10.11.2.1 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-alpha.0/cpp/include/KIM_LanguageName.hpp

10.12 KIM::NUMBERING::Comparator Struct Reference

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


Public Member Functions

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

10.12.1 Detailed Description

Definition at line 63 of file KIM_Numbering.hpp.

10.12.2 Member Function Documentation

10.12.2.1 [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-alpha.0/cpp/include/[KIM_Numbering.hpp](#)

10.13 KIM::SPECIES_NAME::Comparator Struct Reference

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

Public Member Functions

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

10.13.1 Detailed Description

Definition at line 200 of file KIM_SpeciesName.hpp.

10.13.2 Member Function Documentation

10.13.2.1 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-alpha.0/cpp/include/KIM_SpeciesName.hpp

10.14 KIM::LENGTH_UNIT::Comparator Struct Reference

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

Public Member Functions

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

10.14.1 Detailed Description

Definition at line 67 of file KIM_LengthUnit.hpp.

10.14.2 Member Function Documentation

10.14.2.1 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-alpha.0/cpp/include/KIM_LengthUnit.hpp

10.15 KIM::SUPPORT_STATUS::Comparator Struct Reference

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


Public Member Functions

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

10.15.1 Detailed Description

Definition at line 65 of file `KIM_SupportStatus.hpp`.

10.15.2 Member Function Documentation

10.15.2.1 [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-alpha.0/cpp/include/KIM_SupportStatus.hpp`

10.16 KIM::TEMPERATURE_UNIT::Comparator Struct Reference

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

Public Member Functions

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

10.16.1 Detailed Description

Definition at line 64 of file `KIM_TemperatureUnit.hpp`.

10.16.2 Member Function Documentation

10.16.2.1 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-alpha.0/cpp/include/KIM_TemperatureUnit.hpp](#)

10.17 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 [String](#) () const

Public Attributes

- int [dataTypeID](#)

10.17.1 Detailed Description

Definition at line 42 of file KIM_DataType.hpp.

10.17.2 Constructor & Destructor Documentation

10.17.2.1 [DataType](#)() [1/3]

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


10.17.2.2 `DataType()` [2/3]

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

10.17.2.3 `DataType()` [3/3]

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

10.17.3 Member Function Documentation

10.17.3.1 `operator!=()`

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

10.17.3.2 `operator==()`

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

10.17.3.3 `String()`

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

10.17.4 Member Data Documentation

10.17.4.1 `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-alpha.0/cpp/include/KIM_DataType.hpp`

10.18 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 [String](#) () const

Public Attributes

- int [energyUnitID](#)

10.18.1 Detailed Description

Definition at line 42 of file KIM_EnergyUnit.hpp.

10.18.2 Constructor & Destructor Documentation

10.18.2.1 [EnergyUnit\(\)](#) [1/3]

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

10.18.2.2 [EnergyUnit\(\)](#) [2/3]

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

10.18.2.3 [EnergyUnit\(\)](#) [3/3]

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


10.18.3 Member Function Documentation

10.18.3.1 operator!=(())

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

10.18.3.2 operator==(())

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

10.18.3.3 String()

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

10.18.4 Member Data Documentation

10.18.4.1 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-alpha.0/cpp/include/[KIM_EnergyUnit.hpp](#)

10.19 KIM_ArgumentName Struct Reference

```
#include <KIM_ArgumentName.h>
```

Public Attributes

- int [argumentNameID](#)

10.19.1 Detailed Description

Definition at line 45 of file KIM_ArgumentName.h.

10.19.2 Member Data Documentation

10.19.2.1 argumentNameID

```
int KIM_ArgumentName::argumentNameID
```

Definition at line 47 of file KIM_ArgumentName.h.

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

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

10.20 KIM_CallbackName Struct Reference

```
#include <KIM_CallbackName.h>
```

Public Attributes

- int [callbackNameID](#)

10.20.1 Detailed Description

Definition at line 39 of file KIM_CallbackName.h.

10.20.2 Member Data Documentation

10.20.2.1 callbackNameID

```
int KIM_CallbackName::callbackNameID
```

Definition at line 41 of file KIM_CallbackName.h.

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

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

10.21 KIM_ChargeUnit Struct Reference

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

Public Attributes

- int [chargeUnitID](#)

10.21.1 Detailed Description

Definition at line 39 of file KIM_ChargeUnit.h.

10.21.2 Member Data Documentation

10.21.2.1 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-alpha.0/c/include/[KIM_ChargeUnit.h](#)

10.22 KIM_DataType Struct Reference

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

Public Attributes

- int [dataTypeID](#)

10.22.1 Detailed Description

Definition at line 39 of file KIM_DataType.h.

10.22.2 Member Data Documentation

10.22.2.1 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-alpha.0/c/include/[KIM_DataType.h](#)

10.23 KIM_EnergyUnit Struct Reference

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

Public Attributes

- int [energyUnitID](#)

10.23.1 Detailed Description

Definition at line 39 of file KIM_EnergyUnit.h.

10.23.2 Member Data Documentation

10.23.2.1 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-alpha.0/c/include/[KIM_EnergyUnit.h](#)

10.24 KIM_LanguageName Struct Reference

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

Public Attributes

- int [languageNameID](#)

10.24.1 Detailed Description

Definition at line 39 of file KIM_LanguageName.h.

10.24.2 Member Data Documentation

10.24.2.1 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-alpha.0/c/include/KIM_LanguageName.h](#)

10.25 KIM_LengthUnit Struct Reference

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

Public Attributes

- int [lengthUnitID](#)

10.25.1 Detailed Description

Definition at line 39 of file KIM_LengthUnit.h.

10.25.2 Member Data Documentation

10.25.2.1 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-alpha.0/c/include/KIM_LengthUnit.h](#)

10.26 kim_log_module::kim_log_pop_verbosity Interface Reference

10.26.1 Detailed Description

Definition at line 121 of file kim_log_module.f90.

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

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

10.27 KIM_LogVerbosity Struct Reference

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

Public Attributes

- int [logVerbosityID](#)

10.27.1 Detailed Description

Definition at line 42 of file KIM_LogVerbosity.h.

10.27.2 Member Data Documentation

10.27.2.1 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-alpha.0/c/include/[KIM_LogVerbosity.h](#)

10.28 kim_model_module::kim_model_compute Interface Reference

10.28.1 Detailed Description

Definition at line 339 of file kim_model_module.f90.

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

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

10.29 kim_model_compute_module::kim_model_compute_get_model_buffer_pointer Interface Reference

10.29.1 Detailed Description

Definition at line 216 of file kim_model_compute_module.f90.

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

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

10.30 kim_model_compute_module::kim_model_compute_get_neighbor_list Interface Reference

10.30.1 Detailed Description

Definition at line 162 of file kim_model_compute_module.f90.

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

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

10.31 kim_model_compute_module::kim_model_compute_string Interface Reference

10.31.1 Detailed Description

Definition at line 238 of file kim_model_compute_module.f90.

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

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

10.32 kim_model_module::kim_model_create Interface Reference

10.32.1 Detailed Description

Definition at line 225 of file kim_model_module.f90.

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

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

10.33 kim_model_create_module::kim_model_create_convert_unit Interface Reference

10.33.1 Detailed Description

Definition at line 246 of file kim_model_create_module.f90.

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

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

10.34 kim_model_create_module::kim_model_create_log_entry Interface Reference

10.34.1 Detailed Description

Definition at line 282 of file kim_model_create_module.f90.

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

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

10.35 kim_model_create_module::kim_model_create_set_argument_support_status Interface Reference

10.35.1 Detailed Description

Definition at line 191 of file kim_model_create_module.f90.

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

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

10.36 kim_model_create_module::kim_model_create_set_callback_support_status Interface Reference

10.36.1 Detailed Description

Definition at line 204 of file kim_model_create_module.f90.

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

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

10.37 kim_model_create_module::kim_model_create_set_compute_pointer Interface Reference

10.37.1 Detailed Description

Definition at line 167 of file kim_model_create_module.f90.

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

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

10.38 kim_model_create_module::kim_model_create_set_destroy_pointer Interface Reference

10.38.1 Detailed Description

Definition at line 155 of file kim_model_create_module.f90.

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

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

10.39 kim_model_create_module::kim_model_create_set_influence_distance_pointer Interface Reference

10.39.1 Detailed Description

Definition at line 124 of file kim_model_create_module.f90.

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

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

10.40 kim_model_create_module::kim_model_create_set_model_buffer_pointer Interface Reference

10.40.1 Detailed Description

Definition at line 217 of file kim_model_create_module.f90.

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

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

10.41 kim_model_create_module::kim_model_create_set_species_code Interface Reference

10.41.1 Detailed Description

Definition at line 179 of file kim_model_create_module.f90.

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

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

10.42 kim_model_create_module::kim_model_create_string Interface Reference

10.42.1 Detailed Description

Definition at line 295 of file kim_model_create_module.f90.

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

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

10.43 kim_model_module::kim_model_destroy Interface Reference

10.43.1 Detailed Description

Definition at line 249 of file kim_model_module.f90.

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

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

10.44 kim_model_destroy_module::kim_model_destroy_string Interface Reference

10.44.1 Detailed Description

Definition at line 99 of file kim_model_destroy_module.f90.

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

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

10.45 kim_model_driver_create_module::kim_model_driver_create_convert_unit Interface Reference

10.45.1 Detailed Description

Definition at line 284 of file kim_model_driver_create_module.f90.

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

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

10.46 kim_model_driver_create_module::kim_model_driver_create_log_entry Interface Reference

10.46.1 Detailed Description

Definition at line 321 of file kim_model_driver_create_module.f90.

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

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

10.47 kim_model_driver_create_module::kim_model_driver_create_set_argument_↔ support_status Interface Reference

10.47.1 Detailed Description

Definition at line 224 of file kim_model_driver_create_module.f90.

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

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

10.48 kim_model_driver_create_module::kim_model_driver_create_set_callback_↔ support_status Interface Reference

10.48.1 Detailed Description

Definition at line 238 of file kim_model_driver_create_module.f90.

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

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

10.49 kim_model_driver_create_module::kim_model_driver_create_set_compute_pointer Interface Reference

10.49.1 Detailed Description

Definition at line 198 of file kim_model_driver_create_module.f90.

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

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

10.50 kim_model_driver_create_module::kim_model_driver_create_set_destroy_pointer Interface Reference

10.50.1 Detailed Description

Definition at line 185 of file kim_model_driver_create_module.f90.

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

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

10.51 kim_model_driver_create_module::kim_model_driver_create_set_influence_distance_pointer Interface Reference

10.51.1 Detailed Description

Definition at line 151 of file kim_model_driver_create_module.f90.

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

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

10.52 kim_model_driver_create_module::kim_model_driver_create_set_model_buffer_pointer Interface Reference

10.52.1 Detailed Description

Definition at line 252 of file kim_model_driver_create_module.f90.

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

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

10.53 kim_model_driver_create_module::kim_model_driver_create_set_species_code Interface Reference

10.53.1 Detailed Description

Definition at line 211 of file kim_model_driver_create_module.f90.

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

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

10.54 kim_model_driver_create_module::kim_model_driver_create_string Interface Reference

10.54.1 Detailed Description

Definition at line 336 of file kim_model_driver_create_module.f90.

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

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

10.55 kim_model_module::kim_model_get_callback_support_status Interface Reference

10.55.1 Detailed Description

Definition at line 296 of file kim_model_module.f90.

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

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

10.56 kim_model_module::kim_model_get_number_of_parameters Interface Reference

10.56.1 Detailed Description

Definition at line 369 of file kim_model_module.f90.

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

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

10.57 kim_model_module::kim_model_get_units Interface Reference

10.57.1 Detailed Description

Definition at line 324 of file kim_model_module.f90.

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

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

10.58 kim_model_module::kim_model_pop_log_verbosity Interface Reference

10.58.1 Detailed Description

Definition at line 433 of file kim_model_module.f90.

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

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

10.59 kim_model_refresh_module::kim_model_refresh_string Interface Reference

10.59.1 Detailed Description

Definition at line 124 of file kim_model_refresh_module.f90.

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

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

10.60 kim_model_module::kim_model_set_callback_pointer Interface Reference

10.60.1 Detailed Description

Definition at line 309 of file kim_model_module.f90.

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

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

10.61 kim_model_module::kim_model_set_simulator_buffer_pointer Interface Reference

10.61.1 Detailed Description

Definition at line 392 of file kim_model_module.f90.

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

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

10.62 KIM_Numbering Struct Reference

```
#include <KIM_Numbering.h>
```

Public Attributes

- int [numberingID](#)

10.62.1 Detailed Description

Definition at line 39 of file KIM_Numbering.h.

10.62.2 Member Data Documentation

10.62.2.1 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-alpha.0/c/include/[KIM_Numbering.h](#)

10.63 KIM_SpeciesName Struct Reference

```
#include <KIM_SpeciesName.h>
```


Public Attributes

- int [speciesNameID](#)

10.63.1 Detailed Description

Definition at line 39 of file KIM_SpeciesName.h.

10.63.2 Member Data Documentation

10.63.2.1 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-alpha.0/c/include/[KIM_SpeciesName.h](#)

10.64 KIM_SupportStatus Struct Reference

```
#include <KIM_SupportStatus.h>
```

Public Attributes

- int [supportStatusID](#)

10.64.1 Detailed Description

Definition at line 39 of file KIM_SupportStatus.h.

10.64.2 Member Data Documentation

10.64.2.1 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-alpha.0/c/include/KIM_SupportStatus.h](#)

10.65 KIM_TemperatureUnit Struct Reference

```
#include <KIM_TemperatureUnit.h>
```

Public Attributes

- int [temperatureUnitID](#)

10.65.1 Detailed Description

Definition at line 39 of file KIM_TemperatureUnit.h.

10.65.2 Member Data Documentation

10.65.2.1 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-alpha.0/c/include/KIM_TemperatureUnit.h](#)

10.66 KIM_TimeUnit Struct Reference

```
#include <KIM_TimeUnit.h>
```

Public Attributes

- int [timeUnitID](#)

10.66.1 Detailed Description

Definition at line 39 of file KIM_TimeUnit.h.

10.66.2 Member Data Documentation

10.66.2.1 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-alpha.0/c/include/KIM_TimeUnit.h](#)

10.67 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 [String](#) () const

Public Attributes

- int [languageNameID](#)

10.67.1 Detailed Description

Definition at line 41 of file KIM_LanguageName.hpp.

10.67.2 Constructor & Destructor Documentation

10.67.2.1 `LanguageName()` [1/3]

```
KIM::LanguageName::LanguageName ( )
```

10.67.2.2 `LanguageName()` [2/3]

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

10.67.2.3 `LanguageName()` [3/3]

```
KIM::LanguageName::LanguageName (
    std::string const str )
```

10.67.3 Member Function Documentation

10.67.3.1 `operator!=(())`

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

10.67.3.2 `operator==(())`

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

10.67.3.3 `String()`

```
std::string KIM::LanguageName::String ( ) const
```

10.67.4 Member Data Documentation

10.67.4.1 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-alpha.0/cpp/include/[KIM_LanguageName.hpp](#)

10.68 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 [String](#) () const

Public Attributes

- int [lengthUnitID](#)

10.68.1 Detailed Description

Definition at line 42 of file KIM_LengthUnit.hpp.

10.68.2 Constructor & Destructor Documentation

10.68.2.1 LengthUnit() [1/3]

```
KIM::LengthUnit::LengthUnit ( )
```


10.68.2.2 LengthUnit() [2/3]

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

10.68.2.3 LengthUnit() [3/3]

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

10.68.3 Member Function Documentation

10.68.3.1 operator!=(())

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

10.68.3.2 operator==(())

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

10.68.3.3 String()

```
std::string KIM::LengthUnit::String ( ) const
```

10.68.4 Member Data Documentation

10.68.4.1 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-alpha.0/cpp/include/[KIM_LengthUnit.hpp](#)

10.69 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)

10.69.1 Detailed Description

Definition at line 53 of file LennardJones612.hpp.

10.69.2 Constructor & Destructor Documentation

10.69.2.1 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 94 of file LennardJones612.cpp.

10.69.2.2 ~LennardJones612()

```
LennardJones612::~~LennardJones612 ( )
```

Definition at line 114 of file LennardJones612.cpp.

10.69.3 Member Function Documentation

10.69.3.1 Compute()

```
int LennardJones612::Compute (
    KIM::ModelCompute const *const modelCompute ) [static]
```

Definition at line 150 of file LennardJones612.cpp.

10.69.3.2 Destroy()

```
int LennardJones612::Destroy (
    KIM::ModelDestroy *const modelDestroy ) [static]
```

Definition at line 121 of file LennardJones612.cpp.

10.69.3.3 Refresh()

```
int LennardJones612::Refresh (
    KIM::ModelRefresh *const modelRefresh ) [static]
```

Definition at line 138 of file LennardJones612.cpp.

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

- kim-api-v2.0.0-alpha.0/examples/model_drivers/LennardJones612__MD_414112407348_002/LennardJones612.hpp
- kim-api-v2.0.0-alpha.0/examples/model_drivers/LennardJones612__MD_414112407348_002/LennardJones612.cpp

10.70 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)

10.70.1 Detailed Description

Definition at line 74 of file LennardJones612Implementation.hpp.

10.70.2 Constructor & Destructor Documentation

10.70.2.1 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 59 of file LennardJones612Implementation.cpp.

10.70.2.2 ~LennardJones612Implementation()

```
LennardJones612Implementation::~LennardJones612Implementation ( )
```

Definition at line 124 of file LennardJones612Implementation.cpp.

10.70.3 Member Function Documentation

10.70.3.1 Compute()

```
int LennardJones612Implementation::Compute (
    KIM::ModelCompute const *const modelCompute )
```

Definition at line 158 of file LennardJones612Implementation.cpp.

10.70.3.2 Refresh()

```
int LennardJones612Implementation::Refresh (
    KIM::ModelRefresh *const modelRefresh )
```

Definition at line 142 of file LennardJones612Implementation.cpp.

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

- kim-api-v2.0.0-alpha.0/examples/model_drivers/LennardJones612__MD_414112407348_002/[LennardJones612Implementation](#)
- kim-api-v2.0.0-alpha.0/examples/model_drivers/LennardJones612__MD_414112407348_002/[LennardJones612Implementation](#)

10.71 KIM::Log Class Reference

```
#include <KIM_Log.hpp>
```

Public Member Functions

- std::string [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)

10.71.1 Detailed Description

Definition at line 46 of file KIM_Log.hpp.

10.71.2 Member Function Documentation

10.71.2.1 Create()

```
static int KIM::Log::Create (
    Log **const log ) [static]
```


10.71.2.2 Destroy()

```
static void KIM::Log::Destroy (
    Log **const log ) [static]
```

10.71.2.3 GetID()

```
std::string KIM::Log::GetID ( ) const
```

10.71.2.4 LogEntry() [1/2]

```
void KIM::Log::LogEntry (
    LogVerbosity const logVerbosity,
    std::string const & message,
    int const lineNumber,
    std::string const & fileName ) const
```

10.71.2.5 LogEntry() [2/2]

```
void KIM::Log::LogEntry (
    LogVerbosity const logVerbosity,
    std::stringstream const & message,
    int const lineNumber,
    std::string const & fileName ) const
```

10.71.2.6 PopVerbosity()

```
void KIM::Log::PopVerbosity ( )
```

10.71.2.7 PushVerbosity()

```
void KIM::Log::PushVerbosity (
    LogVerbosity const logVerbosity )
```


10.71.2.8 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-alpha.0/cpp/include/[KIM_Log.hpp](#)

10.72 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 [String](#) () const

Public Attributes

- int [logVerbosityID](#)

10.72.1 Detailed Description

Definition at line 46 of file [KIM_LogVerbosity.hpp](#).

10.72.2 Constructor & Destructor Documentation

10.72.2.1 LogVerbosity() [1/3]

```
KIM::LogVerbosity::LogVerbosity ( )
```


10.72.2.2 LogVerbosity() [2/3]

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

10.72.2.3 LogVerbosity() [3/3]

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

10.72.3 Member Function Documentation

10.72.3.1 operator!=(())

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

10.72.3.2 operator<()

```
bool KIM::LogVerbosity::operator< (
    LogVerbosity const & rhs ) const
```

10.72.3.3 operator<=()

```
bool KIM::LogVerbosity::operator<= (
    LogVerbosity const & rhs ) const
```

10.72.3.4 operator==(())

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


10.72.3.5 operator>()

```
bool KIM::LogVerbosity::operator> (
    LogVerbosity const & rhs ) const
```

10.72.3.6 operator>=()

```
bool KIM::LogVerbosity::operator>= (
    LogVerbosity const & rhs ) const
```

10.72.3.7 String()

```
std::string KIM::LogVerbosity::String ( ) const
```

10.72.4 Member Data Documentation

10.72.4.1 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-alpha.0/cpp/include/[KIM_LogVerbosity.hpp](#)

10.73 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
- int [GetArgumentSupportStatus](#) ([ArgumentName](#) const argumentName, [SupportStatus](#) *const supportStatus) const
- int [GetCallbackSupportStatus](#) ([CallbackName](#) const callbackName, [SupportStatus](#) *const supportStatus) const
- void [GetUnits](#) ([LengthUnit](#) *const lengthUnit, [EnergyUnit](#) *const energyUnit, [ChargeUnit](#) *const chargeUnit, [TemperatureUnit](#) *const temperatureUnit, [TimeUnit](#) *const timeUnit) const
- int [SetArgumentPointer](#) ([ArgumentName](#) const argumentName, int const *const ptr)
- int [SetArgumentPointer](#) ([ArgumentName](#) const argumentName, double const *const ptr)
- int [SetCallbackPointer](#) ([CallbackName](#) const callbackName, [LanguageName](#) const languageName, [func](#) *const fptr, void const *const dataObject)
- int [Compute](#) () const
- int [ClearInfluenceDistanceAndCutoffsThenRefreshModel](#) ()
- int [GetSpeciesSupportAndCode](#) ([KIM::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 *const extent, std::string *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 [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)

10.73.1 Detailed Description

Definition at line 62 of file `KIM_Model.hpp`.

10.73.2 Member Function Documentation

10.73.2.1 ClearInfluenceDistanceAndCutoffsThenRefreshModel()

```
int KIM::Model::ClearInfluenceDistanceAndCutoffsThenRefreshModel ( )
```

10.73.2.2 Compute()

```
int KIM::Model::Compute ( ) const
```

10.73.2.3 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]
```

10.73.2.4 Destroy()

```
static void KIM::Model::Destroy (
    Model **const model ) [static]
```

10.73.2.5 GetArgumentSupportStatus()

```
int KIM::Model::GetArgumentSupportStatus (
    ArgumentName const argumentName,
    SupportStatus *const supportStatus ) const
```

10.73.2.6 GetCallbackSupportStatus()

```
int KIM::Model::GetCallbackSupportStatus (
    CallbackName const callbackName,
    SupportStatus *const supportStatus ) const
```


10.73.2.7 GetInfluenceDistance()

```
void KIM::Model::GetInfluenceDistance (
    double *const influenceDistance ) const
```

10.73.2.8 GetNeighborListCutoffsPointer()

```
void KIM::Model::GetNeighborListCutoffsPointer (
    int *const numberOfCutoffs,
    double const **const cutoffs ) const
```

10.73.2.9 GetNumberOfParameters()

```
void KIM::Model::GetNumberOfParameters (
    int *const numberOfParameters ) const
```

10.73.2.10 GetParameter() [1/2]

```
int KIM::Model::GetParameter (
    int const parameterIndex,
    int const arrayIndex,
    int *const parameterValue ) const
```

10.73.2.11 GetParameter() [2/2]

```
int KIM::Model::GetParameter (
    int const parameterIndex,
    int const arrayIndex,
    double *const parameterValue ) const
```

10.73.2.12 GetParameterDataTypeExtentAndDescription()

```
int KIM::Model::GetParameterDataTypeExtentAndDescription (
    int const index,
    DataType *const dataType,
    int * extent,
    std::string *const description ) const
```


10.73.2.13 GetSimulatorBufferPointer()

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

10.73.2.14 GetSpeciesSupportAndCode()

```
int KIM::Model::GetSpeciesSupportAndCode (
    KIM::SpeciesName const speciesName,
    int *const speciesIsSupported,
    int *const code ) const
```

10.73.2.15 GetUnits()

```
void KIM::Model::GetUnits (
    LengthUnit *const lengthUnit,
    EnergyUnit *const energyUnit,
    ChargeUnit *const chargeUnit,
    TemperatureUnit *const temperatureUnit,
    TimeUnit *const timeUnit ) const
```

10.73.2.16 PopLogVerbosity()

```
void KIM::Model::PopLogVerbosity ( )
```

10.73.2.17 PushLogVerbosity()

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

10.73.2.18 SetArgumentPointer() [1/2]

```
int KIM::Model::SetArgumentPointer (
    ArgumentName const argumentName,
    int const *const ptr )
```


10.73.2.19 SetArgumentPointer() [2/2]

```
int KIM::Model::SetArgumentPointer (
    ArgumentName const argumentName,
    double const *const ptr )
```

10.73.2.20 SetCallbackPointer()

```
int KIM::Model::SetCallbackPointer (
    CallbackName const callbackName,
    LanguageName const languageName,
    func *const fptr,
    void const *const dataObject )
```

10.73.2.21 SetLogID()

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

10.73.2.22 SetParameter() [1/2]

```
int KIM::Model::SetParameter (
    int const parameterIndex,
    int const arrayIndex,
    int const parameterValue )
```

10.73.2.23 SetParameter() [2/2]

```
int KIM::Model::SetParameter (
    int const parameterIndex,
    int const arrayIndex,
    double const parameterValue )
```

10.73.2.24 SetSimulatorBufferPointer()

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


10.73.2.25 String()

```
std::string KIM::Model::String ( ) const
```

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

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

10.74 KIM::ModelCompute Class Reference

```
#include <KIM_ModelCompute.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](#) ([ArgumentName](#) const argumentName, int const **const ptr) const
- int [GetArgumentPointer](#) ([ArgumentName](#) const argumentName, int **const ptr) const
- int [GetArgumentPointer](#) ([ArgumentName](#) const argumentName, double const **const ptr) const
- int [GetArgumentPointer](#) ([ArgumentName](#) const argumentName, double **const ptr) const
- int [IsCallbackPresent](#) ([CallbackName](#) const callbackName, int *const present) const
- void [GetModelBufferPointer](#) (void **const ptr) const
- void [LogEntry](#) ([LogVerbosity](#) const logVerbosity, std::string const &message, int const lineNumber, std::string const &fileName) const
- std::string [String](#) () const

10.74.1 Detailed Description

Definition at line 47 of file [KIM_ModelCompute.hpp](#).

10.74.2 Member Function Documentation

10.74.2.1 GetArgumentPointer() [1/4]

```
int KIM::ModelCompute::GetArgumentPointer (
    ArgumentName const argumentName,
    int const **const ptr ) const
```


10.74.2.2 GetArgumentPointer() [2/4]

```
int KIM::ModelCompute::GetArgumentPointer (
    ArgumentName const argumentName,
    int **const ptr ) const
```

10.74.2.3 GetArgumentPointer() [3/4]

```
int KIM::ModelCompute::GetArgumentPointer (
    ArgumentName const argumentName,
    double const **const ptr ) const
```

10.74.2.4 GetArgumentPointer() [4/4]

```
int KIM::ModelCompute::GetArgumentPointer (
    ArgumentName const argumentName,
    double **const ptr ) const
```

10.74.2.5 GetModelBufferPointer()

```
void KIM::ModelCompute::GetModelBufferPointer (
    void **const ptr ) const
```

10.74.2.6 GetNeighborList()

```
int KIM::ModelCompute::GetNeighborList (
    int const neighborListIndex,
    int const particleNumber,
    int *const numberOfNeighbors,
    int const **const neighborsOfParticle ) const
```

10.74.2.7 IsCallbackPresent()

```
int KIM::ModelCompute::IsCallbackPresent (
    CallbackName const callbackName,
    int *const present ) const
```


10.74.2.8 LogEntry()

```
void KIM::ModelCompute::LogEntry (
    LogVerbosity const logVerbosity,
    std::string const & message,
    int const lineNumber,
    std::string const & fileName ) const
```

10.74.2.9 ProcessD2EDr2Term()

```
int KIM::ModelCompute::ProcessD2EDr2Term (
    double const de,
    double const *const r,
    double const *const dx,
    int const *const i,
    int const *const j ) const
```

10.74.2.10 ProcessDEDrTerm()

```
int KIM::ModelCompute::ProcessDEDrTerm (
    double const de,
    double const r,
    double const *const dx,
    int const i,
    int const j ) const
```

10.74.2.11 String()

```
std::string KIM::ModelCompute::String ( ) const
```

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

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

10.75 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 [SetComputePointer](#) ([LanguageName](#) const languageName, [func](#) *const fptr)
- int [SetSpeciesCode](#) ([SpeciesName](#) const speciesName, int const code)
- int [SetArgumentSupportStatus](#) ([ArgumentName](#) const argumentName, [SupportStatus](#) const supportStatus)
- int [SetCallbackSupportStatus](#) ([CallbackName](#) const callbackName, [SupportStatus](#) const supportStatus)
- 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
- std::string [String](#) () const

10.75.1 Detailed Description

Definition at line 61 of file `KIM_ModelCreate.hpp`.

10.75.2 Member Function Documentation

10.75.2.1 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
```


10.75.2.2 LogEntry()

```
void KIM::ModelCreate::LogEntry (
    LogVerbosity const logVerbosity,
    std::string const & message,
    int const lineNumber,
    std::string const & fileName ) const
```

10.75.2.3 SetArgumentSupportStatus()

```
int KIM::ModelCreate::SetArgumentSupportStatus (
    ArgumentName const argumentName,
    SupportStatus const supportStatus )
```

10.75.2.4 SetCallbackSupportStatus()

```
int KIM::ModelCreate::SetCallbackSupportStatus (
    CallbackName const callbackName,
    SupportStatus const supportStatus )
```

10.75.2.5 SetComputePointer()

```
int KIM::ModelCreate::SetComputePointer (
    LanguageName const languageName,
    func *const fptr )
```

10.75.2.6 SetDestroyPointer()

```
int KIM::ModelCreate::SetDestroyPointer (
    LanguageName const languageName,
    func *const fptr )
```

10.75.2.7 SetInfluenceDistancePointer()

```
void KIM::ModelCreate::SetInfluenceDistancePointer (
    double const *const influenceDistance )
```


10.75.2.8 SetModelBufferPointer()

```
void KIM::ModelCreate::SetModelBufferPointer (
    void *const ptr )
```

10.75.2.9 SetModelNumbering()

```
int KIM::ModelCreate::SetModelNumbering (
    Numbering const numbering )
```

10.75.2.10 SetNeighborListCutoffsPointer()

```
void KIM::ModelCreate::SetNeighborListCutoffsPointer (
    int const numberOfCutoffs,
    double const *const cutoffs )
```

10.75.2.11 SetParameterPointer() [1/2]

```
int KIM::ModelCreate::SetParameterPointer (
    int const extent,
    int *const ptr,
    std::string const & description )
```

10.75.2.12 SetParameterPointer() [2/2]

```
int KIM::ModelCreate::SetParameterPointer (
    int const extent,
    double *const ptr,
    std::string const & description )
```

10.75.2.13 SetRefreshPointer()

```
int KIM::ModelCreate::SetRefreshPointer (
    LanguageName const languageName,
    func *const fptr )
```


10.75.2.14 SetSpeciesCode()

```
int KIM::ModelCreate::SetSpeciesCode (
    SpeciesName const speciesName,
    int const code )
```

10.75.2.15 SetUnits()

```
int KIM::ModelCreate::SetUnits (
    LengthUnit const lengthUnit,
    EnergyUnit const energyUnit,
    ChargeUnit const chargeUnit,
    TemperatureUnit const temperatureUnit,
    TimeUnit const timeUnit )
```

10.75.2.16 String()

```
std::string KIM::ModelCreate::String ( ) const
```

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

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

10.76 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
- std::string [String](#) () const

10.76.1 Detailed Description

Definition at line 44 of file [KIM_ModelDestroy.hpp](#).

10.76.2 Member Function Documentation

10.76.2.1 GetModelBufferPointer()

```
void KIM::ModelDestroy::GetModelBufferPointer (
    void **const ptr ) const
```

10.76.2.2 LogEntry()

```
void KIM::ModelDestroy::LogEntry (
    LogVerbosity const logVerbosity,
    std::string const & message,
    int const lineNumber,
    std::string const & fileName ) const
```

10.76.2.3 String()

```
std::string KIM::ModelDestroy::String ( ) const
```

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

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

10.77 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 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 [SetComputePointer](#) ([LanguageName](#) const languageName, [func](#) *const fptr)
- int [SetSpeciesCode](#) ([SpeciesName](#) const speciesName, int const code)
- int [SetArgumentSupportStatus](#) ([ArgumentName](#) const argumentName, [SupportStatus](#) const supportStatus)
- int [SetCallbackSupportStatus](#) ([CallbackName](#) const callbackName, [SupportStatus](#) const supportStatus)
- 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
- std::string [String](#) () const

10.77.1 Detailed Description

Definition at line 61 of file KIM_ModelDriverCreate.hpp.

10.77.2 Member Function Documentation

10.77.2.1 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
```

10.77.2.2 GetNumberOfParameterFiles()

```
void KIM::ModelDriverCreate::GetNumberOfParameterFiles (
    int *const numberOfParameterFiles ) const
```

10.77.2.3 GetParameterFileName()

```
int KIM::ModelDriverCreate::GetParameterFileName (
    int const index,
    std::string *const parameterFileName ) const
```


10.77.2.4 LogEntry()

```
void KIM::ModelDriverCreate::LogEntry (
    LogVerbosity const logVerbosity,
    std::string const & message,
    int const lineNumber,
    std::string const & fileName ) const
```

10.77.2.5 SetArgumentSupportStatus()

```
int KIM::ModelDriverCreate::SetArgumentSupportStatus (
    ArgumentName const argumentName,
    SupportStatus const supportStatus )
```

10.77.2.6 SetCallbackSupportStatus()

```
int KIM::ModelDriverCreate::SetCallbackSupportStatus (
    CallbackName const callbackName,
    SupportStatus const supportStatus )
```

10.77.2.7 SetComputePointer()

```
int KIM::ModelDriverCreate::SetComputePointer (
    LanguageName const languageName,
    func *const fptr )
```

10.77.2.8 SetDestroyPointer()

```
int KIM::ModelDriverCreate::SetDestroyPointer (
    LanguageName const languageName,
    func *const fptr )
```

10.77.2.9 SetInfluenceDistancePointer()

```
void KIM::ModelDriverCreate::SetInfluenceDistancePointer (
    double const *const influenceDistance )
```


10.77.2.10 SetModelBufferPointer()

```
void KIM::ModelDriverCreate::SetModelBufferPointer (
    void *const ptr )
```

10.77.2.11 SetModelNumbering()

```
int KIM::ModelDriverCreate::SetModelNumbering (
    Numbering const numbering )
```

10.77.2.12 SetNeighborListCutoffsPointer()

```
void KIM::ModelDriverCreate::SetNeighborListCutoffsPointer (
    int const numberOfCutoffs,
    double const *const cutoffs )
```

10.77.2.13 SetParameterPointer() [1/2]

```
int KIM::ModelDriverCreate::SetParameterPointer (
    int const extent,
    int *const ptr,
    std::string const & description )
```

10.77.2.14 SetParameterPointer() [2/2]

```
int KIM::ModelDriverCreate::SetParameterPointer (
    int const extent,
    double *const ptr,
    std::string const & description )
```

10.77.2.15 SetRefreshPointer()

```
int KIM::ModelDriverCreate::SetRefreshPointer (
    LanguageName const languageName,
    func *const fptr )
```


10.77.2.16 SetSpeciesCode()

```
int KIM::ModelDriverCreate::SetSpeciesCode (
    SpeciesName const speciesName,
    int const code )
```

10.77.2.17 SetUnits()

```
int KIM::ModelDriverCreate::SetUnits (
    LengthUnit const lengthUnit,
    EnergyUnit const energyUnit,
    ChargeUnit const chargeUnit,
    TemperatureUnit const temperatureUnit,
    TimeUnit const timeUnit )
```

10.77.2.18 String()

```
std::string KIM::ModelDriverCreate::String ( ) const
```

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

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

10.78 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
- std::string [String](#) () const

10.78.1 Detailed Description

Definition at line 50 of file [KIM_ModelRefresh.hpp](#).

10.78.2 Member Function Documentation

10.78.2.1 GetModelBufferPointer()

```
void KIM::ModelRefresh::GetModelBufferPointer (
    void **const ptr ) const
```

10.78.2.2 LogEntry()

```
void KIM::ModelRefresh::LogEntry (
    LogVerbosity const logVerbosity,
    std::string const & message,
    int const lineNumber,
    std::string const & fileName ) const
```

10.78.2.3 SetInfluenceDistancePointer()

```
void KIM::ModelRefresh::SetInfluenceDistancePointer (
    double const *const influenceDistance )
```

10.78.2.4 SetNeighborListCutoffsPointer()

```
void KIM::ModelRefresh::SetNeighborListCutoffsPointer (
    int const numberOfCutoffs,
    double const *const cutoffs )
```

10.78.2.5 String()

```
std::string KIM::ModelRefresh::String ( ) const
```

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

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

10.79 mod_neighborlist::neighobject_type Type Reference**Public Attributes**

- integer(c_int) [number_of_particles](#)
- integer(c_int), dimension(:,:), pointer [neighborlist](#)
- real(c_double), dimension(:,:), pointer [rijlist](#)

10.79.1 Detailed Description

Definition at line 73 of file `ex_test_Ar_fcc_cluster_fortran.F90`.

10.79.2 Member Data Documentation

10.79.2.1 neighborlist

```
integer(c_int), dimension(:, :), pointer mod_neighborlist::neighobject_type::neighborlist
```

Definition at line 75 of file `ex_test_Ar_fcc_cluster_fortran.F90`.

10.79.2.2 number_of_particles

```
integer(c_int) mod_neighborlist::neighobject_type::number_of_particles
```

Definition at line 74 of file `ex_test_Ar_fcc_cluster_fortran.F90`.

10.79.2.3 rijlist

```
real(c_double), dimension(:, :, :), pointer mod_neighborlist::neighobject_type::rijlist
```

Definition at line 76 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-alpha.0/examples/simulators/ex_test_Ar_fcc_cluster_fortran/ex_test_Ar_fcc_cluster_fortran.F90](#)
- [kim-api-v2.0.0-alpha.0/examples/simulators/utility_forces_numer_deriv/utility_forces_numer_deriv.F03](#)

10.80 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 [String](#) () const

Public Attributes

- int [numberingID](#)

10.80.1 Detailed Description

Definition at line 42 of file KIM_Numbering.hpp.

10.80.2 Constructor & Destructor Documentation

10.80.2.1 [Numbering\(\)](#) [1/3]

```
KIM::Numbering::Numbering ( )
```

10.80.2.2 [Numbering\(\)](#) [2/3]

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

10.80.2.3 [Numbering\(\)](#) [3/3]

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

10.80.3 Member Function Documentation

10.80.3.1 [operator!=\(\)](#)

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


10.80.3.2 operator==()

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

10.80.3.3 String()

```
std::string KIM::Numbering::String ( ) const
```

10.80.4 Member Data Documentation

10.80.4.1 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-alpha.0/cpp/include/KIM_Numbering.hpp](#)

10.81 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 [String](#) () const

Public Attributes

- int [speciesNameID](#)

10.81.1 Detailed Description

Definition at line 42 of file KIM_SpeciesName.hpp.

10.81.2 Constructor & Destructor Documentation

10.81.2.1 SpeciesName() [1/3]

```
KIM::SpeciesName::SpeciesName ( )
```

10.81.2.2 SpeciesName() [2/3]

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

10.81.2.3 SpeciesName() [3/3]

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

10.81.3 Member Function Documentation

10.81.3.1 operator!=()

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

10.81.3.2 operator==()

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

10.81.3.3 String()

```
std::string KIM::SpeciesName::String ( ) const
```


10.81.4 Member Data Documentation

10.81.4.1 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-alpha.0/cpp/include/KIM_SpeciesName.hpp](#)

10.82 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 [String](#) () const

Public Attributes

- int [supportStatusID](#)

10.82.1 Detailed Description

Definition at line 42 of file KIM_SupportStatus.hpp.

10.82.2 Constructor & Destructor Documentation

10.82.2.1 SupportStatus() [1/3]

```
KIM::SupportStatus::SupportStatus ( )
```


10.82.2.2 SupportStatus() [2/3]

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

10.82.2.3 SupportStatus() [3/3]

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

10.82.3 Member Function Documentation

10.82.3.1 operator!=(())

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

10.82.3.2 operator==(())

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

10.82.3.3 String()

```
std::string KIM::SupportStatus::String ( ) const
```

10.82.4 Member Data Documentation

10.82.4.1 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-alpha.0/cpp/include/KIM_SupportStatus.hpp](#)

10.83 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 [String](#) () const

Public Attributes

- int [temperatureUnitID](#)

10.83.1 Detailed Description

Definition at line 42 of file KIM_TemperatureUnit.hpp.

10.83.2 Constructor & Destructor Documentation

10.83.2.1 [TemperatureUnit\(\)](#) [1/3]

```
KIM::TemperatureUnit::TemperatureUnit ( )
```

10.83.2.2 [TemperatureUnit\(\)](#) [2/3]

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

10.83.2.3 [TemperatureUnit\(\)](#) [3/3]

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


10.83.3 Member Function Documentation

10.83.3.1 operator!=(())

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

10.83.3.2 operator==(())

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

10.83.3.3 String()

```
std::string KIM::TemperatureUnit::String ( ) const
```

10.83.4 Member Data Documentation

10.83.4.1 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-alpha.0/cpp/include/[KIM_TemperatureUnit.hpp](#)

10.84 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 [String](#) () const

Public Attributes

- int [timeUnitID](#)

10.84.1 Detailed Description

Definition at line 42 of file KIM_TimeUnit.hpp.

10.84.2 Constructor & Destructor Documentation

10.84.2.1 [TimeUnit\(\)](#) [1/3]

```
KIM::TimeUnit::TimeUnit ( )
```

10.84.2.2 [TimeUnit\(\)](#) [2/3]

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

10.84.2.3 [TimeUnit\(\)](#) [3/3]

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

10.84.3 Member Function Documentation

10.84.3.1 operator!=()

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

10.84.3.2 operator==()

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

10.84.3.3 String()

```
std::string KIM::TimeUnit::String ( ) const
```

10.84.4 Member Data Documentation

10.84.4.1 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-alpha.0/cpp/include/[KIM_TimeUnit.hpp](#)

Chapter 11

File Documentation

11.1 kim-api-v2.0.0-alpha.0/c/include/KIM_ArgumentName.h File Reference

Classes

- struct [KIM_ArgumentName](#)

Macros

- `#define` [KIM_DATA_TYPE_DEFINED_](#)
- `#define` [KIM_ARGUMENT_NAME_DEFINED_](#)

Typedefs

- typedef struct [KIM_DataType](#) [KIM_DataType](#)
- typedef struct [KIM_ArgumentName](#) [KIM_ArgumentName](#)

Functions

- [KIM_ArgumentName](#) [KIM_ArgumentNameFromString](#) (char const *const str)
- int [KIM_ArgumentNameEqual](#) ([KIM_ArgumentName](#) const left, [KIM_ArgumentName](#) const right)
- int [KIM_ArgumentNameNotEqual](#) ([KIM_ArgumentName](#) const left, [KIM_ArgumentName](#) const right)
- char const *const [KIM_ArgumentNameString](#) ([KIM_ArgumentName](#) const argumentName)
- void [KIM_ARGUMENT_NAME_GetNumberOfArguments](#) (int *const numberOfArguments)
- int [KIM_ARGUMENT_NAME_GetArgumentName](#) (int const index, [KIM_ArgumentName](#) *const argumentName↵
Name)
- int [KIM_ARGUMENT_NAME_GetArgumentDataType](#) ([KIM_ArgumentName](#) const argumentName,
[KIM_DataType](#) *const dataType)

Variables

- [KIM_ArgumentName](#) const [KIM_ARGUMENT_NAME_numberOfParticles](#)
- [KIM_ArgumentName](#) const [KIM_ARGUMENT_NAME_particleSpeciesCodes](#)
- [KIM_ArgumentName](#) const [KIM_ARGUMENT_NAME_particleContributing](#)
- [KIM_ArgumentName](#) const [KIM_ARGUMENT_NAME_coordinates](#)
- [KIM_ArgumentName](#) const [KIM_ARGUMENT_NAME_partialEnergy](#)
- [KIM_ArgumentName](#) const [KIM_ARGUMENT_NAME_partialForces](#)
- [KIM_ArgumentName](#) const [KIM_ARGUMENT_NAME_partialParticleEnergy](#)
- [KIM_ArgumentName](#) const [KIM_ARGUMENT_NAME_partialVirial](#)
- [KIM_ArgumentName](#) const [KIM_ARGUMENT_NAME_partialParticleVirial](#)

11.1.1 Macro Definition Documentation

11.1.1.1 KIM_ARGUMENT_NAME_DEFINED_

```
#define KIM_ARGUMENT_NAME_DEFINED_
```

Definition at line 50 of file [KIM_ArgumentName.h](#).

11.1.1.2 KIM_DATA_TYPE_DEFINED_

```
#define KIM_DATA_TYPE_DEFINED_
```

Definition at line 41 of file [KIM_ArgumentName.h](#).

11.1.2 Typedef Documentation

11.1.2.1 KIM_ArgumentName

```
typedef struct KIM\_ArgumentName KIM\_ArgumentName
```

Definition at line 51 of file [KIM_ArgumentName.h](#).

11.1.2.2 KIM_DataType

```
typedef struct KIM\_DataType KIM\_DataType
```

Definition at line 42 of file [KIM_ArgumentName.h](#).

11.1.3 Function Documentation

11.1.3.1 KIM_ARGUMENT_NAME_GetArgumentDataType()

```
int KIM_ARGUMENT_NAME_GetArgumentDataType (
    KIM_ArgumentName const argumentName,
    KIM_DataType *const dataType )
```

11.1.3.2 KIM_ARGUMENT_NAME_GetArgumentName()

```
int KIM_ARGUMENT_NAME_GetArgumentName (
    int const index,
    KIM_ArgumentName *const argumentName )
```

11.1.3.3 KIM_ARGUMENT_NAME_GetNumberOfArguments()

```
void KIM_ARGUMENT_NAME_GetNumberOfArguments (
    int *const numberOfArguments )
```

11.1.3.4 KIM_ArgumentNameEqual()

```
int KIM_ArgumentNameEqual (
    KIM_ArgumentName const left,
    KIM_ArgumentName const right )
```

11.1.3.5 KIM_ArgumentNameFromString()

```
KIM_ArgumentName KIM_ArgumentNameFromString (
    char const *const str )
```

11.1.3.6 KIM_ArgumentNameNotEqual()

```
int KIM_ArgumentNameNotEqual (
    KIM_ArgumentName const left,
    KIM_ArgumentName const right )
```


11.1.3.7 KIM_ArgumentNameString()

```
char const* const KIM_ArgumentNameString (
    KIM_ArgumentName const argumentName )
```

11.1.4 Variable Documentation

11.1.4.1 KIM_ARGUMENT_NAME_coordinates

```
KIM_ArgumentName const KIM_ARGUMENT_NAME_coordinates
```

11.1.4.2 KIM_ARGUMENT_NAME_numberOfParticles

```
KIM_ArgumentName const KIM_ARGUMENT_NAME_numberOfParticles
```

11.1.4.3 KIM_ARGUMENT_NAME_partialEnergy

```
KIM_ArgumentName const KIM_ARGUMENT_NAME_partialEnergy
```

11.1.4.4 KIM_ARGUMENT_NAME_partialForces

```
KIM_ArgumentName const KIM_ARGUMENT_NAME_partialForces
```

11.1.4.5 KIM_ARGUMENT_NAME_partialParticleEnergy

```
KIM_ArgumentName const KIM_ARGUMENT_NAME_partialParticleEnergy
```

11.1.4.6 KIM_ARGUMENT_NAME_partialParticleVirial

```
KIM_ArgumentName const KIM_ARGUMENT_NAME_partialParticleVirial
```


11.1.4.7 KIM_ARGUMENT_NAME_partialVirial

`KIM_ArgumentName` const KIM_ARGUMENT_NAME_partialVirial

11.1.4.8 KIM_ARGUMENT_NAME_particleContributing

`KIM_ArgumentName` const KIM_ARGUMENT_NAME_particleContributing

11.1.4.9 KIM_ARGUMENT_NAME_particleSpeciesCodes

`KIM_ArgumentName` const KIM_ARGUMENT_NAME_particleSpeciesCodes

11.2 kim-api-v2.0.0-alpha.0/c/include/KIM_CallbackName.h File Reference

Classes

- struct `KIM_CallbackName`

Macros

- `#define KIM_CALLBACK_NAME_DEFINED_`

Typedefs

- typedef struct `KIM_CallbackName` `KIM_CallbackName`

Functions

- `KIM_CallbackName` `KIM_CallbackNameFromString` (char const *const str)
- int `KIM_CallbackNameEqual` (`KIM_CallbackName` const left, `KIM_CallbackName` const right)
- int `KIM_CallbackNameNotEqual` (`KIM_CallbackName` const left, `KIM_CallbackName` const right)
- char const *const `KIM_CallbackNameString` (`KIM_CallbackName` const callbackName)
- void `KIM_CALLBACK_NAME_GetNumberOfCallbacks` (int *const numberOfCallbacks)
- int `KIM_CALLBACK_NAME_GetCallbackName` (int const index, `KIM_CallbackName` *const callbackName)

Variables

- `KIM_CallbackName` const `KIM_CALLBACK_NAME_GetNeighborList`
- `KIM_CallbackName` const `KIM_CALLBACK_NAME_ProcessDEDrTerm`
- `KIM_CallbackName` const `KIM_CALLBACK_NAME_ProcessD2EDr2Term`

11.2.1 Macro Definition Documentation

11.2.1.1 KIM_CALLBACK_NAME_DEFINED_

```
#define KIM_CALLBACK_NAME_DEFINED_
```

Definition at line 44 of file KIM_CallbackName.h.

11.2.2 Typedef Documentation

11.2.2.1 KIM_CallbackName

```
typedef struct KIM_CallbackName KIM_CallbackName
```

Definition at line 45 of file KIM_CallbackName.h.

11.2.3 Function Documentation

11.2.3.1 KIM_CALLBACK_NAME_GetCallbackName()

```
int KIM_CALLBACK_NAME_GetCallbackName (
    int const index,
    KIM_CallbackName *const callbackName )
```

11.2.3.2 KIM_CALLBACK_NAME_GetNumberOfCallbacks()

```
void KIM_CALLBACK_NAME_GetNumberOfCallbacks (
    int *const numberOfCallbacks )
```

11.2.3.3 KIM_CallbackNameEqual()

```
int KIM_CallbackNameEqual (
    KIM_CallbackName const left,
    KIM_CallbackName const right )
```


11.2.3.4 KIM_CallbackNameFromString()

```
KIM_CallbackName KIM_CallbackNameFromString (
    char const *const str )
```

11.2.3.5 KIM_CallbackNameNotEqual()

```
int KIM_CallbackNameNotEqual (
    KIM_CallbackName const left,
    KIM_CallbackName const right )
```

11.2.3.6 KIM_CallbackNameString()

```
char const* const KIM_CallbackNameString (
    KIM_CallbackName const callbackName )
```

11.2.4 Variable Documentation

11.2.4.1 KIM_CALLBACK_NAME_GetNeighborList

```
KIM_CallbackName const KIM_CALLBACK_NAME_GetNeighborList
```

11.2.4.2 KIM_CALLBACK_NAME_ProcessD2EDr2Term

```
KIM_CallbackName const KIM_CALLBACK_NAME_ProcessD2EDr2Term
```

11.2.4.3 KIM_CALLBACK_NAME_ProcessDEDrTerm

```
KIM_CallbackName const KIM_CALLBACK_NAME_ProcessDEDrTerm
```

11.3 kim-api-v2.0.0-alpha.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_ChargeUnitFromString` (char const *const str)
- `int KIM_ChargeUnitEqual` (KIM_ChargeUnit const left, KIM_ChargeUnit right)
- `int KIM_ChargeUnitNotEqual` (KIM_ChargeUnit const left, KIM_ChargeUnit right)
- `char const *const KIM_ChargeUnitString` (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`

11.3.1 Macro Definition Documentation

11.3.1.1 KIM_CHARGE_UNIT_DEFINED_

```
#define KIM_CHARGE_UNIT_DEFINED_
```

Definition at line 44 of file KIM_ChargeUnit.h.

11.3.2 Typedef Documentation

11.3.2.1 KIM_ChargeUnit

```
typedef struct KIM_ChargeUnit KIM_ChargeUnit
```

Definition at line 45 of file KIM_ChargeUnit.h.

11.3.3 Function Documentation

11.3.3.1 KIM_ChargeUnitEqual()

```
int KIM_ChargeUnitEqual (
    KIM_ChargeUnit const left,
    KIM_ChargeUnit right )
```

11.3.3.2 KIM_ChargeUnitFromString()

```
KIM_ChargeUnit KIM_ChargeUnitFromString (
    char const *const str )
```

11.3.3.3 KIM_ChargeUnitNotEqual()

```
int KIM_ChargeUnitNotEqual (
    KIM_ChargeUnit const left,
    KIM_ChargeUnit right )
```

11.3.3.4 KIM_ChargeUnitString()

```
char const* const KIM_ChargeUnitString (
    KIM_ChargeUnit const chargeUnit )
```

11.3.4 Variable Documentation

11.3.4.1 KIM_CHARGE_UNIT_C

```
KIM_ChargeUnit const KIM_CHARGE_UNIT_C
```

11.3.4.2 KIM_CHARGE_UNIT_e

```
KIM_ChargeUnit const KIM_CHARGE_UNIT_e
```


11.3.4.3 KIM_CHARGE_UNIT_statC

`KIM_ChargeUnit` const KIM_CHARGE_UNIT_statC

11.3.4.4 KIM_CHARGE_UNIT_unused

`KIM_ChargeUnit` const KIM_CHARGE_UNIT_unused

11.4 kim-api-v2.0.0-alpha.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_DataTypeFromString` (char const *const str)
- int `KIM_DataTypeEqual` (`KIM_DataType` const left, `KIM_DataType` const right)
- int `KIM_DataTypeNotEqual` (`KIM_DataType` const left, `KIM_DataType` const right)
- char const *const `KIM_DataTypeString` (`KIM_DataType` const dataType)

Variables

- `KIM_DataType` const `KIM_DATA_TYPE_Integer`
- `KIM_DataType` const `KIM_DATA_TYPE_Double`

11.4.1 Macro Definition Documentation

11.4.1.1 KIM_DATA_TYPE_DEFINED_

```
#define KIM_DATA_TYPE_DEFINED_
```

Definition at line 44 of file `KIM_DataType.h`.

11.4.2 Typedef Documentation

11.4.2.1 KIM_DataType

```
typedef struct KIM_DataType KIM_DataType
```

Definition at line 45 of file KIM_DataType.h.

11.4.3 Function Documentation

11.4.3.1 KIM_DataTypeEqual()

```
int KIM_DataTypeEqual (
    KIM_DataType const left,
    KIM_DataType const right )
```

11.4.3.2 KIM_DataTypeFromString()

```
KIM_DataType KIM_DataTypeFromString (
    char const *const str )
```

11.4.3.3 KIM_DataTypeNotEqual()

```
int KIM_DataTypeNotEqual (
    KIM_DataType const left,
    KIM_DataType const right )
```

11.4.3.4 KIM_DataTypeString()

```
char const* const KIM_DataTypeString (
    KIM_DataType const dataType )
```

11.4.4 Variable Documentation

11.4.4.1 KIM_DATA_TYPE_Double

`KIM_DataType` const KIM_DATA_TYPE_Double

11.4.4.2 KIM_DATA_TYPE_Integer

`KIM_DataType` const KIM_DATA_TYPE_Integer

11.5 kim-api-v2.0.0-alpha.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_EnergyUnitFromString` (char const *const str)
- int `KIM_EnergyUnitEqual` (`KIM_EnergyUnit` const left, `KIM_EnergyUnit` const right)
- int `KIM_EnergyUnitNotEqual` (`KIM_EnergyUnit` const left, `KIM_EnergyUnit` const right)
- char const *const `KIM_EnergyUnitString` (`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`

11.5.1 Macro Definition Documentation

11.5.1.1 KIM_ENERGY_UNIT_DEFINED_

```
#define KIM_ENERGY_UNIT_DEFINED_
```

Definition at line 44 of file KIM_EnergyUnit.h.

11.5.2 Typedef Documentation

11.5.2.1 KIM_EnergyUnit

```
typedef struct KIM_EnergyUnit KIM_EnergyUnit
```

Definition at line 45 of file KIM_EnergyUnit.h.

11.5.3 Function Documentation

11.5.3.1 KIM_EnergyUnitEqual()

```
int KIM_EnergyUnitEqual (
    KIM_EnergyUnit const left,
    KIM_EnergyUnit const right )
```

11.5.3.2 KIM_EnergyUnitFromString()

```
KIM_EnergyUnit KIM_EnergyUnitFromString (
    char const *const str )
```

11.5.3.3 KIM_EnergyUnitNotEqual()

```
int KIM_EnergyUnitNotEqual (
    KIM_EnergyUnit const left,
    KIM_EnergyUnit const right )
```


11.5.3.4 KIM_EnergyUnitString()

```
char const* const KIM_EnergyUnitString (
    KIM_EnergyUnit const energyUnit )
```

11.5.4 Variable Documentation

11.5.4.1 KIM_ENERGY_UNIT_amu_A2_per_ps2

```
KIM_EnergyUnit const KIM_ENERGY_UNIT_amu_A2_per_ps2
```

11.5.4.2 KIM_ENERGY_UNIT_erg

```
KIM_EnergyUnit const KIM_ENERGY_UNIT_erg
```

11.5.4.3 KIM_ENERGY_UNIT_eV

```
KIM_EnergyUnit const KIM_ENERGY_UNIT_eV
```

11.5.4.4 KIM_ENERGY_UNIT_Hartree

```
KIM_EnergyUnit const KIM_ENERGY_UNIT_Hartree
```

11.5.4.5 KIM_ENERGY_UNIT_J

```
KIM_EnergyUnit const KIM_ENERGY_UNIT_J
```

11.5.4.6 KIM_ENERGY_UNIT_kcal_mol

```
KIM_EnergyUnit const KIM_ENERGY_UNIT_kcal_mol
```


11.5.4.7 KIM_ENERGY_UNIT_unused

`KIM_EnergyUnit` `const KIM_ENERGY_UNIT_unused`

11.6 kim-api-v2.0.0-alpha.0/c/include/KIM_func.h File Reference

Typedefs

- typedef void() `func()`

11.6.1 Typedef Documentation

11.6.1.1 func

```
typedef void() func()
```

Definition at line 39 of file `KIM_func.h`.

11.7 kim-api-v2.0.0-alpha.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_LanguageNameFromString` (`char const *const str`)
- int `KIM_LanguageNameEqual` (`KIM_LanguageName` `const left`, `KIM_LanguageName` `const right`)
- int `KIM_LanguageNameNotEqual` (`KIM_LanguageName` `const left`, `KIM_LanguageName` `const right`)
- `char const *const` `KIM_LanguageNameString` (`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](#)

11.7.1 Macro Definition Documentation

11.7.1.1 KIM_LANGUAGE_NAME_DEFINED_

```
#define KIM_LANGUAGE_NAME_DEFINED_
```

Definition at line 44 of file [KIM_LanguageName.h](#).

11.7.2 Typedef Documentation

11.7.2.1 KIM_LanguageName

```
typedef struct KIM\_LanguageName KIM\_LanguageName
```

Definition at line 45 of file [KIM_LanguageName.h](#).

11.7.3 Function Documentation

11.7.3.1 KIM_LanguageNameEqual()

```
int KIM_LanguageNameEqual (
    KIM\_LanguageName const left,
    KIM\_LanguageName const right )
```

11.7.3.2 KIM_LanguageNameFromString()

```
KIM\_LanguageName KIM_LanguageNameFromString (
    char const *const str )
```


11.7.3.3 KIM_LanguageNameNotEqual()

```
int KIM_LanguageNameNotEqual (
    KIM_LanguageName const left,
    KIM_LanguageName const right )
```

11.7.3.4 KIM_LanguageNameString()

```
char const* const KIM_LanguageNameString (
    KIM_LanguageName const languageName )
```

11.7.4 Variable Documentation

11.7.4.1 KIM_LANGUAGE_NAME_c

```
KIM_LanguageName const KIM_LANGUAGE_NAME_c
```

11.7.4.2 KIM_LANGUAGE_NAME_cpp

```
KIM_LanguageName const KIM_LANGUAGE_NAME_cpp
```

11.7.4.3 KIM_LANGUAGE_NAME_fortran

```
KIM_LanguageName const KIM_LANGUAGE_NAME_fortran
```

11.8 kim-api-v2.0.0-alpha.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_LengthUnitFromString](#) (char const *const str)
- int [KIM_LengthUnitEqual](#) ([KIM_LengthUnit](#) left, [KIM_LengthUnit](#) right)
- int [KIM_LengthUnitNotEqual](#) ([KIM_LengthUnit](#) left, [KIM_LengthUnit](#) right)
- char const *const [KIM_LengthUnitString](#) ([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](#)

11.8.1 Macro Definition Documentation

11.8.1.1 [KIM_LENGTH_UNIT_DEFINED_](#)

```
#define KIM\_LENGTH\_UNIT\_DEFINED\_
```

Definition at line 44 of file [KIM_LengthUnit.h](#).

11.8.2 Typedef Documentation

11.8.2.1 [KIM_LengthUnit](#)

```
typedef struct KIM\_LengthUnit KIM\_LengthUnit
```

Definition at line 45 of file [KIM_LengthUnit.h](#).

11.8.3 Function Documentation

11.8.3.1 KIM_LengthUnitEqual()

```
int KIM_LengthUnitEqual (
    KIM_LengthUnit left,
    KIM_LengthUnit right )
```

11.8.3.2 KIM_LengthUnitFromString()

```
KIM_LengthUnit KIM_LengthUnitFromString (
    char const *const str )
```

11.8.3.3 KIM_LengthUnitNotEqual()

```
int KIM_LengthUnitNotEqual (
    KIM_LengthUnit left,
    KIM_LengthUnit right )
```

11.8.3.4 KIM_LengthUnitString()

```
char const* const KIM_LengthUnitString (
    KIM_LengthUnit const lengthUnit )
```

11.8.4 Variable Documentation

11.8.4.1 KIM_LENGTH_UNIT_A

```
KIM_LengthUnit const KIM_LENGTH_UNIT_A
```

11.8.4.2 KIM_LENGTH_UNIT_Bohr

```
KIM_LengthUnit const KIM_LENGTH_UNIT_Bohr
```


11.8.4.3 KIM_LENGTH_UNIT_cm

`KIM_LengthUnit` const KIM_LENGTH_UNIT_cm

11.8.4.4 KIM_LENGTH_UNIT_m

`KIM_LengthUnit` const KIM_LENGTH_UNIT_m

11.8.4.5 KIM_LENGTH_UNIT_nm

`KIM_LengthUnit` const KIM_LENGTH_UNIT_nm

11.8.4.6 KIM_LENGTH_UNIT_unused

`KIM_LengthUnit` const KIM_LENGTH_UNIT_unused

11.9 kim-api-v2.0.0-alpha.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_PopVerboisty` (`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)

11.9.1 Macro Definition Documentation

11.9.1.1 KIM_LOG_DEFINED_

```
#define KIM_LOG_DEFINED_
```

Definition at line 48 of file KIM_Log.h.

11.9.1.2 KIM_LOG_VERBOSITY_DEFINED_

```
#define KIM_LOG_VERBOSITY_DEFINED_
```

Definition at line 41 of file KIM_Log.h.

11.9.2 Typedef Documentation

11.9.2.1 KIM_Log

```
typedef struct KIM_Log KIM_Log
```

Definition at line 49 of file KIM_Log.h.

11.9.2.2 KIM_LogVerbosity

```
typedef struct KIM_LogVerbosity KIM_LogVerbosity
```

Definition at line 42 of file KIM_Log.h.

11.9.3 Function Documentation

11.9.3.1 KIM_Log_Create()

```
int KIM_Log_Create (
    KIM_Log **const log )
```


11.9.3.2 KIM_Log_Destroy()

```
void KIM_Log_Destroy (
    KIM_Log **const log )
```

11.9.3.3 KIM_Log_GetID()

```
char const* const KIM_Log_GetID (
    KIM_Log const *const log )
```

11.9.3.4 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 )
```

11.9.3.5 KIM_Log_PopVerbosity()

```
void KIM_Log_PopVerbosity (
    KIM_Log *const log )
```

11.9.3.6 KIM_Log_PushVerbosity()

```
void KIM_Log_PushVerbosity (
    KIM_Log *const log,
    KIM_LogVerbosity const logVerbosity )
```

11.9.3.7 KIM_Log_SetID()

```
void KIM_Log_SetID (
    KIM_Log *const log,
    char const *const id )
```


11.10 kim-api-v2.0.0-alpha.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_LogVerbosityFromString](#) (char const *const str)
- int [KIM_LogVerbosityLessThan](#) ([KIM_LogVerbosity](#) const left, [KIM_LogVerbosity](#) const right)
- int [KIM_LogVerbosityGreaterThan](#) ([KIM_LogVerbosity](#) const left, [KIM_LogVerbosity](#) const right)
- int [KIM_LogVerbosityLessThanEqual](#) ([KIM_LogVerbosity](#) const left, [KIM_LogVerbosity](#) const right)
- int [KIM_LogVerbosityGreaterThanEqual](#) ([KIM_LogVerbosity](#) const left, [KIM_LogVerbosity](#) const right)
- int [KIM_LogVerbosityEqual](#) ([KIM_LogVerbosity](#) const left, [KIM_LogVerbosity](#) const right)
- int [KIM_LogVerbosityNotEqual](#) ([KIM_LogVerbosity](#) const left, [KIM_LogVerbosity](#) const right)
- char const *const [KIM_LogVerbosityString](#) ([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](#)

11.10.1 Macro Definition Documentation

11.10.1.1 KIM_LOG_VERBOSITY_DEFINED_

```
#define KIM_LOG_VERBOSITY_DEFINED_
```

Definition at line 47 of file [KIM_LogVerbosity.h](#).

11.10.2 Typedef Documentation

11.10.2.1 KIM_LogVerbosity

```
typedef struct KIM_LogVerbosity KIM_LogVerbosity
```

Definition at line 48 of file KIM_LogVerbosity.h.

11.10.3 Function Documentation

11.10.3.1 KIM_LogVerbosityEqual()

```
int KIM_LogVerbosityEqual (
    KIM_LogVerbosity const left,
    KIM_LogVerbosity const right )
```

11.10.3.2 KIM_LogVerbosityFromString()

```
KIM_LogVerbosity KIM_LogVerbosityFromString (
    char const *const str )
```

11.10.3.3 KIM_LogVerbosityGreaterThan()

```
int KIM_LogVerbosityGreaterThan (
    KIM_LogVerbosity const left,
    KIM_LogVerbosity const right )
```

11.10.3.4 KIM_LogVerbosityGreaterThanOrEqualTo()

```
int KIM_LogVerbosityGreaterThanOrEqualTo (
    KIM_LogVerbosity const left,
    KIM_LogVerbosity const right )
```


11.10.3.5 KIM_LogVerbosityLessThan()

```
int KIM_LogVerbosityLessThan (
    KIM_LogVerbosity const left,
    KIM_LogVerbosity const right )
```

11.10.3.6 KIM_LogVerbosityLessThanEqual()

```
int KIM_LogVerbosityLessThanEqual (
    KIM_LogVerbosity const left,
    KIM_LogVerbosity const right )
```

11.10.3.7 KIM_LogVerbosityNotEqual()

```
int KIM_LogVerbosityNotEqual (
    KIM_LogVerbosity const left,
    KIM_LogVerbosity const right )
```

11.10.3.8 KIM_LogVerbosityString()

```
char const* const KIM_LogVerbosityString (
    KIM_LogVerbosity const logVerbosity )
```

11.10.4 Variable Documentation

11.10.4.1 KIM_LOG_VERBOSITY_debug

```
KIM_LogVerbosity const KIM_LOG_VERBOSITY_debug
```

11.10.4.2 KIM_LOG_VERBOSITY_error

```
KIM_LogVerbosity const KIM_LOG_VERBOSITY_error
```


11.10.4.3 KIM_LOG_VERBOSITY_fatal

```
KIM_LogVerbosity const KIM_LOG_VERBOSITY_fatal
```

11.10.4.4 KIM_LOG_VERBOSITY_information

```
KIM_LogVerbosity const KIM_LOG_VERBOSITY_information
```

11.10.4.5 KIM_LOG_VERBOSITY_silent

```
KIM_LogVerbosity const KIM_LOG_VERBOSITY_silent
```

11.10.4.6 KIM_LOG_VERBOSITY_warning

```
KIM_LogVerbosity const KIM_LOG_VERBOSITY_warning
```

11.11 kim-api-v2.0.0-alpha.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_ARGUMENT_NAME_DEFINED_`
- `#define KIM_CALLBACK_NAME_DEFINED_`
- `#define KIM_SUPPORT_STATUS_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_ArgumentName](#) [KIM_ArgumentName](#)
- typedef struct [KIM_CallbackName](#) [KIM_CallbackName](#)
- typedef struct [KIM_SupportStatus](#) [KIM_SupportStatus](#)
- typedef struct [KIM_Model](#) [KIM_Model](#)

Functions

- 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)
- 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 numberOfCutoffs, double const **const cutoffs)
- int [KIM_Model_GetArgumentSupportStatus](#) ([KIM_Model](#) const *const model, [KIM_ArgumentName](#) const argumentName, [KIM_SupportStatus](#) *const supportStatus)
- int [KIM_Model_GetCallbackSupportStatus](#) ([KIM_Model](#) const *const model, [KIM_CallbackName](#) const callbackName, [KIM_SupportStatus](#) *const supportStatus)
- 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_SetArgumentPointerInteger](#) ([KIM_Model](#) *const model, [KIM_ArgumentName](#) const argumentName, int const *const ptr)
- int [KIM_Model_SetArgumentPointerDouble](#) ([KIM_Model](#) *const model, [KIM_ArgumentName](#) const argumentName, double const *const ptr)
- int [KIM_Model_SetCallbackPointer](#) ([KIM_Model](#) *const model, [KIM_CallbackName](#) const callbackName, [KIM_LanguageName](#) const languageName, func *const fptr, void const *const dataObject)
- int [KIM_Model_Compute](#) ([KIM_Model](#) const *const model)
- 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 numberOfParameters)
- 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 arrayIndex, 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)

11.11.1 Macro Definition Documentation

11.11.1.1 KIM_ARGUMENT_NAME_DEFINED_

```
#define KIM_ARGUMENT_NAME_DEFINED_
```

Definition at line 95 of file [KIM_Model.h](#).

11.11.1.2 KIM_CALLBACK_NAME_DEFINED_

```
#define KIM_CALLBACK_NAME_DEFINED_
```

Definition at line 100 of file [KIM_Model.h](#).

11.11.1.3 KIM_CHARGE_UNIT_DEFINED_

```
#define KIM_CHARGE_UNIT_DEFINED_
```

Definition at line 80 of file [KIM_Model.h](#).

11.11.1.4 KIM_DATA_TYPE_DEFINED_

```
#define KIM_DATA_TYPE_DEFINED_
```

Definition at line 70 of file [KIM_Model.h](#).

11.11.1.5 KIM_ENERGY_UNIT_DEFINED_

```
#define KIM_ENERGY_UNIT_DEFINED_
```

Definition at line 75 of file KIM_Model.h.

11.11.1.6 KIM_LANGUAGE_NAME_DEFINED_

```
#define KIM_LANGUAGE_NAME_DEFINED_
```

Definition at line 55 of file KIM_Model.h.

11.11.1.7 KIM_LENGTH_UNIT_DEFINED_

```
#define KIM_LENGTH_UNIT_DEFINED_
```

Definition at line 65 of file KIM_Model.h.

11.11.1.8 KIM_LOG_VERBOSITY_DEFINED_

```
#define KIM_LOG_VERBOSITY_DEFINED_
```

Definition at line 45 of file KIM_Model.h.

11.11.1.9 KIM_MODEL_DEFINED_

```
#define KIM_MODEL_DEFINED_
```

Definition at line 113 of file KIM_Model.h.

11.11.1.10 KIM_NUMBERING_DEFINED_

```
#define KIM_NUMBERING_DEFINED_
```

Definition at line 60 of file KIM_Model.h.

11.11.1.11 KIM_SPECIES_NAME_DEFINED_

```
#define KIM_SPECIES_NAME_DEFINED_
```

Definition at line 50 of file KIM_Model.h.

11.11.1.12 KIM_SUPPORT_STATUS_DEFINED_

```
#define KIM_SUPPORT_STATUS_DEFINED_
```

Definition at line 105 of file KIM_Model.h.

11.11.1.13 KIM_TEMPERATURE_UNIT_DEFINED_

```
#define KIM_TEMPERATURE_UNIT_DEFINED_
```

Definition at line 85 of file KIM_Model.h.

11.11.1.14 KIM_TIME_UNIT_DEFINED_

```
#define KIM_TIME_UNIT_DEFINED_
```

Definition at line 90 of file KIM_Model.h.

11.11.2 Typedef Documentation

11.11.2.1 KIM_ArgumentName

```
typedef struct KIM_ArgumentName KIM_ArgumentName
```

Definition at line 96 of file KIM_Model.h.

11.11.2.2 KIM_CallbackName

```
typedef struct KIM_CallbackName KIM_CallbackName
```

Definition at line 101 of file KIM_Model.h.

11.11.2.3 KIM_ChargeUnit

```
typedef struct KIM_ChargeUnit KIM_ChargeUnit
```

Definition at line 81 of file KIM_Model.h.

11.11.2.4 KIM_DataType

```
typedef struct KIM_DataType KIM_DataType
```

Definition at line 71 of file KIM_Model.h.

11.11.2.5 KIM_EnergyUnit

```
typedef struct KIM_EnergyUnit KIM_EnergyUnit
```

Definition at line 76 of file KIM_Model.h.

11.11.2.6 KIM_LanguageName

```
typedef struct KIM_LanguageName KIM_LanguageName
```

Definition at line 56 of file KIM_Model.h.

11.11.2.7 KIM_LengthUnit

```
typedef struct KIM_LengthUnit KIM_LengthUnit
```

Definition at line 66 of file KIM_Model.h.

11.11.2.8 KIM_LogVerbosity

```
typedef struct KIM_LogVerbosity KIM_LogVerbosity
```

Definition at line 46 of file KIM_Model.h.

11.11.2.9 KIM_Model

```
typedef struct KIM_Model KIM_Model
```

Definition at line 114 of file KIM_Model.h.

11.11.2.10 KIM_Numbering

```
typedef struct KIM_Numbering KIM_Numbering
```

Definition at line 61 of file KIM_Model.h.

11.11.2.11 KIM_SpeciesName

```
typedef struct KIM_SpeciesName KIM_SpeciesName
```

Definition at line 51 of file KIM_Model.h.

11.11.2.12 KIM_SupportStatus

```
typedef struct KIM_SupportStatus KIM_SupportStatus
```

Definition at line 106 of file KIM_Model.h.

11.11.2.13 KIM_TemperatureUnit

```
typedef struct KIM_TemperatureUnit KIM_TemperatureUnit
```

Definition at line 86 of file KIM_Model.h.

11.11.2.14 KIM_TimeUnit

```
typedef struct KIM_TimeUnit KIM_TimeUnit
```

Definition at line 91 of file KIM_Model.h.

11.11.3 Function Documentation

11.11.3.1 KIM_Model_ClearInfluenceDistanceAndCutoffsThenRefreshModel()

```
int KIM_Model_ClearInfluenceDistanceAndCutoffsThenRefreshModel (
    KIM_Model *const model )
```

11.11.3.2 KIM_Model_Compute()

```
int KIM_Model_Compute (
    KIM_Model const *const model )
```

11.11.3.3 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 )
```

11.11.3.4 KIM_Model_Destroy()

```
void KIM_Model_Destroy (
    KIM_Model **const model )
```

11.11.3.5 KIM_Model_GetArgumentSupportStatus()

```
int KIM_Model_GetArgumentSupportStatus (
    KIM_Model const *const model,
    KIM_ArgumentName const argumentName,
    KIM_SupportStatus *const supportStatus )
```


11.11.3.6 KIM_Model_GetCallbackSupportStatus()

```
int KIM_Model_GetCallbackSupportStatus (
    KIM_Model const *const model,
    KIM_CallbackName const callbackName,
    KIM_SupportStatus *const supportStatus )
```

11.11.3.7 KIM_Model_GetInfluenceDistance()

```
void KIM_Model_GetInfluenceDistance (
    KIM_Model const *const model,
    double *const influenceDistance )
```

11.11.3.8 KIM_Model_GetNeighborListCutoffsPointer()

```
void KIM_Model_GetNeighborListCutoffsPointer (
    KIM_Model const *const model,
    int *const numberOfCutoffs,
    double const **const cutoffs )
```

11.11.3.9 KIM_Model_GetNumberOfParameters()

```
void KIM_Model_GetNumberOfParameters (
    KIM_Model const *const model,
    int *const numberOfParameters )
```

11.11.3.10 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 )
```


11.11.3.11 KIM_Model_GetParameterDouble()

```
int KIM_Model_GetParameterDouble (
    KIM_Model const *const model,
    int const parameterIndex,
    int const arrayIndex,
    double *const parameterValue )
```

11.11.3.12 KIM_Model_GetParameterInteger()

```
int KIM_Model_GetParameterInteger (
    KIM_Model const *const model,
    int const parameterIndex,
    int const arrayIndex,
    int *const parameterValue )
```

11.11.3.13 KIM_Model_GetSimulatorBufferPointer()

```
void KIM_Model_GetSimulatorBufferPointer (
    KIM_Model const *const model,
    void **const ptr )
```

11.11.3.14 KIM_Model_GetSpeciesSupportAndCode()

```
int KIM_Model_GetSpeciesSupportAndCode (
    KIM_Model const *const model,
    KIM_SpeciesName const speciesName,
    int *const speciesIsSupported,
    int *const code )
```

11.11.3.15 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 )
```


11.11.3.16 KIM_Model_PopLogVerbosity()

```
void KIM_Model_PopLogVerbosity (
    KIM_Model *const model )
```

11.11.3.17 KIM_Model_PushLogVerbosity()

```
void KIM_Model_PushLogVerbosity (
    KIM_Model *const model,
    KIM_LogVerbosity const logVerbosity )
```

11.11.3.18 KIM_Model_SetArgumentPointerDouble()

```
int KIM_Model_SetArgumentPointerDouble (
    KIM_Model *const model,
    KIM_ArgumentName const argumentName,
    double const *const ptr )
```

11.11.3.19 KIM_Model_SetArgumentPointerInteger()

```
int KIM_Model_SetArgumentPointerInteger (
    KIM_Model *const model,
    KIM_ArgumentName const argumentName,
    int const *const ptr )
```

11.11.3.20 KIM_Model_SetCallbackPointer()

```
int KIM_Model_SetCallbackPointer (
    KIM_Model *const model,
    KIM_CallbackName const callbackName,
    KIM_LanguageName const languageName,
    func *const fptr,
    void const *const dataObject )
```

11.11.3.21 KIM_Model_SetLogID()

```
void KIM_Model_SetLogID (
    KIM_Model *const model,
    char const *const logID )
```


11.11.3.22 KIM_Model_SetParameterDouble()

```
int KIM_Model_SetParameterDouble (
    KIM_Model *const model,
    int const parameterIndex,
    int const arrayIndex,
    double const parameterValue )
```

11.11.3.23 KIM_Model_SetParameterInteger()

```
int KIM_Model_SetParameterInteger (
    KIM_Model *const model,
    int const parameterIndex,
    int const arrayIndex,
    int const parameterValue )
```

11.11.3.24 KIM_Model_SetSimulatorBufferPointer()

```
void KIM_Model_SetSimulatorBufferPointer (
    KIM_Model *const model,
    void *const ptr )
```

11.11.3.25 KIM_Model_String()

```
char const* const KIM_Model_String (
    KIM_Model const *const model )
```

11.12 kim-api-v2.0.0-alpha.0/c/include/KIM_ModelCompute.h File Reference

Macros

- `#define KIM_LOG_VERBOSITY_DEFINED_`
- `#define KIM_ARGUMENT_NAME_DEFINED_`
- `#define KIM_CALLBACK_NAME_DEFINED_`
- `#define KIM_MODEL_COMPUTE_DEFINED_`

Typedefs

- `typedef struct KIM_LogVerbosity KIM_LogVerbosity`
- `typedef struct KIM_ArgumentName KIM_ArgumentName`
- `typedef struct KIM_CallbackName KIM_CallbackName`
- `typedef struct KIM_ModelCompute KIM_ModelCompute`

Functions

- int [KIM_ModelCompute_GetNeighborList](#) ([KIM_ModelCompute](#) const *const modelCompute, int const neighborListIndex, int const particleNumber, int *const numberOfNeighbors, int const **const neighbors←OfParticle)
- int [KIM_ModelCompute_ProcessDEDrTerm](#) ([KIM_ModelCompute](#) const *const modelCompute, double const de, double const r, double const *const dx, int const i, int const j)
- int [KIM_ModelCompute_ProcessD2EDr2Term](#) ([KIM_ModelCompute](#) const *const modelCompute, double const de, double const *const r, double const *const dx, int const *const i, int const *const j)
- int [KIM_ModelCompute_GetArgumentPointerInteger](#) ([KIM_ModelCompute](#) const *const modelCompute, [KIM_ArgumentName](#) const argumentName, int **const ptr)
- int [KIM_ModelCompute_GetArgumentPointerDouble](#) ([KIM_ModelCompute](#) const *const modelCompute, [KIM_ArgumentName](#) const argumentName, double **const ptr)
- int [KIM_ModelCompute_IsCallbackPresent](#) ([KIM_ModelCompute](#) const *const modelCompute, [KIM_CallbackName](#) const callbackName, int *const present)
- 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)

11.12.1 Macro Definition Documentation

11.12.1.1 KIM_ARGUMENT_NAME_DEFINED_

```
#define KIM_ARGUMENT_NAME_DEFINED_
```

Definition at line 46 of file [KIM_ModelCompute.h](#).

11.12.1.2 KIM_CALLBACK_NAME_DEFINED_

```
#define KIM_CALLBACK_NAME_DEFINED_
```

Definition at line 51 of file [KIM_ModelCompute.h](#).

11.12.1.3 KIM_LOG_VERBOSITY_DEFINED_

```
#define KIM_LOG_VERBOSITY_DEFINED_
```

Definition at line 41 of file [KIM_ModelCompute.h](#).

11.12.1.4 KIM_MODEL_COMPUTE_DEFINED_

```
#define KIM_MODEL_COMPUTE_DEFINED_
```

Definition at line 59 of file KIM_ModelCompute.h.

11.12.2 Typedef Documentation

11.12.2.1 KIM_ArgumentName

```
typedef struct KIM_ArgumentName KIM_ArgumentName
```

Definition at line 47 of file KIM_ModelCompute.h.

11.12.2.2 KIM_CallbackName

```
typedef struct KIM_CallbackName KIM_CallbackName
```

Definition at line 52 of file KIM_ModelCompute.h.

11.12.2.3 KIM_LogVerbosity

```
typedef struct KIM_LogVerbosity KIM_LogVerbosity
```

Definition at line 42 of file KIM_ModelCompute.h.

11.12.2.4 KIM_ModelCompute

```
typedef struct KIM_ModelCompute KIM_ModelCompute
```

Definition at line 60 of file KIM_ModelCompute.h.

11.12.3 Function Documentation

11.12.3.1 KIM_ModelCompute_GetArgumentPointerDouble()

```
int KIM_ModelCompute_GetArgumentPointerDouble (
    KIM_ModelCompute const *const modelCompute,
    KIM_ArgumentName const argumentName,
    double **const ptr )
```

11.12.3.2 KIM_ModelCompute_GetArgumentPointerInteger()

```
int KIM_ModelCompute_GetArgumentPointerInteger (
    KIM_ModelCompute const *const modelCompute,
    KIM_ArgumentName const argumentName,
    int **const ptr )
```

11.12.3.3 KIM_ModelCompute_GetModelBufferPointer()

```
void KIM_ModelCompute_GetModelBufferPointer (
    KIM_ModelCompute const *const modelCompute,
    void **const ptr )
```

11.12.3.4 KIM_ModelCompute_GetNeighborList()

```
int KIM_ModelCompute_GetNeighborList (
    KIM_ModelCompute const *const modelCompute,
    int const neighborListIndex,
    int const particleNumber,
    int *const numberOfNeighbors,
    int const **const neighborsOfParticle )
```

11.12.3.5 KIM_ModelCompute_IsCallbackPresent()

```
int KIM_ModelCompute_IsCallbackPresent (
    KIM_ModelCompute const *const modelCompute,
    KIM_CallbackName const callbackName,
    int *const present )
```


11.12.3.6 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 )
```

11.12.3.7 KIM_ModelCompute_ProcessD2EDr2Term()

```
int KIM_ModelCompute_ProcessD2EDr2Term (
    KIM_ModelCompute const *const modelCompute,
    double const de,
    double const *const r,
    double const *const dx,
    int const *const i,
    int const *const j )
```

11.12.3.8 KIM_ModelCompute_ProcessDEDrTerm()

```
int KIM_ModelCompute_ProcessDEDrTerm (
    KIM_ModelCompute const *const modelCompute,
    double const de,
    double const r,
    double const *const dx,
    int const i,
    int const j )
```

11.12.3.9 KIM_ModelCompute_String()

```
char const* const KIM_ModelCompute_String (
    KIM_ModelCompute const *const modelCompute )
```

11.13 kim-api-v2.0.0-alpha.0/c/include/KIM_ModelComputeLogMacros.h File Reference

Macros

- #define [LOG_FATAL](#)(message)
- #define [LOG_ERROR](#)(message)
- #define [LOG_WARNING](#)(message)
- #define [LOG_INFORMATION](#)(message)
- #define [LOG_DEBUG](#)(message)

11.13.1 Macro Definition Documentation

11.13.1.1 LOG_DEBUG

```
#define LOG_DEBUG(  
    message )
```

Value:

```
KIM_ModelCompute_LogEntry(modelCompute,  
    KIM_LOG_VERBOSITY_debug, message,  
    __LINE__, __FILE__)
```

Definition at line 88 of file KIM_ModelComputeLogMacros.h.

11.13.1.2 LOG_ERROR

```
#define LOG_ERROR(  
    message )
```

Value:

```
KIM_ModelCompute_LogEntry(modelCompute,  
    KIM_LOG_VERBOSITY_error, message,  
    __LINE__, __FILE__)
```

Definition at line 52 of file KIM_ModelComputeLogMacros.h.

11.13.1.3 LOG_FATAL

```
#define LOG_FATAL(  
    message )
```

Value:

```
KIM_ModelCompute_LogEntry(modelCompute,  
    KIM_LOG_VERBOSITY_fatal, message,  
    __LINE__, __FILE__)
```

Definition at line 40 of file KIM_ModelComputeLogMacros.h.

11.13.1.4 LOG_INFORMATION

```
#define LOG_INFORMATION(  
    message )
```

Value:

```
KIM_ModelCompute_LogEntry (modelCompute,  
                            KIM_LOG_VERBOSITY_information, message,  
                            __LINE__, __FILE__)
```

Definition at line 76 of file KIM_ModelComputeLogMacros.h.

11.13.1.5 LOG_WARNING

```
#define LOG_WARNING(  
    message )
```

Value:

```
KIM_ModelCompute_LogEntry (modelCompute,  
                            KIM_LOG_VERBOSITY_warning, message,  
                            __LINE__, __FILE__)
```

Definition at line 64 of file KIM_ModelComputeLogMacros.h.

11.14 kim-api-v2.0.0-alpha.0/c/include/KIM_ModelCreate.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_ENERGY_UNIT_DEFINED_](#)
- #define [KIM_CHARGE_UNIT_DEFINED_](#)
- #define [KIM_TEMPERATURE_UNIT_DEFINED_](#)
- #define [KIM_TIME_UNIT_DEFINED_](#)
- #define [KIM_SUPPORT_STATUS_DEFINED_](#)
- #define [KIM_ARGUMENT_NAME_DEFINED_](#)
- #define [KIM_CALLBACK_NAME_DEFINED_](#)
- #define [KIM_MODEL_CREATE_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_EnergyUnit](#) [KIM_EnergyUnit](#)
- typedef struct [KIM_ChargeUnit](#) [KIM_ChargeUnit](#)
- typedef struct [KIM_TemperatureUnit](#) [KIM_TemperatureUnit](#)
- typedef struct [KIM_TimeUnit](#) [KIM_TimeUnit](#)
- typedef struct [KIM_SupportStatus](#) [KIM_SupportStatus](#)
- typedef struct [KIM_ArgumentName](#) [KIM_ArgumentName](#)
- typedef struct [KIM_CallbackName](#) [KIM_CallbackName](#)
- 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_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_SetArgumentSupportStatus](#) ([KIM_ModelCreate](#) *const modelCreate, [KIM_ArgumentName](#) const argumentName, [KIM_SupportStatus](#) const supportStatus)
- int [KIM_ModelCreate_SetCallbackSupportStatus](#) ([KIM_ModelCreate](#) *const modelCreate, [KIM_CallbackName](#) const callbackName, [KIM_SupportStatus](#) const supportStatus)
- 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)

11.14.1 Macro Definition Documentation

11.14.1.1 KIM_ARGUMENT_NAME_DEFINED_

```
#define KIM_ARGUMENT_NAME_DEFINED_
```

Definition at line 95 of file KIM_ModelCreate.h.

11.14.1.2 KIM_CALLBACK_NAME_DEFINED_

```
#define KIM_CALLBACK_NAME_DEFINED_
```

Definition at line 100 of file KIM_ModelCreate.h.

11.14.1.3 KIM_CHARGE_UNIT_DEFINED_

```
#define KIM_CHARGE_UNIT_DEFINED_
```

Definition at line 75 of file KIM_ModelCreate.h.

11.14.1.4 KIM_ENERGY_UNIT_DEFINED_

```
#define KIM_ENERGY_UNIT_DEFINED_
```

Definition at line 70 of file KIM_ModelCreate.h.

11.14.1.5 KIM_LANGUAGE_NAME_DEFINED_

```
#define KIM_LANGUAGE_NAME_DEFINED_
```

Definition at line 55 of file KIM_ModelCreate.h.

11.14.1.6 KIM_LENGTH_UNIT_DEFINED_

```
#define KIM_LENGTH_UNIT_DEFINED_
```

Definition at line 65 of file KIM_ModelCreate.h.

11.14.1.7 KIM_LOG_VERBOSITY_DEFINED_

```
#define KIM_LOG_VERBOSITY_DEFINED_
```

Definition at line 45 of file KIM_ModelCreate.h.

11.14.1.8 KIM_MODEL_CREATE_DEFINED_

```
#define KIM_MODEL_CREATE_DEFINED_
```

Definition at line 108 of file KIM_ModelCreate.h.

11.14.1.9 KIM_NUMBERING_DEFINED_

```
#define KIM_NUMBERING_DEFINED_
```

Definition at line 60 of file KIM_ModelCreate.h.

11.14.1.10 KIM_SPECIES_NAME_DEFINED_

```
#define KIM_SPECIES_NAME_DEFINED_
```

Definition at line 50 of file KIM_ModelCreate.h.

11.14.1.11 KIM_SUPPORT_STATUS_DEFINED_

```
#define KIM_SUPPORT_STATUS_DEFINED_
```

Definition at line 90 of file KIM_ModelCreate.h.

11.14.1.12 KIM_TEMPERATURE_UNIT_DEFINED_

```
#define KIM_TEMPERATURE_UNIT_DEFINED_
```

Definition at line 80 of file KIM_ModelCreate.h.

11.14.1.13 KIM_TIME_UNIT_DEFINED_

```
#define KIM_TIME_UNIT_DEFINED_
```

Definition at line 85 of file KIM_ModelCreate.h.

11.14.2 Typedef Documentation

11.14.2.1 KIM_ArgumentName

```
typedef struct KIM_ArgumentName KIM_ArgumentName
```

Definition at line 96 of file KIM_ModelCreate.h.

11.14.2.2 KIM_CallbackName

```
typedef struct KIM_CallbackName KIM_CallbackName
```

Definition at line 101 of file KIM_ModelCreate.h.

11.14.2.3 KIM_ChargeUnit

```
typedef struct KIM_ChargeUnit KIM_ChargeUnit
```

Definition at line 76 of file KIM_ModelCreate.h.

11.14.2.4 KIM_EnergyUnit

```
typedef struct KIM_EnergyUnit KIM_EnergyUnit
```

Definition at line 71 of file KIM_ModelCreate.h.

11.14.2.5 KIM_LanguageName

```
typedef struct KIM_LanguageName KIM_LanguageName
```

Definition at line 56 of file KIM_ModelCreate.h.

11.14.2.6 KIM_LengthUnit

```
typedef struct KIM_LengthUnit KIM_LengthUnit
```

Definition at line 66 of file KIM_ModelCreate.h.

11.14.2.7 KIM_LogVerbosity

```
typedef struct KIM_LogVerbosity KIM_LogVerbosity
```

Definition at line 46 of file KIM_ModelCreate.h.

11.14.2.8 KIM_ModelCreate

```
typedef struct KIM_ModelCreate KIM_ModelCreate
```

Definition at line 109 of file KIM_ModelCreate.h.

11.14.2.9 KIM_Numbering

```
typedef struct KIM_Numbering KIM_Numbering
```

Definition at line 61 of file KIM_ModelCreate.h.

11.14.2.10 KIM_SpeciesName

```
typedef struct KIM_SpeciesName KIM_SpeciesName
```

Definition at line 51 of file KIM_ModelCreate.h.

11.14.2.11 KIM_SupportStatus

```
typedef struct KIM_SupportStatus KIM_SupportStatus
```

Definition at line 91 of file KIM_ModelCreate.h.

11.14.2.12 KIM_TemperatureUnit

```
typedef struct KIM_TemperatureUnit KIM_TemperatureUnit
```

Definition at line 81 of file KIM_ModelCreate.h.

11.14.2.13 KIM_TimeUnit

```
typedef struct KIM_TimeUnit KIM_TimeUnit
```

Definition at line 86 of file KIM_ModelCreate.h.

11.14.3 Function Documentation

11.14.3.1 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 )
```


11.14.3.2 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 )
```

11.14.3.3 KIM_ModelCreate_SetArgumentSupportStatus()

```
int KIM_ModelCreate_SetArgumentSupportStatus (
    KIM_ModelCreate *const modelCreate,
    KIM_ArgumentName const argumentName,
    KIM_SupportStatus const supportStatus )
```

11.14.3.4 KIM_ModelCreate_SetCallbackSupportStatus()

```
int KIM_ModelCreate_SetCallbackSupportStatus (
    KIM_ModelCreate *const modelCreate,
    KIM_CallbackName const callbackName,
    KIM_SupportStatus const supportStatus )
```

11.14.3.5 KIM_ModelCreate_SetComputePointer()

```
int KIM_ModelCreate_SetComputePointer (
    KIM_ModelCreate *const modelCreate,
    KIM_LanguageName const languageName,
    func *const fptr )
```

11.14.3.6 KIM_ModelCreate_SetDestroyPointer()

```
int KIM_ModelCreate_SetDestroyPointer (
    KIM_ModelCreate *const modelCreate,
    KIM_LanguageName const languageName,
    func *const fptr )
```


11.14.3.7 KIM_ModelCreate_SetInfluenceDistancePointer()

```
void KIM_ModelCreate_SetInfluenceDistancePointer (
    KIM_ModelCreate *const modelCreate,
    double *const influenceDistance )
```

11.14.3.8 KIM_ModelCreate_SetModelBufferPointer()

```
void KIM_ModelCreate_SetModelBufferPointer (
    KIM_ModelCreate *const modelCreate,
    void *const ptr )
```

11.14.3.9 KIM_ModelCreate_SetModelNumbering()

```
int KIM_ModelCreate_SetModelNumbering (
    KIM_ModelCreate *const modelCreate,
    KIM_Numbering const numbering )
```

11.14.3.10 KIM_ModelCreate_SetNeighborListCutoffsPointer()

```
void KIM_ModelCreate_SetNeighborListCutoffsPointer (
    KIM_ModelCreate *const modelCreate,
    int const numberOfCutoffs,
    double const *const cutoffs )
```

11.14.3.11 KIM_ModelCreate_SetParameterPointerDouble()

```
int KIM_ModelCreate_SetParameterPointerDouble (
    KIM_ModelCreate *const modelCreate,
    int const extent,
    double *const ptr,
    char const *const description )
```

11.14.3.12 KIM_ModelCreate_SetParameterPointerInteger()

```
int KIM_ModelCreate_SetParameterPointerInteger (
    KIM_ModelCreate *const modelCreate,
    int const extent,
    int *const ptr,
    char const *const description )
```


11.14.3.13 KIM_ModelCreate_SetRefreshPointer()

```
int KIM_ModelCreate_SetRefreshPointer (
    KIM_ModelCreate *const modelCreate,
    KIM_LanguageName const languageName,
    func *const fptr )
```

11.14.3.14 KIM_ModelCreate_SetSpeciesCode()

```
int KIM_ModelCreate_SetSpeciesCode (
    KIM_ModelCreate *const modelCreate,
    KIM_SpeciesName const speciesName,
    int const code )
```

11.14.3.15 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 )
```

11.14.3.16 KIM_ModelCreate_String()

```
char const* const KIM_ModelCreate_String (
    KIM_ModelCreate const *const modelCreate )
```

11.15 kim-api-v2.0.0-alpha.0/c/include/KIM_ModelCreateLogMacros.h File Reference

Macros

- #define [LOG_FATAL](#)(message)
- #define [LOG_ERROR](#)(message)
- #define [LOG_WARNING](#)(message)
- #define [LOG_INFORMATION](#)(message)
- #define [LOG_DEBUG](#)(message)

11.15.1 Macro Definition Documentation

11.15.1.1 LOG_DEBUG

```
#define LOG_DEBUG(  
    message )
```

Value:

```
KIM_ModelCreate_LogEntry(modelCreate,  
    KIM_LOG_VERBOSITY_debug, message,  
    __LINE__, __FILE__)
```

Definition at line 88 of file KIM_ModelCreateLogMacros.h.

11.15.1.2 LOG_ERROR

```
#define LOG_ERROR(  
    message )
```

Value:

```
KIM_ModelCreate_LogEntry(modelCreate,  
    KIM_LOG_VERBOSITY_error, message,  
    __LINE__, __FILE__)
```

Definition at line 52 of file KIM_ModelCreateLogMacros.h.

11.15.1.3 LOG_FATAL

```
#define LOG_FATAL(  
    message )
```

Value:

```
KIM_ModelCreate_LogEntry(modelCreate,  
    KIM_LOG_VERBOSITY_fatal, message,  
    __LINE__, __FILE__)
```

Definition at line 40 of file KIM_ModelCreateLogMacros.h.

11.15.1.4 LOG_INFORMATION

```
#define LOG_INFORMATION(  
    message )
```

Value:

```
KIM_ModelCreate_LogEntry(modelCreate,  
    KIM_LOG_VERBOSITY_information, message,  
    __LINE__, __FILE__)
```

Definition at line 76 of file KIM_ModelCreateLogMacros.h.

11.15.1.5 LOG_WARNING

```
#define LOG_WARNING(  
    message )
```

Value:

```
KIM_ModelCreate_LogEntry(modelCreate,  
    KIM_LOG_VERBOSITY_warning, message,  
    __LINE__, __FILE__)
```

Definition at line 64 of file KIM_ModelCreateLogMacros.h.

11.16 kim-api-v2.0.0-alpha.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)

11.16.1 Macro Definition Documentation

11.16.1.1 KIM_LOG_VERBOSITY_DEFINED_

```
#define KIM_LOG_VERBOSITY_DEFINED_
```

Definition at line 41 of file KIM_ModelDestroy.h.

11.16.1.2 KIM_MODEL_DESTROY_DEFINED_

```
#define KIM_MODEL_DESTROY_DEFINED_
```

Definition at line 49 of file KIM_ModelDestroy.h.

11.16.2 Typedef Documentation

11.16.2.1 KIM_LogVerbosity

```
typedef struct KIM_LogVerbosity KIM_LogVerbosity
```

Definition at line 42 of file KIM_ModelDestroy.h.

11.16.2.2 KIM_ModelDestroy

```
typedef struct KIM_ModelDestroy KIM_ModelDestroy
```

Definition at line 50 of file KIM_ModelDestroy.h.

11.16.3 Function Documentation

11.16.3.1 KIM_ModelDestroy_GetModelBufferPointer()

```
void KIM_ModelDestroy_GetModelBufferPointer (
    KIM_ModelDestroy const *const modelDestroy,
    void **const ptr )
```


11.16.3.2 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 )
```

11.16.3.3 KIM_ModelDestroy_String()

```
char const* const KIM_ModelDestroy_String (
    KIM_ModelDestroy const *const modelDestroy )
```

11.17 kim-api-v2.0.0-alpha.0/c/include/KIM_ModelDestroyLogMacros.h File Reference

Macros

- #define [LOG_FATAL](#)(message)
- #define [LOG_ERROR](#)(message)
- #define [LOG_WARNING](#)(message)
- #define [LOG_INFORMATION](#)(message)
- #define [LOG_DEBUG](#)(message)

11.17.1 Macro Definition Documentation

11.17.1.1 LOG_DEBUG

```
#define LOG_DEBUG(
    message )
```

Value:

```
KIM_ModelDestroy_LogEntry(modelDestroy,
    KIM_LOG_VERBOSITY_debug, message,
    __LINE__, __FILE__)
```

Definition at line 88 of file KIM_ModelDestroyLogMacros.h.

11.17.1.2 LOG_ERROR

```
#define LOG_ERROR(  
    message )
```

Value:

```
KIM_ModelDestroy_LogEntry (modelDestroy,  
    KIM_LOG_VERBOSITY_error, message,  
    __LINE__, __FILE__)
```

Definition at line 52 of file KIM_ModelDestroyLogMacros.h.

11.17.1.3 LOG_FATAL

```
#define LOG_FATAL(  
    message )
```

Value:

```
KIM_ModelDestroy_LogEntry (modelDestroy,  
    KIM_LOG_VERBOSITY_fatal, message,  
    __LINE__, __FILE__)
```

Definition at line 40 of file KIM_ModelDestroyLogMacros.h.

11.17.1.4 LOG_INFORMATION

```
#define LOG_INFORMATION(  
    message )
```

Value:

```
KIM_ModelDestroy_LogEntry (modelDestroy,  
    KIM_LOG_VERBOSITY_information, message,  
    __LINE__, __FILE__)
```

Definition at line 76 of file KIM_ModelDestroyLogMacros.h.

11.17.1.5 LOG_WARNING

```
#define LOG_WARNING(  
    message )
```

Value:

```
KIM_ModelDestroy_LogEntry (modelDestroy,  
    KIM_LOG_VERBOSITY_warning, message,  
    __LINE__, __FILE__)
```

Definition at line 64 of file KIM_ModelDestroyLogMacros.h.

11.18 kim-api-v2.0.0-alpha.0/c/include/KIM_ModelDriverCreate.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_ENERGY_UNIT_DEFINED_`
- `#define KIM_CHARGE_UNIT_DEFINED_`
- `#define KIM_TEMPERATURE_UNIT_DEFINED_`
- `#define KIM_TIME_UNIT_DEFINED_`
- `#define KIM_SUPPORT_STATUS_DEFINED_`
- `#define KIM_ARGUMENT_NAME_DEFINED_`
- `#define KIM_CALLBACK_NAME_DEFINED_`
- `#define KIM_MODEL_DRIVER_CREATE_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_EnergyUnit KIM_EnergyUnit`
- `typedef struct KIM_ChargeUnit KIM_ChargeUnit`
- `typedef struct KIM_TemperatureUnit KIM_TemperatureUnit`
- `typedef struct KIM_TimeUnit KIM_TimeUnit`
- `typedef struct KIM_SupportStatus KIM_SupportStatus`
- `typedef struct KIM_ArgumentName KIM_ArgumentName`
- `typedef struct KIM_CallbackName KIM_CallbackName`
- `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_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_SetArgumentSupportStatus](#) (KIM_ModelDriverCreate *const modelDriverCreate, KIM_ArgumentName const argumentName, KIM_SupportStatus const supportStatus)
- int [KIM_ModelDriverCreate_SetCallbackSupportStatus](#) (KIM_ModelDriverCreate *const modelDriverCreate, KIM_CallbackName const callbackName, KIM_SupportStatus const supportStatus)
- 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)

11.18.1 Macro Definition Documentation

11.18.1.1 KIM_ARGUMENT_NAME_DEFINED_

```
#define KIM_ARGUMENT_NAME_DEFINED_
```

Definition at line 95 of file KIM_ModelDriverCreate.h.

11.18.1.2 KIM_CALLBACK_NAME_DEFINED_

```
#define KIM_CALLBACK_NAME_DEFINED_
```

Definition at line 100 of file KIM_ModelDriverCreate.h.

11.18.1.3 KIM_CHARGE_UNIT_DEFINED_

```
#define KIM_CHARGE_UNIT_DEFINED_
```

Definition at line 75 of file KIM_ModelDriverCreate.h.

11.18.1.4 KIM_ENERGY_UNIT_DEFINED_

```
#define KIM_ENERGY_UNIT_DEFINED_
```

Definition at line 70 of file KIM_ModelDriverCreate.h.

11.18.1.5 KIM_LANGUAGE_NAME_DEFINED_

```
#define KIM_LANGUAGE_NAME_DEFINED_
```

Definition at line 55 of file KIM_ModelDriverCreate.h.

11.18.1.6 KIM_LENGTH_UNIT_DEFINED_

```
#define KIM_LENGTH_UNIT_DEFINED_
```

Definition at line 65 of file KIM_ModelDriverCreate.h.

11.18.1.7 KIM_LOG_VERBOSITY_DEFINED_

```
#define KIM_LOG_VERBOSITY_DEFINED_
```

Definition at line 45 of file KIM_ModelDriverCreate.h.

11.18.1.8 KIM_MODEL_DRIVER_CREATE_DEFINED_

```
#define KIM_MODEL_DRIVER_CREATE_DEFINED_
```

Definition at line 108 of file KIM_ModelDriverCreate.h.

11.18.1.9 KIM_NUMBERING_DEFINED_

```
#define KIM_NUMBERING_DEFINED_
```

Definition at line 60 of file KIM_ModelDriverCreate.h.

11.18.1.10 KIM_SPECIES_NAME_DEFINED_

```
#define KIM_SPECIES_NAME_DEFINED_
```

Definition at line 50 of file KIM_ModelDriverCreate.h.

11.18.1.11 KIM_SUPPORT_STATUS_DEFINED_

```
#define KIM_SUPPORT_STATUS_DEFINED_
```

Definition at line 90 of file KIM_ModelDriverCreate.h.

11.18.1.12 KIM_TEMPERATURE_UNIT_DEFINED_

```
#define KIM_TEMPERATURE_UNIT_DEFINED_
```

Definition at line 80 of file KIM_ModelDriverCreate.h.

11.18.1.13 KIM_TIME_UNIT_DEFINED_

```
#define KIM_TIME_UNIT_DEFINED_
```

Definition at line 85 of file KIM_ModelDriverCreate.h.

11.18.2 Typedef Documentation

11.18.2.1 KIM_ArgumentName

```
typedef struct KIM_ArgumentName KIM_ArgumentName
```

Definition at line 96 of file KIM_ModelDriverCreate.h.

11.18.2.2 KIM_CallbackName

```
typedef struct KIM_CallbackName KIM_CallbackName
```

Definition at line 101 of file KIM_ModelDriverCreate.h.

11.18.2.3 KIM_ChargeUnit

```
typedef struct KIM_ChargeUnit KIM_ChargeUnit
```

Definition at line 76 of file KIM_ModelDriverCreate.h.

11.18.2.4 KIM_EnergyUnit

```
typedef struct KIM_EnergyUnit KIM_EnergyUnit
```

Definition at line 71 of file KIM_ModelDriverCreate.h.

11.18.2.5 KIM_LanguageName

```
typedef struct KIM_LanguageName KIM_LanguageName
```

Definition at line 56 of file KIM_ModelDriverCreate.h.

11.18.2.6 KIM_LengthUnit

```
typedef struct KIM_LengthUnit KIM_LengthUnit
```

Definition at line 66 of file KIM_ModelDriverCreate.h.

11.18.2.7 KIM_LogVerbosity

```
typedef struct KIM_LogVerbosity KIM_LogVerbosity
```

Definition at line 46 of file KIM_ModelDriverCreate.h.

11.18.2.8 KIM_ModelDriverCreate

```
typedef struct KIM_ModelDriverCreate KIM_ModelDriverCreate
```

Definition at line 109 of file KIM_ModelDriverCreate.h.

11.18.2.9 KIM_Numbering

```
typedef struct KIM_Numbering KIM_Numbering
```

Definition at line 61 of file KIM_ModelDriverCreate.h.

11.18.2.10 KIM_SpeciesName

```
typedef struct KIM_SpeciesName KIM_SpeciesName
```

Definition at line 51 of file KIM_ModelDriverCreate.h.

11.18.2.11 KIM_SupportStatus

```
typedef struct KIM_SupportStatus KIM_SupportStatus
```

Definition at line 91 of file KIM_ModelDriverCreate.h.

11.18.2.12 KIM_TemperatureUnit

```
typedef struct KIM_TemperatureUnit KIM_TemperatureUnit
```

Definition at line 81 of file KIM_ModelDriverCreate.h.

11.18.2.13 KIM_TimeUnit

```
typedef struct KIM_TimeUnit KIM_TimeUnit
```

Definition at line 86 of file KIM_ModelDriverCreate.h.

11.18.3 Function Documentation

11.18.3.1 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 )
```

11.18.3.2 KIM_ModelDriverCreate_GetNumberOfParameterFiles()

```
void KIM_ModelDriverCreate_GetNumberOfParameterFiles (
    KIM_ModelDriverCreate *const modelDriverCreate,
    int *const numberOfParameterFiles )
```

11.18.3.3 KIM_ModelDriverCreate_GetParameterFileName()

```
int KIM_ModelDriverCreate_GetParameterFileName (
    KIM_ModelDriverCreate *const modelDriverCreate,
    int const index,
    char const **const parameterFileName )
```

11.18.3.4 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 )
```


11.18.3.5 KIM_ModelDriverCreate_SetArgumentSupportStatus()

```
int KIM_ModelDriverCreate_SetArgumentSupportStatus (
    KIM_ModelDriverCreate *const modelDriverCreate,
    KIM_ArgumentName const argumentName,
    KIM_SupportStatus const supportStatus )
```

11.18.3.6 KIM_ModelDriverCreate_SetCallbackSupportStatus()

```
int KIM_ModelDriverCreate_SetCallbackSupportStatus (
    KIM_ModelDriverCreate *const modelDriverCreate,
    KIM_CallbackName const callbackName,
    KIM_SupportStatus const supportStatus )
```

11.18.3.7 KIM_ModelDriverCreate_SetComputePointer()

```
int KIM_ModelDriverCreate_SetComputePointer (
    KIM_ModelDriverCreate *const modelDriverCreate,
    KIM_LanguageName const languageName,
    func *const fptr )
```

11.18.3.8 KIM_ModelDriverCreate_SetDestroyPointer()

```
int KIM_ModelDriverCreate_SetDestroyPointer (
    KIM_ModelDriverCreate *const modelDriverCreate,
    KIM_LanguageName const languageName,
    func *const fptr )
```

11.18.3.9 KIM_ModelDriverCreate_SetInfluenceDistancePointer()

```
void KIM_ModelDriverCreate_SetInfluenceDistancePointer (
    KIM_ModelDriverCreate *const modelDriverCreate,
    double *const influenceDistance )
```

11.18.3.10 KIM_ModelDriverCreate_SetModelBufferPointer()

```
void KIM_ModelDriverCreate_SetModelBufferPointer (
    KIM_ModelDriverCreate *const modelDriverCreate,
    void *const ptr )
```


11.18.3.11 KIM_ModelDriverCreate_SetModelNumbering()

```
int KIM_ModelDriverCreate_SetModelNumbering (
    KIM_ModelDriverCreate *const modelDriverCreate,
    KIM_Numbering const numbering )
```

11.18.3.12 KIM_ModelDriverCreate_SetNeighborListCutoffsPointer()

```
void KIM_ModelDriverCreate_SetNeighborListCutoffsPointer (
    KIM_ModelDriverCreate *const modelDriverCreate,
    int const numberOfCutoffs,
    double const *const cutoffs )
```

11.18.3.13 KIM_ModelDriverCreate_SetParameterPointerDouble()

```
int KIM_ModelDriverCreate_SetParameterPointerDouble (
    KIM_ModelDriverCreate *const modelDriverCreate,
    int const extent,
    double *const ptr,
    char const *const description )
```

11.18.3.14 KIM_ModelDriverCreate_SetParameterPointerInteger()

```
int KIM_ModelDriverCreate_SetParameterPointerInteger (
    KIM_ModelDriverCreate *const modelDriverCreate,
    int const extent,
    int *const ptr,
    char const *const description )
```

11.18.3.15 KIM_ModelDriverCreate_SetRefreshPointer()

```
int KIM_ModelDriverCreate_SetRefreshPointer (
    KIM_ModelDriverCreate *const modelDriverCreate,
    KIM_LanguageName const languageName,
    func *const fptr )
```


11.18.3.16 KIM_ModelDriverCreate_SetSpeciesCode()

```
int KIM_ModelDriverCreate_SetSpeciesCode (
    KIM_ModelDriverCreate *const modelDriverCreate,
    KIM_SpeciesName const speciesName,
    int const code )
```

11.18.3.17 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 )
```

11.18.3.18 KIM_ModelDriverCreate_String()

```
char const* const KIM_ModelDriverCreate_String (
    KIM_ModelDriverCreate const *const modelDriverCreate )
```

11.19 kim-api-v2.0.0-alpha.0/c/include/KIM_ModelDriverCreateLogMacros.h File Reference

Macros

- #define [LOG_FATAL](#)(message)
- #define [LOG_ERROR](#)(message)
- #define [LOG_WARNING](#)(message)
- #define [LOG_INFORMATION](#)(message)
- #define [LOG_DEBUG](#)(message)

11.19.1 Macro Definition Documentation

11.19.1.1 LOG_DEBUG

```
#define LOG_DEBUG(  
    message )
```

Value:

```
KIM_ModelDriverCreate_LogEntry(modelDriverCreate,  
    KIM_LOG_VERBOSITY_debug, message, \  
    __LINE__, __FILE__)
```

Definition at line 88 of file KIM_ModelDriverCreateLogMacros.h.

11.19.1.2 LOG_ERROR

```
#define LOG_ERROR(  
    message )
```

Value:

```
KIM_ModelDriverCreate_LogEntry(modelDriverCreate,  
    KIM_LOG_VERBOSITY_error, message, \  
    __LINE__, __FILE__)
```

Definition at line 52 of file KIM_ModelDriverCreateLogMacros.h.

11.19.1.3 LOG_FATAL

```
#define LOG_FATAL(  
    message )
```

Value:

```
KIM_ModelDriverCreate_LogEntry(modelDriverCreate,  
    KIM_LOG_VERBOSITY_fatal, message, \  
    __LINE__, __FILE__)
```

Definition at line 40 of file KIM_ModelDriverCreateLogMacros.h.

11.19.1.4 LOG_INFORMATION

```
#define LOG_INFORMATION(  
    message )
```

Value:

```
KIM_ModelDriverCreate_LogEntry(modelDriverCreate,  
                                KIM_LOG_VERBOSITY_information, message, \  
                                __LINE__, __FILE__)
```

Definition at line 76 of file KIM_ModelDriverCreateLogMacros.h.

11.19.1.5 LOG_WARNING

```
#define LOG_WARNING(  
    message )
```

Value:

```
KIM_ModelDriverCreate_LogEntry(modelDriverCreate,  
                                KIM_LOG_VERBOSITY_warning, message, \  
                                __LINE__, __FILE__)
```

Definition at line 64 of file KIM_ModelDriverCreateLogMacros.h.

11.20 kim-api-v2.0.0-alpha.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_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)
- void [KIM_ModelRefresh_GetModelBufferPointer](#) (KIM_ModelRefresh const *const modelRefresh, void **const ptr)

11.20.1 Macro Definition Documentation

11.20.1.1 KIM_LOG_VERBOSITY_DEFINED_

```
#define KIM_LOG_VERBOSITY_DEFINED_
```

Definition at line 42 of file KIM_ModelRefresh.h.

11.20.1.2 KIM_MODEL_REFRESH_DEFINED_

```
#define KIM_MODEL_REFRESH_DEFINED_
```

Definition at line 47 of file KIM_ModelRefresh.h.

11.20.2 Typedef Documentation

11.20.2.1 KIM_LogVerbosity

```
typedef struct KIM_LogVerbosity KIM_LogVerbosity
```

Definition at line 43 of file KIM_ModelRefresh.h.

11.20.2.2 KIM_ModelRefresh

```
typedef struct KIM_ModelRefresh KIM_ModelRefresh
```

Definition at line 48 of file KIM_ModelRefresh.h.

11.20.3 Function Documentation

11.20.3.1 KIM_ModelRefresh_GetModelBufferPointer()

```
void KIM_ModelRefresh_GetModelBufferPointer (
    KIM_ModelRefresh const *const modelRefresh,
    void **const ptr )
```


11.20.3.2 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 )
```

11.20.3.3 KIM_ModelRefresh_SetInfluenceDistancePointer()

```
void KIM_ModelRefresh_SetInfluenceDistancePointer (
    KIM_ModelRefresh *const modelRefresh,
    double *const influenceDistance )
```

11.20.3.4 KIM_ModelRefresh_SetNeighborListCutoffsPointer()

```
void KIM_ModelRefresh_SetNeighborListCutoffsPointer (
    KIM_ModelRefresh *const modelRefresh,
    int const numberOfCutoffs,
    double const *const cutoffs )
```

11.20.3.5 KIM_ModelRefresh_string()

```
char const* const KIM_ModelRefresh_string (
    KIM_ModelRefresh const *const modelRefresh )
```

11.21 kim-api-v2.0.0-alpha.0/c/include/KIM_ModelRefreshLogMacros.h File Reference

Macros

- #define [LOG_FATAL](#)(message)
- #define [LOG_ERROR](#)(message)
- #define [LOG_WARNING](#)(message)
- #define [LOG_INFORMATION](#)(message)
- #define [LOG_DEBUG](#)(message)

11.21.1 Macro Definition Documentation

11.21.1.1 LOG_DEBUG

```
#define LOG_DEBUG(  
    message )
```

Value:

```
KIM_ModelRefresh_LogEntry(modelRefresh,  
    KIM_LOG_VERBOSITY_debug, message,  
    __LINE__, __FILE__)
```

Definition at line 88 of file KIM_ModelRefreshLogMacros.h.

11.21.1.2 LOG_ERROR

```
#define LOG_ERROR(  
    message )
```

Value:

```
KIM_ModelRefresh_LogEntry(modelRefresh,  
    KIM_LOG_VERBOSITY_error, message,  
    __LINE__, __FILE__)
```

Definition at line 52 of file KIM_ModelRefreshLogMacros.h.

11.21.1.3 LOG_FATAL

```
#define LOG_FATAL(  
    message )
```

Value:

```
KIM_ModelRefresh_LogEntry(modelRefresh,  
    KIM_LOG_VERBOSITY_fatal, message,  
    __LINE__, __FILE__)
```

Definition at line 40 of file KIM_ModelRefreshLogMacros.h.

11.21.1.4 LOG_INFORMATION

```
#define LOG_INFORMATION(  
    message )
```

Value:

```
KIM_ModelRefresh_LogEntry(modelRefresh,  
    KIM_LOG_VERBOSITY_information, message, \  
    __LINE__, __FILE__)
```

Definition at line 76 of file KIM_ModelRefreshLogMacros.h.

11.21.1.5 LOG_WARNING

```
#define LOG_WARNING(  
    message )
```

Value:

```
KIM_ModelRefresh_LogEntry(modelRefresh,  
    KIM_LOG_VERBOSITY_warning, message, \  
    __LINE__, __FILE__)
```

Definition at line 64 of file KIM_ModelRefreshLogMacros.h.

11.22 kim-api-v2.0.0-alpha.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_NumberingFromString](#) (char const *const str)
- int [KIM_NumberingEqual](#) ([KIM_Numbering](#) const left, [KIM_Numbering](#) const right)
- int [KIM_NumberingNotEqual](#) ([KIM_Numbering](#) const left, [KIM_Numbering](#) const right)
- char const *const [KIM_NumberingString](#) ([KIM_Numbering](#) const numbering)

Variables

- [KIM_Numbering](#) const [KIM_NUMBERING_zeroBased](#)
- [KIM_Numbering](#) const [KIM_NUMBERING_oneBased](#)

11.22.1 Macro Definition Documentation

11.22.1.1 KIM_NUMBERING_DEFINED_

```
#define KIM_NUMBERING_DEFINED_
```

Definition at line 44 of file [KIM_Numbering.h](#).

11.22.2 Typedef Documentation

11.22.2.1 KIM_Numbering

```
typedef struct KIM\_Numbering KIM\_Numbering
```

Definition at line 45 of file [KIM_Numbering.h](#).

11.22.3 Function Documentation

11.22.3.1 KIM_NumberingEqual()

```
int KIM_NumberingEqual (  
    KIM\_Numbering const left,  
    KIM\_Numbering const right )
```

11.22.3.2 KIM_NumberingFromString()

```
KIM\_Numbering KIM_NumberingFromString (  
    char const *const str )
```


11.22.3.3 KIM_NumberingNotEqual()

```
int KIM_NumberingNotEqual (
    KIM_Numbering const left,
    KIM_Numbering const right )
```

11.22.3.4 KIM_NumberingString()

```
char const* const KIM_NumberingString (
    KIM_Numbering const numbering )
```

11.22.4 Variable Documentation

11.22.4.1 KIM_NUMBERING_oneBased

```
KIM_Numbering const KIM_NUMBERING_oneBased
```

11.22.4.2 KIM_NUMBERING_zeroBased

```
KIM_Numbering const KIM_NUMBERING_zeroBased
```

11.23 kim-api-v2.0.0-alpha.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 **const prerelease, char const **const buildMetadata)

11.23.1 Function Documentation

11.23.1.1 KIM_SEM_VER_GetSemVer()

```
void KIM_SEM_VER_GetSemVer (
    char const **const version )
```

11.23.1.2 KIM_SEM_VER_IsLessThan()

```
int KIM_SEM_VER_IsLessThan (
    char const *const versionA,
    char const *const versionB,
    int *const isLessThan )
```

11.23.1.3 KIM_SEM_VER_ParseSemVer()

```
int KIM_SEM_VER_ParseSemVer (
    char const *const version,
    int *const major,
    int *const minor,
    int *const patch,
    char const **const prerelease,
    char const **const buildMetadata )
```

11.24 kim-api-v2.0.0-alpha.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_SpeciesNameFromString](#) (char const *const str)
- int [KIM_SpeciesNameEqual](#) ([KIM_SpeciesName](#) const left, [KIM_SpeciesName](#) const right)
- int [KIM_SpeciesNameNotEqual](#) ([KIM_SpeciesName](#) const left, [KIM_SpeciesName](#) const right)
- char const *const [KIM_SpeciesNameString](#) ([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_FI](#)
- [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](#)

11.24.1 Macro Definition Documentation

11.24.1.1 KIM_SPECIES_NAME_DEFINED_

```
#define KIM_SPECIES_NAME_DEFINED_
```

Definition at line 45 of file [KIM_SpeciesName.h](#).

11.24.2 Typedef Documentation

11.24.2.1 KIM_SpeciesName

```
typedef struct KIM_SpeciesName KIM_SpeciesName
```

Definition at line 46 of file [KIM_SpeciesName.h](#).

11.24.3 Function Documentation

11.24.3.1 KIM_SPECIES_NAME_GetNumberOfSpeciesNames()

```
void KIM_SPECIES_NAME_GetNumberOfSpeciesNames (
    int *const numberOfSpeciesNames )
```

11.24.3.2 KIM_SPECIES_NAME_GetSpeciesName()

```
int KIM_SPECIES_NAME_GetSpeciesName (
    int const index,
    KIM_SpeciesName *const speciesName )
```

11.24.3.3 KIM_SpeciesNameEqual()

```
int KIM_SpeciesNameEqual (
    KIM_SpeciesName const left,
    KIM_SpeciesName const right )
```

11.24.3.4 KIM_SpeciesNameFromString()

```
KIM_SpeciesName KIM_SpeciesNameFromString (
    char const *const str )
```

11.24.3.5 KIM_SpeciesNameNotEqual()

```
int KIM_SpeciesNameNotEqual (
    KIM_SpeciesName const left,
    KIM_SpeciesName const right )
```

11.24.3.6 KIM_SpeciesNameString()

```
char const* const KIM_SpeciesNameString (
    KIM_SpeciesName const speciesName )
```


11.24.4 Variable Documentation

11.24.4.1 KIM_SPECIES_NAME_Ac

`KIM_SpeciesName` const KIM_SPECIES_NAME_Ac

11.24.4.2 KIM_SPECIES_NAME_Ag

`KIM_SpeciesName` const KIM_SPECIES_NAME_Ag

11.24.4.3 KIM_SPECIES_NAME_Al

`KIM_SpeciesName` const KIM_SPECIES_NAME_Al

11.24.4.4 KIM_SPECIES_NAME_Am

`KIM_SpeciesName` const KIM_SPECIES_NAME_Am

11.24.4.5 KIM_SPECIES_NAME_Ar

`KIM_SpeciesName` const KIM_SPECIES_NAME_Ar

11.24.4.6 KIM_SPECIES_NAME_As

`KIM_SpeciesName` const KIM_SPECIES_NAME_As

11.24.4.7 KIM_SPECIES_NAME_At

`KIM_SpeciesName` const KIM_SPECIES_NAME_At

11.24.4.8 KIM_SPECIES_NAME_Au

`KIM_SpeciesName` const KIM_SPECIES_NAME_Au

11.24.4.9 KIM_SPECIES_NAME_B

`KIM_SpeciesName` const KIM_SPECIES_NAME_B

11.24.4.10 KIM_SPECIES_NAME_Ba

`KIM_SpeciesName` const KIM_SPECIES_NAME_Ba

11.24.4.11 KIM_SPECIES_NAME_Be

`KIM_SpeciesName` const KIM_SPECIES_NAME_Be

11.24.4.12 KIM_SPECIES_NAME_Bh

`KIM_SpeciesName` const KIM_SPECIES_NAME_Bh

11.24.4.13 KIM_SPECIES_NAME_Bi

`KIM_SpeciesName` const KIM_SPECIES_NAME_Bi

11.24.4.14 KIM_SPECIES_NAME_Bk

`KIM_SpeciesName` const KIM_SPECIES_NAME_Bk

11.24.4.15 KIM_SPECIES_NAME_Br

`KIM_SpeciesName` const KIM_SPECIES_NAME_Br

11.24.4.16 KIM_SPECIES_NAME_C

`KIM_SpeciesName` const KIM_SPECIES_NAME_C

11.24.4.17 KIM_SPECIES_NAME_Ca

`KIM_SpeciesName` const KIM_SPECIES_NAME_Ca

11.24.4.18 KIM_SPECIES_NAME_Cd

`KIM_SpeciesName` const KIM_SPECIES_NAME_Cd

11.24.4.19 KIM_SPECIES_NAME_Ce

`KIM_SpeciesName` const KIM_SPECIES_NAME_Ce

11.24.4.20 KIM_SPECIES_NAME_Cf

`KIM_SpeciesName` const KIM_SPECIES_NAME_Cf

11.24.4.21 KIM_SPECIES_NAME_Cl

`KIM_SpeciesName` const KIM_SPECIES_NAME_Cl

11.24.4.22 KIM_SPECIES_NAME_Cm

`KIM_SpeciesName` const KIM_SPECIES_NAME_Cm

11.24.4.23 KIM_SPECIES_NAME_Cn

`KIM_SpeciesName` const KIM_SPECIES_NAME_Cn

11.24.4.24 KIM_SPECIES_NAME_Co

`KIM_SpeciesName` const KIM_SPECIES_NAME_Co

11.24.4.25 KIM_SPECIES_NAME_Cr

`KIM_SpeciesName` const KIM_SPECIES_NAME_Cr

11.24.4.26 KIM_SPECIES_NAME-Cs

`KIM_SpeciesName` const KIM_SPECIES_NAME-Cs

11.24.4.27 KIM_SPECIES_NAME_Cu

`KIM_SpeciesName` const KIM_SPECIES_NAME_Cu

11.24.4.28 KIM_SPECIES_NAME_Db

`KIM_SpeciesName` const KIM_SPECIES_NAME_Db

11.24.4.29 KIM_SPECIES_NAME_Ds

`KIM_SpeciesName` const KIM_SPECIES_NAME_Ds

11.24.4.30 KIM_SPECIES_NAME_Dy

`KIM_SpeciesName` const KIM_SPECIES_NAME_Dy

11.24.4.31 KIM_SPECIES_NAME_electron

`KIM_SpeciesName` const KIM_SPECIES_NAME_electron

11.24.4.32 KIM_SPECIES_NAME_Er

`KIM_SpeciesName` const KIM_SPECIES_NAME_Er

11.24.4.33 KIM_SPECIES_NAME_Es

`KIM_SpeciesName` const KIM_SPECIES_NAME_Es

11.24.4.34 KIM_SPECIES_NAME_Eu

`KIM_SpeciesName` const KIM_SPECIES_NAME_Eu

11.24.4.35 KIM_SPECIES_NAME_F

`KIM_SpeciesName` const KIM_SPECIES_NAME_F

11.24.4.36 KIM_SPECIES_NAME_Fe

`KIM_SpeciesName` const KIM_SPECIES_NAME_Fe

11.24.4.37 KIM_SPECIES_NAME_FI

`KIM_SpeciesName` const KIM_SPECIES_NAME_FI

11.24.4.38 KIM_SPECIES_NAME_Fm

`KIM_SpeciesName` const KIM_SPECIES_NAME_Fm

11.24.4.39 KIM_SPECIES_NAME_Fr

`KIM_SpeciesName` const KIM_SPECIES_NAME_Fr

11.24.4.40 KIM_SPECIES_NAME_Ga

`KIM_SpeciesName` const KIM_SPECIES_NAME_Ga

11.24.4.41 KIM_SPECIES_NAME_Gd

`KIM_SpeciesName` const KIM_SPECIES_NAME_Gd

11.24.4.42 KIM_SPECIES_NAME_Ge

`KIM_SpeciesName` const KIM_SPECIES_NAME_Ge

11.24.4.43 KIM_SPECIES_NAME_H

`KIM_SpeciesName` const KIM_SPECIES_NAME_H

11.24.4.44 KIM_SPECIES_NAME_He

`KIM_SpeciesName` const KIM_SPECIES_NAME_He

11.24.4.45 KIM_SPECIES_NAME_Hf

`KIM_SpeciesName` const KIM_SPECIES_NAME_Hf

11.24.4.46 KIM_SPECIES_NAME_Hg

`KIM_SpeciesName` const KIM_SPECIES_NAME_Hg

11.24.4.47 KIM_SPECIES_NAME_Ho

`KIM_SpeciesName` const KIM_SPECIES_NAME_Ho

11.24.4.48 KIM_SPECIES_NAME_Hs

`KIM_SpeciesName` const KIM_SPECIES_NAME_Hs

11.24.4.49 KIM_SPECIES_NAME_I

`KIM_SpeciesName` const KIM_SPECIES_NAME_I

11.24.4.50 KIM_SPECIES_NAME_In

`KIM_SpeciesName` const KIM_SPECIES_NAME_In

11.24.4.51 KIM_SPECIES_NAME_Ir

`KIM_SpeciesName` const KIM_SPECIES_NAME_Ir

11.24.4.52 KIM_SPECIES_NAME_K

`KIM_SpeciesName` const KIM_SPECIES_NAME_K

11.24.4.53 KIM_SPECIES_NAME_Kr

`KIM_SpeciesName` const KIM_SPECIES_NAME_Kr

11.24.4.54 KIM_SPECIES_NAME_La

`KIM_SpeciesName` const KIM_SPECIES_NAME_La

11.24.4.55 KIM_SPECIES_NAME_Li

`KIM_SpeciesName` const KIM_SPECIES_NAME_Li

11.24.4.56 KIM_SPECIES_NAME_Lr

`KIM_SpeciesName` const KIM_SPECIES_NAME_Lr

11.24.4.57 KIM_SPECIES_NAME_Lu

`KIM_SpeciesName` const KIM_SPECIES_NAME_Lu

11.24.4.58 KIM_SPECIES_NAME_Lv

`KIM_SpeciesName` const KIM_SPECIES_NAME_Lv

11.24.4.59 KIM_SPECIES_NAME_Md

`KIM_SpeciesName` const KIM_SPECIES_NAME_Md

11.24.4.60 KIM_SPECIES_NAME_Mg

`KIM_SpeciesName` const KIM_SPECIES_NAME_Mg

11.24.4.61 KIM_SPECIES_NAME_Mn

`KIM_SpeciesName` const KIM_SPECIES_NAME_Mn

11.24.4.62 KIM_SPECIES_NAME_Mo

`KIM_SpeciesName` const KIM_SPECIES_NAME_Mo

11.24.4.63 KIM_SPECIES_NAME_Mt

`KIM_SpeciesName` const KIM_SPECIES_NAME_Mt

11.24.4.64 KIM_SPECIES_NAME_N

`KIM_SpeciesName` const KIM_SPECIES_NAME_N

11.24.4.65 KIM_SPECIES_NAME_Na

`KIM_SpeciesName` const KIM_SPECIES_NAME_Na

11.24.4.66 KIM_SPECIES_NAME_Nb

`KIM_SpeciesName` const KIM_SPECIES_NAME_Nb

11.24.4.67 KIM_SPECIES_NAME_Nd

`KIM_SpeciesName` const KIM_SPECIES_NAME_Nd

11.24.4.68 KIM_SPECIES_NAME_Ne

`KIM_SpeciesName` const KIM_SPECIES_NAME_Ne

11.24.4.69 KIM_SPECIES_NAME_Ni

`KIM_SpeciesName` const KIM_SPECIES_NAME_Ni

11.24.4.70 KIM_SPECIES_NAME_No

`KIM_SpeciesName` const KIM_SPECIES_NAME_No

11.24.4.71 KIM_SPECIES_NAME_Np

`KIM_SpeciesName` const KIM_SPECIES_NAME_Np

11.24.4.72 KIM_SPECIES_NAME_O

`KIM_SpeciesName` const KIM_SPECIES_NAME_O

11.24.4.73 KIM_SPECIES_NAME_Os

`KIM_SpeciesName` const KIM_SPECIES_NAME_Os

11.24.4.74 KIM_SPECIES_NAME_P

`KIM_SpeciesName` const KIM_SPECIES_NAME_P

11.24.4.75 KIM_SPECIES_NAME_Pa

`KIM_SpeciesName` const KIM_SPECIES_NAME_Pa

11.24.4.76 KIM_SPECIES_NAME_Pb

`KIM_SpeciesName` const KIM_SPECIES_NAME_Pb

11.24.4.77 KIM_SPECIES_NAME_Pd

`KIM_SpeciesName` const KIM_SPECIES_NAME_Pd

11.24.4.78 KIM_SPECIES_NAME_Pm

`KIM_SpeciesName` const KIM_SPECIES_NAME_Pm

11.24.4.79 KIM_SPECIES_NAME_Po

`KIM_SpeciesName` const KIM_SPECIES_NAME_Po

11.24.4.80 KIM_SPECIES_NAME_Pr

`KIM_SpeciesName` const KIM_SPECIES_NAME_Pr

11.24.4.81 KIM_SPECIES_NAME_Pt

`KIM_SpeciesName` const KIM_SPECIES_NAME_Pt

11.24.4.82 KIM_SPECIES_NAME_Pu

`KIM_SpeciesName` const KIM_SPECIES_NAME_Pu

11.24.4.83 KIM_SPECIES_NAME_Ra

`KIM_SpeciesName` const KIM_SPECIES_NAME_Ra

11.24.4.84 KIM_SPECIES_NAME_Rb

`KIM_SpeciesName` const KIM_SPECIES_NAME_Rb

11.24.4.85 KIM_SPECIES_NAME_Re

`KIM_SpeciesName` const KIM_SPECIES_NAME_Re

11.24.4.86 KIM_SPECIES_NAME_Rf

`KIM_SpeciesName` const KIM_SPECIES_NAME_Rf

11.24.4.87 KIM_SPECIES_NAME_Rg

`KIM_SpeciesName` const KIM_SPECIES_NAME_Rg

11.24.4.88 KIM_SPECIES_NAME_Rh

`KIM_SpeciesName` const KIM_SPECIES_NAME_Rh

11.24.4.89 KIM_SPECIES_NAME_Rn

`KIM_SpeciesName` const KIM_SPECIES_NAME_Rn

11.24.4.90 KIM_SPECIES_NAME_Ru

`KIM_SpeciesName` const KIM_SPECIES_NAME_Ru

11.24.4.91 KIM_SPECIES_NAME_S

`KIM_SpeciesName` const KIM_SPECIES_NAME_S

11.24.4.92 KIM_SPECIES_NAME_Sb

`KIM_SpeciesName` const KIM_SPECIES_NAME_Sb

11.24.4.93 KIM_SPECIES_NAME_Sc

`KIM_SpeciesName` const KIM_SPECIES_NAME_Sc

11.24.4.94 KIM_SPECIES_NAME_Se

`KIM_SpeciesName` const KIM_SPECIES_NAME_Se

11.24.4.95 KIM_SPECIES_NAME_Sg

`KIM_SpeciesName` const KIM_SPECIES_NAME_Sg

11.24.4.96 KIM_SPECIES_NAME_Si

`KIM_SpeciesName` const KIM_SPECIES_NAME_Si

11.24.4.97 KIM_SPECIES_NAME_Sm

`KIM_SpeciesName` const KIM_SPECIES_NAME_Sm

11.24.4.98 KIM_SPECIES_NAME_Sn

`KIM_SpeciesName` const KIM_SPECIES_NAME_Sn

11.24.4.99 KIM_SPECIES_NAME_Sr

`KIM_SpeciesName` const KIM_SPECIES_NAME_Sr

11.24.4.100 KIM_SPECIES_NAME-Ta

`KIM_SpeciesName` const KIM_SPECIES_NAME-Ta

11.24.4.101 KIM_SPECIES_NAME_Tb

`KIM_SpeciesName` const KIM_SPECIES_NAME_Tb

11.24.4.102 KIM_SPECIES_NAME_Tc

`KIM_SpeciesName` const KIM_SPECIES_NAME_Tc

11.24.4.103 KIM_SPECIES_NAME_Te

`KIM_SpeciesName` const KIM_SPECIES_NAME_Te

11.24.4.104 KIM_SPECIES_NAME_Th

`KIM_SpeciesName` const KIM_SPECIES_NAME_Th

11.24.4.105 KIM_SPECIES_NAME_Ti

`KIM_SpeciesName` const KIM_SPECIES_NAME_Ti

11.24.4.106 KIM_SPECIES_NAME_Tl

`KIM_SpeciesName` const KIM_SPECIES_NAME_Tl

11.24.4.107 KIM_SPECIES_NAME_Tm

`KIM_SpeciesName` const KIM_SPECIES_NAME_Tm

11.24.4.108 KIM_SPECIES_NAME_U

`KIM_SpeciesName` const KIM_SPECIES_NAME_U

11.24.4.109 KIM_SPECIES_NAME_user01

`KIM_SpeciesName` const KIM_SPECIES_NAME_user01

11.24.4.110 KIM_SPECIES_NAME_user02

`KIM_SpeciesName` const KIM_SPECIES_NAME_user02

11.24.4.111 KIM_SPECIES_NAME_user03

`KIM_SpeciesName` const KIM_SPECIES_NAME_user03

11.24.4.112 KIM_SPECIES_NAME_user04

`KIM_SpeciesName` const KIM_SPECIES_NAME_user04

11.24.4.113 KIM_SPECIES_NAME_user05

`KIM_SpeciesName` const KIM_SPECIES_NAME_user05

11.24.4.114 KIM_SPECIES_NAME_user06

`KIM_SpeciesName` const KIM_SPECIES_NAME_user06

11.24.4.115 KIM_SPECIES_NAME_user07

`KIM_SpeciesName` const KIM_SPECIES_NAME_user07

11.24.4.116 KIM_SPECIES_NAME_user08

`KIM_SpeciesName` const KIM_SPECIES_NAME_user08

11.24.4.117 KIM_SPECIES_NAME_user09

`KIM_SpeciesName` const KIM_SPECIES_NAME_user09

11.24.4.118 KIM_SPECIES_NAME_user10

`KIM_SpeciesName` const KIM_SPECIES_NAME_user10

11.24.4.119 KIM_SPECIES_NAME_user11

`KIM_SpeciesName` const KIM_SPECIES_NAME_user11

11.24.4.120 KIM_SPECIES_NAME_user12

`KIM_SpeciesName` const KIM_SPECIES_NAME_user12

11.24.4.121 KIM_SPECIES_NAME_user13

`KIM_SpeciesName` const KIM_SPECIES_NAME_user13

11.24.4.122 KIM_SPECIES_NAME_user14

`KIM_SpeciesName` const KIM_SPECIES_NAME_user14

11.24.4.123 KIM_SPECIES_NAME_user15

`KIM_SpeciesName` const KIM_SPECIES_NAME_user15

11.24.4.124 KIM_SPECIES_NAME_user16

`KIM_SpeciesName` const KIM_SPECIES_NAME_user16

11.24.4.125 KIM_SPECIES_NAME_user17

`KIM_SpeciesName` const KIM_SPECIES_NAME_user17

11.24.4.126 KIM_SPECIES_NAME_user18

`KIM_SpeciesName` const KIM_SPECIES_NAME_user18

11.24.4.127 KIM_SPECIES_NAME_user19

`KIM_SpeciesName` const KIM_SPECIES_NAME_user19

11.24.4.128 KIM_SPECIES_NAME_user20

`KIM_SpeciesName` const KIM_SPECIES_NAME_user20

11.24.4.129 KIM_SPECIES_NAME_Uuo

`KIM_SpeciesName` const KIM_SPECIES_NAME_Uuo

11.24.4.130 KIM_SPECIES_NAME_Uup

`KIM_SpeciesName` const KIM_SPECIES_NAME_Uup

11.24.4.131 KIM_SPECIES_NAME_Uus

`KIM_SpeciesName` const KIM_SPECIES_NAME_Uus

11.24.4.132 KIM_SPECIES_NAME_Uut

`KIM_SpeciesName` const KIM_SPECIES_NAME_Uut

11.24.4.133 KIM_SPECIES_NAME_V

`KIM_SpeciesName` const KIM_SPECIES_NAME_V

11.24.4.134 KIM_SPECIES_NAME_W

`KIM_SpeciesName` const KIM_SPECIES_NAME_W

11.24.4.135 KIM_SPECIES_NAME_Xe

`KIM_SpeciesName` const KIM_SPECIES_NAME_Xe

11.24.4.136 KIM_SPECIES_NAME_Y

`KIM_SpeciesName` const KIM_SPECIES_NAME_Y

11.24.4.137 KIM_SPECIES_NAME_Yb

`KIM_SpeciesName` const KIM_SPECIES_NAME_Yb

11.24.4.138 KIM_SPECIES_NAME_Zn

`KIM_SpeciesName` const KIM_SPECIES_NAME_Zn

11.24.4.139 KIM_SPECIES_NAME_Zr

`KIM_SpeciesName` const KIM_SPECIES_NAME_Zr

11.25 kim-api-v2.0.0-alpha.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_SupportStatusFromString` (char const *const str)
- int `KIM_SupportStatusEqual` (`KIM_SupportStatus` const left, `KIM_SupportStatus` const right)
- int `KIM_SupportStatusNotEqual` (`KIM_SupportStatus` const left, `KIM_SupportStatus` const right)
- char const *const `KIM_SupportStatusString` (`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`

11.25.1 Macro Definition Documentation

11.25.1.1 KIM_SUPPORT_STATUS_DEFINED_

```
#define KIM_SUPPORT_STATUS_DEFINED_
```

Definition at line 44 of file `KIM_SupportStatus.h`.

11.25.2 Typedef Documentation

11.25.2.1 KIM_SupportStatus

```
typedef struct KIM_SupportStatus KIM_SupportStatus
```

Definition at line 45 of file `KIM_SupportStatus.h`.

11.25.3 Function Documentation

11.25.3.1 KIM_SupportStatusEqual()

```
int KIM_SupportStatusEqual (
    KIM_SupportStatus const left,
    KIM_SupportStatus const right )
```

11.25.3.2 KIM_SupportStatusFromString()

```
KIM_SupportStatus KIM_SupportStatusFromString (
    char const *const str )
```


11.25.3.3 KIM_SupportStatusNotEqual()

```
int KIM_SupportStatusNotEqual (
    KIM_SupportStatus const left,
    KIM_SupportStatus const right )
```

11.25.3.4 KIM_SupportStatusString()

```
char const* const KIM_SupportStatusString (
    KIM_SupportStatus const supportStatus )
```

11.25.4 Variable Documentation

11.25.4.1 KIM_SUPPORT_STATUS_notSupported

```
KIM_SupportStatus const KIM_SUPPORT_STATUS_notSupported
```

11.25.4.2 KIM_SUPPORT_STATUS_optional

```
KIM_SupportStatus const KIM_SUPPORT_STATUS_optional
```

11.25.4.3 KIM_SUPPORT_STATUS_required

```
KIM_SupportStatus const KIM_SUPPORT_STATUS_required
```

11.25.4.4 KIM_SUPPORT_STATUS_requiredByAPI

```
KIM_SupportStatus const KIM_SUPPORT_STATUS_requiredByAPI
```

11.26 kim-api-v2.0.0-alpha.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_TemperatureUnitFromString` (char const *const str)
- `int KIM_TemperatureUnitEqual` (KIM_TemperatureUnit const left, KIM_TemperatureUnit const right)
- `int KIM_TemperatureUnitNotEqual` (KIM_TemperatureUnit const left, KIM_TemperatureUnit const right)
- `char const *const KIM_TemperatureUnitString` (KIM_TemperatureUnit const temperatureUnit)

Variables

- `KIM_TemperatureUnit` const `KIM_TEMPERATURE_UNIT_unused`
- `KIM_TemperatureUnit` const `KIM_TEMPERATURE_UNIT_K`

11.26.1 Macro Definition Documentation

11.26.1.1 KIM_TEMPERATURE_UNIT_DEFINED_

```
#define KIM_TEMPERATURE_UNIT_DEFINED_
```

Definition at line 44 of file KIM_TemperatureUnit.h.

11.26.2 Typedef Documentation

11.26.2.1 KIM_TemperatureUnit

```
typedef struct KIM_TemperatureUnit KIM_TemperatureUnit
```

Definition at line 45 of file KIM_TemperatureUnit.h.

11.26.3 Function Documentation

11.26.3.1 KIM_TemperatureUnitEqual()

```
int KIM_TemperatureUnitEqual (
    KIM_TemperatureUnit const left,
    KIM_TemperatureUnit const right )
```

11.26.3.2 KIM_TemperatureUnitFromString()

```
KIM_TemperatureUnit KIM_TemperatureUnitFromString (
    char const *const str )
```

11.26.3.3 KIM_TemperatureUnitNotEqual()

```
int KIM_TemperatureUnitNotEqual (
    KIM_TemperatureUnit const left,
    KIM_TemperatureUnit const right )
```

11.26.3.4 KIM_TemperatureUnitString()

```
char const* const KIM_TemperatureUnitString (
    KIM_TemperatureUnit const temperatureUnit )
```

11.26.4 Variable Documentation

11.26.4.1 KIM_TEMPERATURE_UNIT_K

```
KIM_TemperatureUnit const KIM_TEMPERATURE_UNIT_K
```

11.26.4.2 KIM_TEMPERATURE_UNIT_unused

```
KIM_TemperatureUnit const KIM_TEMPERATURE_UNIT_unused
```

11.27 kim-api-v2.0.0-alpha.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_TimeUnitFromString` (char const *const str)
- `int KIM_TimeUnitEqual` (KIM_TimeUnit const left, KIM_TimeUnit right)
- `int KIM_TimeUnitNotEqual` (KIM_TimeUnit const left, KIM_TimeUnit right)
- `char const *const KIM_TimeUnitString` (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`

11.27.1 Macro Definition Documentation

11.27.1.1 KIM_TIME_UNIT_DEFINED_

```
#define KIM_TIME_UNIT_DEFINED_
```

Definition at line 44 of file KIM_TimeUnit.h.

11.27.2 Typedef Documentation

11.27.2.1 KIM_TimeUnit

```
typedef struct KIM_TimeUnit KIM_TimeUnit
```

Definition at line 45 of file KIM_TimeUnit.h.

11.27.3 Function Documentation

11.27.3.1 KIM_TimeUnitEqual()

```
int KIM_TimeUnitEqual (
    KIM_TimeUnit const left,
    KIM_TimeUnit right )
```

11.27.3.2 KIM_TimeUnitFromString()

```
KIM_TimeUnit KIM_TimeUnitFromString (
    char const *const str )
```

11.27.3.3 KIM_TimeUnitNotEqual()

```
int KIM_TimeUnitNotEqual (
    KIM_TimeUnit const left,
    KIM_TimeUnit right )
```

11.27.3.4 KIM_TimeUnitString()

```
char const* const KIM_TimeUnitString (
    KIM_TimeUnit const timeUnit )
```

11.27.4 Variable Documentation

11.27.4.1 KIM_TIME_UNIT_fs

```
KIM_TimeUnit const KIM_TIME_UNIT_fs
```

11.27.4.2 KIM_TIME_UNIT_ns

```
KIM_TimeUnit const KIM_TIME_UNIT_ns
```


11.27.4.3 KIM_TIME_UNIT_ps

```
KIM_TimeUnit const KIM_TIME_UNIT_ps
```

11.27.4.4 KIM_TIME_UNIT_s

```
KIM_TimeUnit const KIM_TIME_UNIT_s
```

11.27.4.5 KIM_TIME_UNIT_unused

```
KIM_TimeUnit const KIM_TIME_UNIT_unused
```

11.28 kim-api-v2.0.0-alpha.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"
```

11.29 kim-api-v2.0.0-alpha.0/cpp/include/KIM_ArgumentName.hpp File Reference

```
#include <string>
```

Classes

- class [KIM::ArgumentName](#)
- struct [KIM::ARGUMENT_NAME::Comparator](#)

Namespaces

- [KIM](#)
- [KIM::ARGUMENT_NAME](#)

Functions

- void [KIM::ARGUMENT_NAME::GetNumberOfArguments](#) (int *const numberOfArguments)
- int [KIM::ARGUMENT_NAME::GetArgumentName](#) (int const index, ArgumentName *const argumentName)
- int [KIM::ARGUMENT_NAME::GetArgumentDataType](#) (ArgumentName const argumentName, DataType *const dataType)

Variables

- ArgumentName const [KIM::ARGUMENT_NAME::numberOfParticles](#)
- ArgumentName const [KIM::ARGUMENT_NAME::particleSpeciesCodes](#)
- ArgumentName const [KIM::ARGUMENT_NAME::particleContributing](#)
- ArgumentName const [KIM::ARGUMENT_NAME::coordinates](#)
- ArgumentName const [KIM::ARGUMENT_NAME::partialEnergy](#)
- ArgumentName const [KIM::ARGUMENT_NAME::partialForces](#)
- ArgumentName const [KIM::ARGUMENT_NAME::partialParticleEnergy](#)
- ArgumentName const [KIM::ARGUMENT_NAME::partialVirial](#)
- ArgumentName const [KIM::ARGUMENT_NAME::partialParticleVirial](#)

11.30 kim-api-v2.0.0-alpha.0/cpp/include/KIM_CallbackName.hpp File Reference

```
#include <string>
```

Classes

- class [KIM::CallbackName](#)
- struct [KIM::CALLBACK_NAME::Comparator](#)

Namespaces

- [KIM](#)
- [KIM::CALLBACK_NAME](#)

Functions

- void [KIM::CALLBACK_NAME::GetNumberOfCallbacks](#) (int *const numberOfCallbacks)
- int [KIM::CALLBACK_NAME::GetCallbackName](#) (int const index, CallbackName *const callbackName)

Variables

- CallbackName const [KIM::CALLBACK_NAME::GetNeighborList](#)
- CallbackName const [KIM::CALLBACK_NAME::ProcessDEDrTerm](#)
- CallbackName const [KIM::CALLBACK_NAME::ProcessD2EDr2Term](#)

11.31 kim-api-v2.0.0-alpha.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](#)

11.32 kim-api-v2.0.0-alpha.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](#)

11.33 kim-api-v2.0.0-alpha.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](#)

11.34 kim-api-v2.0.0-alpha.0/cpp/include/KIM_func.hpp File Reference

Namespaces

- [KIM](#)

Typedefs

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

11.35 kim-api-v2.0.0-alpha.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](#)

11.36 kim-api-v2.0.0-alpha.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](#)

11.37 kim-api-v2.0.0-alpha.0/cpp/include/KIM_Log.hpp File Reference

```
#include <string>
#include <sstream>
```

Classes

- class [KIM::Log](#)

Namespaces

- [KIM](#)

11.38 kim-api-v2.0.0-alpha.0/cpp/include/KIM_LOG_DEFINES.inc File Reference

```
#include "KIM_LOG_MAXIMUM_LEVEL.inc"
```

11.39 kim-api-v2.0.0-alpha.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::GetNumberOfLogVerbosities](#) (int *const numberOfLogVerbosities)
- 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](#)

11.40 kim-api-v2.0.0-alpha.0/cpp/include/KIM_Model.hpp File Reference

```
#include <string>
#include "KIM_func.hpp"
```

Classes

- class [KIM::Model](#)

Namespaces

- [KIM](#)

11.41 kim-api-v2.0.0-alpha.0/cpp/include/KIM_ModelCompute.hpp File Reference

```
#include <string>
```

Classes

- class [KIM::ModelCompute](#)

Namespaces

- [KIM](#)

11.42 kim-api-v2.0.0-alpha.0/cpp/include/KIM_ModelComputeLogMacros.hpp File Reference

Macros

- #define [LOG_FATAL](#)(message)
- #define [LOG_ERROR](#)(message)
- #define [LOG_WARNING](#)(message)
- #define [LOG_INFORMATION](#)(message)
- #define [LOG_DEBUG](#)(message)

11.42.1 Macro Definition Documentation

11.42.1.1 LOG_DEBUG

```
#define LOG_DEBUG(  
    message )
```

Value:

```
modelCompute->LogEntry(KIM::LOG\_VERBOSITY::debug, message, \
    __LINE__, __FILE__)
```

Definition at line 82 of file KIM_ModelComputeLogMacros.hpp.

11.42.1.2 LOG_ERROR

```
#define LOG_ERROR(  
    message )
```

Value:

```
modelCompute->LogEntry(KIM::LOG\_VERBOSITY::error, message, \
    __LINE__, __FILE__)
```

Definition at line 49 of file KIM_ModelComputeLogMacros.hpp.

11.42.1.3 LOG_FATAL

```
#define LOG_FATAL(  
    message )
```

Value:

```
modelCompute->LogEntry (KIM::LOG_VERBOSITY::fatal, message, \br/>    __LINE__, __FILE__)
```

Definition at line 38 of file KIM_ModelComputeLogMacros.hpp.

11.42.1.4 LOG_INFORMATION

```
#define LOG_INFORMATION(  
    message )
```

Value:

```
modelCompute->LogEntry (KIM::LOG_VERBOSITY::information, message, \br/>    __LINE__, __FILE__)
```

Definition at line 71 of file KIM_ModelComputeLogMacros.hpp.

11.42.1.5 LOG_WARNING

```
#define LOG_WARNING(  
    message )
```

Value:

```
modelCompute->LogEntry (KIM::LOG_VERBOSITY::warning, message, \br/>    __LINE__, __FILE__)
```

Definition at line 60 of file KIM_ModelComputeLogMacros.hpp.

11.43 kim-api-v2.0.0-alpha.0/cpp/include/KIM_ModelCreate.hpp File Reference

```
#include <string>  
#include "KIM_func.hpp"
```


Classes

- class [KIM::ModelCreate](#)

Namespaces

- [KIM](#)

11.44 kim-api-v2.0.0-alpha.0/cpp/include/KIM_ModelCreateLogMacros.hpp File Reference

Macros

- #define [LOG_FATAL](#)(message)
- #define [LOG_ERROR](#)(message)
- #define [LOG_WARNING](#)(message)
- #define [LOG_INFORMATION](#)(message)
- #define [LOG_DEBUG](#)(message)

11.44.1 Macro Definition Documentation

11.44.1.1 LOG_DEBUG

```
#define LOG_DEBUG(  
    message )
```

Value:

```
modelCreate->LogEntry (KIM::LOG_VERBOSITY::debug, message, \
    __LINE__, __FILE__)
```

Definition at line 82 of file KIM_ModelCreateLogMacros.hpp.

11.44.1.2 LOG_ERROR

```
#define LOG_ERROR(  
    message )
```

Value:

```
modelCreate->LogEntry (KIM::LOG_VERBOSITY::error, message, \
    __LINE__, __FILE__)
```

Definition at line 49 of file KIM_ModelCreateLogMacros.hpp.

11.44.1.3 LOG_FATAL

```
#define LOG_FATAL(  
    message )
```

Value:

```
modelCreate->LogEntry (KIM::LOG_VERBOSITY::fatal, message, \  
    __LINE__, __FILE__)
```

Definition at line 38 of file KIM_ModelCreateLogMacros.hpp.

11.44.1.4 LOG_INFORMATION

```
#define LOG_INFORMATION(  
    message )
```

Value:

```
modelCreate->LogEntry (KIM::LOG_VERBOSITY::information, message, \  
    __LINE__, __FILE__)
```

Definition at line 71 of file KIM_ModelCreateLogMacros.hpp.

11.44.1.5 LOG_WARNING

```
#define LOG_WARNING(  
    message )
```

Value:

```
modelCreate->LogEntry (KIM::LOG_VERBOSITY::warning, message, \  
    __LINE__, __FILE__)
```

Definition at line 60 of file KIM_ModelCreateLogMacros.hpp.

11.45 kim-api-v2.0.0-alpha.0/cpp/include/KIM_ModelDestroy.hpp File Reference

```
#include <string>
```

Classes

- class [KIM::ModelDestroy](#)

Namespaces

- [KIM](#)

11.46 kim-api-v2.0.0-alpha.0/cpp/include/KIM_ModelDestroyLogMacros.hpp File Reference

Macros

- #define [LOG_FATAL](#)(message)
- #define [LOG_ERROR](#)(message)
- #define [LOG_WARNING](#)(message)
- #define [LOG_INFORMATION](#)(message)
- #define [LOG_DEBUG](#)(message)

11.46.1 Macro Definition Documentation

11.46.1.1 LOG_DEBUG

```
#define LOG_DEBUG(  
    message )
```

Value:

```
modelDestroy->LogEntry(KIM\_LOG\_VERBOSITY\_debug, message, \n    __LINE__, __FILE__)
```

Definition at line 82 of file KIM_ModelDestroyLogMacros.hpp.

11.46.1.2 LOG_ERROR

```
#define LOG_ERROR(  
    message )
```

Value:

```
modelDestroy->LogEntry(KIM\_LOG\_VERBOSITY\_error, message, \n    __LINE__, __FILE__)
```

Definition at line 49 of file KIM_ModelDestroyLogMacros.hpp.

11.46.1.3 LOG_FATAL

```
#define LOG_FATAL(  
    message )
```

Value:

```
modelDestroy->LogEntry(KIM_LOG_VERBOSITY_fatal, message, \br/>    __LINE__, __FILE__)
```

Definition at line 38 of file KIM_ModelDestroyLogMacros.hpp.

11.46.1.4 LOG_INFORMATION

```
#define LOG_INFORMATION(  
    message )
```

Value:

```
modelDestroy->LogEntry(KIM_LOG_VERBOSITY_information, message, \br/>    __LINE__, __FILE__)
```

Definition at line 71 of file KIM_ModelDestroyLogMacros.hpp.

11.46.1.5 LOG_WARNING

```
#define LOG_WARNING(  
    message )
```

Value:

```
modelDestroy->LogEntry(KIM_LOG_VERBOSITY_warning, message, \br/>    __LINE__, __FILE__)
```

Definition at line 60 of file KIM_ModelDestroyLogMacros.hpp.

11.47 kim-api-v2.0.0-alpha.0/cpp/include/KIM_ModelDriverCreate.hpp File Reference

```
#include <string>  
#include "KIM_func.hpp"
```


Classes

- class [KIM::ModelDriverCreate](#)

Namespaces

- [KIM](#)

11.48 kim-api-v2.0.0-alpha.0/cpp/include/KIM_ModelDriverCreateLogMacros.hpp File Reference

Macros

- #define [LOG_FATAL](#)(message)
- #define [LOG_ERROR](#)(message)
- #define [LOG_WARNING](#)(message)
- #define [LOG_INFORMATION](#)(message)
- #define [LOG_DEBUG](#)(message)

11.48.1 Macro Definition Documentation

11.48.1.1 LOG_DEBUG

```
#define LOG_DEBUG(  
    message )
```

Value:

```
modelDriverCreate->LogEntry(KIM::LOG\_VERBOSITY::debug, message, \
    __LINE__, __FILE__)
```

Definition at line 82 of file `KIM_ModelDriverCreateLogMacros.hpp`.

11.48.1.2 LOG_ERROR

```
#define LOG_ERROR(  
    message )
```

Value:

```
modelDriverCreate->LogEntry(KIM::LOG\_VERBOSITY::error, message, \
    __LINE__, __FILE__)
```

Definition at line 49 of file `KIM_ModelDriverCreateLogMacros.hpp`.

11.48.1.3 LOG_FATAL

```
#define LOG_FATAL(  
    message )
```

Value:

```
modelDriverCreate->LogEntry(KIM::LOG\_VERBOSITY::fatal, message, \  
    __LINE__, __FILE__)
```

Definition at line 38 of file KIM_ModelDriverCreateLogMacros.hpp.

11.48.1.4 LOG_INFORMATION

```
#define LOG_INFORMATION(  
    message )
```

Value:

```
modelDriverCreate->LogEntry(KIM::LOG\_VERBOSITY::information, message, \  
    __LINE__, __FILE__)
```

Definition at line 71 of file KIM_ModelDriverCreateLogMacros.hpp.

11.48.1.5 LOG_WARNING

```
#define LOG_WARNING(  
    message )
```

Value:

```
modelDriverCreate->LogEntry(KIM::LOG\_VERBOSITY::warning, message, \  
    __LINE__, __FILE__)
```

Definition at line 60 of file KIM_ModelDriverCreateLogMacros.hpp.

11.49 kim-api-v2.0.0-alpha.0/cpp/include/KIM_ModelRefresh.hpp File Reference

```
#include <string>
```

Classes

- class [KIM::ModelRefresh](#)

Namespaces

- [KIM](#)

11.50 kim-api-v2.0.0-alpha.0/cpp/include/KIM_ModelRefreshLogMacros.hpp File Reference

Macros

- `#define LOG_FATAL(message)`
- `#define LOG_ERROR(message)`
- `#define LOG_WARNING(message)`
- `#define LOG_INFORMATION(message)`
- `#define LOG_DEBUG(message)`

11.50.1 Macro Definition Documentation

11.50.1.1 LOG_DEBUG

```
#define LOG_DEBUG(  
    message )
```

Value:

```
modelRefresh->LogEntry(KIM\_LOG\_VERBOSITY\_debug, message, \n  
    __LINE__, __FILE__)
```

Definition at line 82 of file KIM_ModelRefreshLogMacros.hpp.

11.50.1.2 LOG_ERROR

```
#define LOG_ERROR(  
    message )
```

Value:

```
modelRefresh->LogEntry(KIM\_LOG\_VERBOSITY\_error, message, \n  
    __LINE__, __FILE__)
```

Definition at line 49 of file KIM_ModelRefreshLogMacros.hpp.

11.50.1.3 LOG_FATAL

```
#define LOG_FATAL(  
    message )
```

Value:

```
modelRefresh->LogEntry(KIM_LOG_VERBOSITY_fatal, message, \  
    __LINE__, __FILE__)
```

Definition at line 38 of file KIM_ModelRefreshLogMacros.hpp.

11.50.1.4 LOG_INFORMATION

```
#define LOG_INFORMATION(  
    message )
```

Value:

```
modelRefresh->LogEntry(KIM_LOG_VERBOSITY_information, message, \  
    __LINE__, __FILE__)
```

Definition at line 71 of file KIM_ModelRefreshLogMacros.hpp.

11.50.1.5 LOG_WARNING

```
#define LOG_WARNING(  
    message )
```

Value:

```
modelRefresh->LogEntry(KIM_LOG_VERBOSITY_warning, message, \  
    __LINE__, __FILE__)
```

Definition at line 60 of file KIM_ModelRefreshLogMacros.hpp.

11.51 kim-api-v2.0.0-alpha.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](#)

11.52 kim-api-v2.0.0-alpha.0/cpp/include/KIM_SemVer.hpp File Reference

```
#include <string>
```

Namespaces

- [KIM](#)
- [KIM::SEM_VER](#)

Functions

- void [KIM::SEM_VER::GetSemVer](#) (std::string *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)

11.53 kim-api-v2.0.0-alpha.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::FI](#)
- 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](#)

11.54 kim-api-v2.0.0-alpha.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](#)

11.55 kim-api-v2.0.0-alpha.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](#)

11.56 kim-api-v2.0.0-alpha.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](#)

11.57 kim-api-v2.0.0-alpha.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"
```


11.58 kim-api-v2.0.0-alpha.0/docs/src/features.txt File Reference

11.59 kim-api-v2.0.0-alpha.0/docs/src/implementation.txt File Reference

11.60 kim-api-v2.0.0-alpha.0/docs/src/introduction.txt File Reference

11.61 kim-api-v2.0.0-alpha.0/docs/src/theory.txt File Reference

11.62 kim-api-v2.0.0-alpha.0/docs/src/version2-differences.txt File Reference

11.63 kim-api-v2.0.0-alpha.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_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, 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 [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

11.63.1 Function/Subroutine Documentation

11.63.1.1 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 551 of file ex_model_driver_P_LJ.F90.

11.64 kim-api-v2.0.0-alpha.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_LogVerbosity.h"
#include "KIM_LengthUnit.h"
#include "KIM_EnergyUnit.h"
#include "KIM_ChargeUnit.h"
#include "KIM_TemperatureUnit.h"
#include "KIM_TimeUnit.h"
#include "KIM_LanguageName.h"
#include "KIM_SpeciesName.h"
#include "KIM_SupportStatus.h"
#include "KIM_ArgumentName.h"
#include "KIM_CallbackName.h"
#include "KIM_ModelDriverCreate.h"
#include "KIM_ModelRefresh.h"
#include "KIM_ModelCompute.h"
#include "KIM_ModelDestroy.h"
#include "KIM_ModelComputeLogMacros.h"
#include "KIM_ModelDriverCreateLogMacros.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)
- 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)

11.64.1 Macro Definition Documentation

11.64.1.1 DIM

```
#define DIM 3 /* dimensionality of space */
```

Definition at line 71 of file `ex_model_driver_P_Morse.c`.

11.64.1.2 FALSE

```
#define FALSE 0
```

Definition at line 66 of file `ex_model_driver_P_Morse.c`.

11.64.1.3 SPECCODE

```
#define SPECCODE 1 /* internal species code */
```

Definition at line 72 of file `ex_model_driver_P_Morse.c`.

11.64.1.4 TRUE

```
#define TRUE 1
```

Definition at line 65 of file `ex_model_driver_P_Morse.c`.

11.64.2 Function Documentation11.64.2.1 `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 121 of file `ex_model_driver_P_Morse.c`.

11.64.2.2 `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 148 of file `ex_model_driver_P_Morse.c`.

11.64.2.3 `compute()`

```
static int compute (
    KIM\_ModelCompute const *const modelCompute ) [static]
```

Definition at line 179 of file `ex_model_driver_P_Morse.c`.

11.64.2.4 `destroy()`

```
static int destroy (
    KIM\_ModelDestroy *const modelDestroy ) [static]
```

Definition at line 587 of file `ex_model_driver_P_Morse.c`.

11.64.2.5 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 397 of file ex_model_driver_P_Morse.c.

11.64.2.6 refresh()

```
static int refresh (
    KIM_ModelRefresh *const modelRefresh ) [static]
```

Definition at line 570 of file ex_model_driver_P_Morse.c.

11.65 kim-api-v2.0.0-alpha.0/examples/model_drivers/LennardJones612__MD_414112407348__002/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)

11.65.1 Function Documentation

11.65.1.1 `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.

11.66 kim-api-v2.0.0-alpha.0/examples/model_drivers/LennardJones612__MD_414112407348_002/LennardJones612.hpp File Reference

```
#include "KIM_UnitSystem.hpp"
#include "KIM_ModelDriverCreate.hpp"
#include "KIM_ModelRefresh.hpp"
#include "KIM_ModelDestroy.hpp"
#include "KIM_ModelCompute.hpp"
```

Classes

- class [LennardJones612](#)

Functions

- int `model_driver_create` (KIM::ModelDriverCreate *const modelDriverCreate, KIM::LengthUnit const requestedLengthUnit, KIM::EnergyUnit const requestedEnergyUnit, KIM::ChargeUnit const requested↵ChargeUnit, KIM::TemperatureUnit const requestedTemperatureUnit, KIM::TimeUnit const requestedTime↵Unit)

11.66.1 Function Documentation

11.66.1.1 `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.

11.67 kim-api-v2.0.0-alpha.0/examples/model_drivers/LennardJones612__MD_414112407348__002/LennardJones612Implementation.cpp File Reference

```
#include <cmath>
#include <cstdlib>
#include <cstring>
#include <fstream>
#include <iostream>
#include <map>
#include "LennardJones612Implementation.hpp"
#include "KIM_Numbering.hpp"
#include "KIM_LanguageName.hpp"
#include "KIM_SpeciesName.hpp"
#include "KIM_SupportStatus.hpp"
#include "KIM_ArgumentName.hpp"
#include "KIM_CallbackName.hpp"
#include "KIM_ModelDriverCreateLogMacros.hpp"
#include "LennardJones612ImplementationComputeDispatch.cpp"
#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)

11.67.1 Macro Definition Documentation

11.67.1.1 IGNORE_RESULT

```
#define IGNORE_RESULT(  
    fn ) if(fn){}
```

Definition at line 48 of file LennardJones612Implementation.cpp.

11.67.1.2 MAXLINE

```
#define MAXLINE 1024
```

Definition at line 47 of file LennardJones612Implementation.cpp.

11.67.2 Function Documentation

11.67.2.1 AllocateAndInitialize2DArray()

```
void AllocateAndInitialize2DArray (
    double **& arrayPtr,
    int const extentZero,
    int const extentOne )
```

Definition at line 859 of file LennardJones612Implementation.cpp.

11.67.2.2 Deallocate2DArray()

```
void Deallocate2DArray (
    double **& arrayPtr )
```

Definition at line 880 of file LennardJones612Implementation.cpp.

11.68 kim-api-v2.0.0-alpha.0/examples/model_drivers/LennardJones612__MD_414112407348_002/LennardJones612Implementation.hpp File Reference

```
#include <vector>
#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](#)]

Functions

- void [AllocateAndInitialize2DArray](#) (double **&arrayPtr, int const extentZero, int const extentOne)
- void [Deallocate2DArray](#) (double **&arrayPtr)

11.68.1 Macro Definition Documentation

11.68.1.1 DIMENSION

```
#define DIMENSION 3
```

Definition at line 38 of file LennardJones612Implementation.hpp.

11.68.1.2 HALF

```
#define HALF 0.5
```

Definition at line 40 of file LennardJones612Implementation.hpp.

11.68.1.3 LENNARD_JONES_PHI

```
#define LENNARD_JONES_PHI(  
    exshift )
```

Value:

```
phi = r6iv * (constFourEpsSig12_2D[iSpecies][jSpecies]*r6iv -  
             constFourEpsSig6_2D[iSpecies][jSpecies]) exshift; \
```

Definition at line 237 of file LennardJones612Implementation.hpp.

11.68.1.4 MAX_PARAMETER_FILES

```
#define MAX_PARAMETER_FILES 1
```

Definition at line 42 of file LennardJones612Implementation.hpp.

11.68.1.5 ONE

```
#define ONE 1.0
```

Definition at line 39 of file LennardJones612Implementation.hpp.

11.68.1.6 PARAM_CUTOFFS_INDEX

```
#define PARAM_CUTOFFS_INDEX 1
```

Definition at line 45 of file LennardJones612Implementation.hpp.

11.68.1.7 PARAM_EPSILONS_INDEX

```
#define PARAM_EPSILONS_INDEX 2
```

Definition at line 46 of file LennardJones612Implementation.hpp.

11.68.1.8 PARAM_SHIFT_INDEX

```
#define PARAM_SHIFT_INDEX 0
```

Definition at line 44 of file LennardJones612Implementation.hpp.

11.68.1.9 PARAM_SIGMAS_INDEX

```
#define PARAM_SIGMAS_INDEX 3
```

Definition at line 47 of file LennardJones612Implementation.hpp.

11.68.2 Typedef Documentation

11.68.2.1 GetNeighborFunction

```
typedef int() GetNeighborFunction(void const *const, int const, int *const, int const **const)
```

Definition at line 57 of file LennardJones612Implementation.hpp.

11.68.2.2 VectorOfSizeDIM

```
typedef double VectorOfSizeDIM[DIMENSION]
```

Definition at line 60 of file LennardJones612Implementation.hpp.

11.68.3 Function Documentation

11.68.3.1 AllocateAndInitialize2DArray()

```
void AllocateAndInitialize2DArray (
    double **& arrayPtr,
    int const extentZero,
    int const extentOne )
```

Definition at line 859 of file LennardJones612Implementation.cpp.

11.68.3.2 Deallocate2DArray()

```
void Deallocate2DArray (
    double **& arrayPtr )
```

Definition at line 880 of file LennardJones612Implementation.cpp.

11.69 kim-api-v2.0.0-alpha.0/examples/models/ex_model_Ar_P_LJ/ex_model_Ar_P_LJ.params File Reference

11.70 kim-api-v2.0.0-alpha.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_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, 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 [model_create_routine](#) (model_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_ar_p_mlj_f03::speccode](#) = 1
- real(c_double), parameter, public [ex_model_ar_p_mlj_f03::model_cutoff](#) = 8.15_cd

11.70.1 Function/Subroutine Documentation

11.70.1.1 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 427 of file `ex_model_Ar_P_MLJ_F03.F03`.

11.71 kim-api-v2.0.0-alpha.0/examples/models/ex_model_Ar_P_Morse/ex_model_Ar_P_Morse.params File Reference

11.72 kim-api-v2.0.0-alpha.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_Numbering.h"
#include "KIM_LanguageName.h"
#include "KIM_SpeciesName.h"
#include "KIM_SupportStatus.h"
#include "KIM_ArgumentName.h"
#include "KIM_CallbackName.h"
#include "KIM_LogVerbosity.h"
#include "KIM_UnitSystem.h"
#include "KIM_ModelCreate.h"
#include "KIM_ModelRefresh.h"
#include "KIM_ModelCompute.h"
#include "KIM_ModelDestroy.h"
#include "KIM_ModelComputeLogMacros.h"
#include "KIM_ModelCreateLogMacros.h"
#include "KIM_ModelRefreshLogMacros.h"
#include "KIM_ModelDestroyLogMacros.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 */

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)
- 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)

11.72.1 Macro Definition Documentation

11.72.1.1 CUTOFF

```
#define CUTOFF 8.15 /* Angstroms */
```

Definition at line 70 of file ex_model_Ar_P_Morse_07C.c.

11.72.1.2 DIM

```
#define DIM 3 /* dimensionality of space */
```

Definition at line 68 of file ex_model_Ar_P_Morse_07C.c.

11.72.1.3 EPSILON

```
#define EPSILON -0.0134783698072604 /* eV */
```

Definition at line 71 of file ex_model_Ar_P_Morse_07C.c.

11.72.1.4 FALSE

```
#define FALSE 0
```

Definition at line 63 of file ex_model_Ar_P_Morse_07C.c.

11.72.1.5 PARAM_C

```
#define PARAM_C 1.545 /* 1/Angstroms */
```

Definition at line 72 of file ex_model_Ar_P_Morse_07C.c.

11.72.1.6 RZERO

```
#define RZERO 3.786 /* Angstroms */
```

Definition at line 73 of file `ex_model_Ar_P_Morse_07C.c`.

11.72.1.7 SPECCODE

```
#define SPECCODE 1 /* internal species code */
```

Definition at line 69 of file `ex_model_Ar_P_Morse_07C.c`.

11.72.1.8 TRUE

```
#define TRUE 1
```

Definition at line 62 of file `ex_model_Ar_P_Morse_07C.c`.

11.72.2 Function Documentation

11.72.2.1 `calc_phi()`

```
static void calc_phi (  
    double * epsilon,  
    double * C,  
    double * Rzero,  
    double * shift,  
    double * cutoff,  
    double r,  
    double * phi ) [static]
```

Definition at line 110 of file `ex_model_Ar_P_Morse_07C.c`.

11.72.2.2 `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 155 of file `ex_model_Ar_P_Morse_07C.c`.

11.72.2.3 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 131 of file ex_model_Ar_P_Morse_07C.c.

11.72.2.4 compute()

```
static int compute (
    KIM_ModelCompute const *const modelCompute ) [static]
```

Definition at line 182 of file ex_model_Ar_P_Morse_07C.c.

11.72.2.5 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 )
```

Definition at line 423 of file ex_model_Ar_P_Morse_07C.c.

11.72.2.6 model_destroy()

```
int model_destroy (
    KIM_ModelDestroy *const modelDestroy ) [static]
```

Definition at line 540 of file ex_model_Ar_P_Morse_07C.c.

11.72.2.7 model_refresh()

```
static int model_refresh (
    KIM_ModelRefresh *const modelRefresh ) [static]
```

Definition at line 519 of file ex_model_Ar_P_Morse_07C.c.

11.73 kim-api-v2.0.0-alpha.0/examples/models/LennardJones612_Universal__MO_↔ 826355984548_002/LennardJones612_Universal.params File Reference

11.74 kim-api-v2.0.0-alpha.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_LanguageName.h"
#include "KIM_SpeciesName.h"
#include "KIM_Numbering.h"
#include "KIM_Model.h"
#include "KIM_SupportStatus.h"
#include "KIM_ArgumentName.h"
#include "KIM_CallbackName.h"
#include "KIM_UnitSystem.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 allOrOne, int numberOfParticles, double *coords, double cutoff, NeighList *nl)
- int [get_cluster_neigh](#) (void const *const dataObject, 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](#) ()

11.74.1 Macro Definition Documentation

11.74.1.1 DIM

```
#define DIM 3
```

Definition at line 55 of file `ex_test_Ar_fcc_cluster.c`.

11.74.1.2 FALSE

```
#define FALSE 0
```

Definition at line 50 of file ex_test_Ar_fcc_cluster.c.

11.74.1.3 FCCSPACING

```
#define FCCSPACING 5.260
```

Definition at line 54 of file ex_test_Ar_fcc_cluster.c.

11.74.1.4 MY_ERROR

```
#define MY_ERROR(  
    message )
```

Value:

```
{  
    printf("* Error : \"%s\" %d:%s\n", message,  
        __LINE__, __FILE__);  
    exit(1);  
}
```

\\
\\
\\

Definition at line 62 of file ex_test_Ar_fcc_cluster.c.

11.74.1.5 MY_WARNING

```
#define MY_WARNING(  
    message )
```

Value:

```
{  
    printf("* Error : \"%s\" %d:%s\n", message,  
        __LINE__, __FILE__);  
}
```

\\
\\
\\

Definition at line 69 of file ex_test_Ar_fcc_cluster.c.

11.74.1.6 NAMESTRLEN

```
#define NAMESTRLEN 128
```

Definition at line 52 of file `ex_test_Ar_fcc_cluster.c`.

11.74.1.7 NCELLSPERSIDE

```
#define NCELLSPERSIDE 2
```

Definition at line 56 of file `ex_test_Ar_fcc_cluster.c`.

11.74.1.8 NCLUSTERPARTS

```
#define NCLUSTERPARTS
```

Value:

```
(4*(NCELLSPERSIDE*NCELLSPERSIDE*NCELLSPERSIDE) + \
      6*(NCELLSPERSIDE*NCELLSPERSIDE)           \
      + 3*(NCELLSPERSIDE) + 1)
```

Definition at line 57 of file `ex_test_Ar_fcc_cluster.c`.

11.74.1.9 TRUE

```
#define TRUE 1
```

Definition at line 49 of file `ex_test_Ar_fcc_cluster.c`.

11.74.2 Function Documentation

11.74.2.1 create_FCC_cluster()

```
void create_FCC_cluster (
    double FCCspacing,
    int nCellsPerSide,
    double * coords )
```

Definition at line 324 of file `ex_test_Ar_fcc_cluster.c`.

11.74.2.2 fcc_cluster_neighborlist()

```
void fcc_cluster_neighborlist (
    int allOrOne,
    int numberOfParticles,
    double * coords,
    double cutoff,
    NeighList * nl )
```

Definition at line 442 of file ex_test_Ar_fcc_cluster.c.

11.74.2.3 get_cluster_neigh()

```
int get_cluster_neigh (
    void const *const dataObject,
    int const neighborListIndex,
    int const particleNumber,
    int *const numberOfNeighbors,
    int const **const neighborsOfParticle )
```

Definition at line 485 of file ex_test_Ar_fcc_cluster.c.

11.74.2.4 main()

```
int main ( )
```

Definition at line 99 of file ex_test_Ar_fcc_cluster.c.

11.75 kim-api-v2.0.0-alpha.0/examples/simulators/ex_test_Ar_fcc_cluster_cpp/ex_test_Ar_fcc_cluster_cpp.cpp File Reference

```
#include <stdlib.h>
#include <iostream>
#include <iomanip>
#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 neighborListIndex, int const particleNumber, int *const numberOfNeighbors, int const **const neighborsOfParticle)
- `void create_FCC_cluster` (double FCCspacing, int nCellsPerSide, double *coords)
- `int main` ()

11.75.1 Macro Definition Documentation

11.75.1.1 DIM

```
#define DIM 3
```

Definition at line 53 of file `ex_test_Ar_fcc_cluster_cpp.cpp`.

11.75.1.2 FCCSPACING

```
#define FCCSPACING 5.260
```

Definition at line 52 of file `ex_test_Ar_fcc_cluster_cpp.cpp`.

11.75.1.3 MY_ERROR

```
#define MY_ERROR(  
    message )
```

Value:

```
{  
    std::cout << "* Error : \"" << message << "\" : "  
    << __LINE__ << " : " << __FILE__ << std::endl;  
    exit(1);  
}
```

Definition at line 59 of file `ex_test_Ar_fcc_cluster_cpp.cpp`.

11.75.1.4 MY_WARNING

```
#define MY_WARNING(
    message )
```

Value:

```
{
    std::cout << "* Error : \"" << message << "\" : "
               << __LINE__ << " : " << __FILE__ << std::endl;
}
```

Definition at line 66 of file ex_test_Ar_fcc_cluster_cpp.cpp.

11.75.1.5 NAMESTRLEN

```
#define NAMESTRLEN 128
```

Definition at line 50 of file ex_test_Ar_fcc_cluster_cpp.cpp.

11.75.1.6 NCELLSPERSIDE

```
#define NCELLSPERSIDE 2
```

Definition at line 54 of file ex_test_Ar_fcc_cluster_cpp.cpp.

11.75.1.7 NCLUSTERPARTS

```
#define NCLUSTERPARTS
```

Value:

```
(4*(NCELLSPERSIDE*NCELLSPERSIDE*NCELLSPERSIDE) + \
 6*(NCELLSPERSIDE*NCELLSPERSIDE)
+ 3*(NCELLSPERSIDE) + 1)
```

Definition at line 55 of file ex_test_Ar_fcc_cluster_cpp.cpp.

11.75.2 Function Documentation

11.75.2.1 create_FCC_cluster()

```
void create_FCC_cluster (
    double FCCspacing,
    int nCellsPerSide,
    double * coords )
```

Definition at line 345 of file `ex_test_Ar_fcc_cluster_cpp.cpp`.

11.75.2.2 fcc_cluster_neighborlist()

```
void fcc_cluster_neighborlist (
    int half,
    int numberOfParticles,
    double * coords,
    double cutoff,
    NeighList * nl )
```

Definition at line 463 of file `ex_test_Ar_fcc_cluster_cpp.cpp`.

11.75.2.3 get_cluster_neigh()

```
int get_cluster_neigh (
    void const *const dataObject,
    int const neighborListIndex,
    int const particleNumber,
    int *const numberOfNeighbors,
    int const **const neighborsOfParticle )
```

Definition at line 507 of file `ex_test_Ar_fcc_cluster_cpp.cpp`.

11.75.2.4 main()

```
int main ( )
```

Definition at line 95 of file `ex_test_Ar_fcc_cluster_cpp.cpp`.

11.76 kim-api-v2.0.0-alpha.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](#)

Functions/Subroutines

- subroutine [error::my_error](#) (message, line, file)
- subroutine [error::my_warning](#) (message, line, file)
- subroutine, public [mod_neighborlist::get_neigh](#) (data_object, neighbor_list_index, request, numnei, pnei1part, ierr)
- subroutine [neigh_pure_cluster_neighborlist](#) (half, numberOfParticles, coords, cutoff, neighObject)
- subroutine [create_fcc_configuration](#) (FCCspacing, nCellsPerSide, periodic, coords, MiddlePartId)
- program [ex_test_ar_fcc_cluster](#)

11.76.1 Function/Subroutine Documentation

11.76.1.1 [create_fcc_configuration\(\)](#)

```
subroutine 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 202 of file `ex_test_Ar_fcc_cluster_fortran.F90`.

11.76.1.2 [ex_test_ar_fcc_cluster\(\)](#)

```
program ex_test_ar_fcc_cluster ( )
```

Definition at line 314 of file `ex_test_Ar_fcc_cluster_fortran.F90`.

11.76.1.3 [neigh_pure_cluster_neighborlist\(\)](#)

```
subroutine 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 141 of file `ex_test_Ar_fcc_cluster_fortran.F90`.

11.77 kim-api-v2.0.0-alpha.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](#)

Functions/Subroutines

- subroutine [error::my_error](#) (message, line, file)
- subroutine [error::my_warning](#) (message, line, file)
- subroutine, public [mod_neighborlist::get_neigh](#) (data_object, neighbor_list_index, request, numnei, pnei1part, ierr)
- program [vc_forces_numer_deriv](#)
- subroutine [check_model_compatibility](#) (model_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, DIM, N, coords, cutoff, cutpad, energy, do_update_list, coordsave, neighObject, deriv, deriv_err, ierr)
- real(c_double) function [dfridr](#) (h, err)

11.77.1 Function/Subroutine Documentation

11.77.1.1 [check_model_compatibility\(\)](#)

```
subroutine check_model_compatibility (
    type(kim_model_handle_type), intent(in) model_handle,
    logical, intent(out) forces_optional,
    logical, intent(out) model_is_compatible,
    integer(c_int), intent(out) ierr )
```

Definition at line 506 of file `utility_forces_numer_deriv.F03`.

11.77.1.2 compute_numer_deriv()

```

subroutine compute_numer_deriv (
    integer(c_int), intent(in) partnum,
    integer(c_int), intent(in) dir,
    type(kim_model_handle_type), intent(in) model_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 909 of file utility_forces_numer_deriv.F03.

11.77.1.3 create_fcc_configuration()

```

subroutine 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 809 of file utility_forces_numer_deriv.F03.

11.77.1.4 dfridr()

```

real(c_double) function compute_numer_deriv::dfridr (
    real(c_double), intent(inout) h,
    real(c_double), intent(out) err )

```

Definition at line 987 of file utility_forces_numer_deriv.F03.

11.77.1.5 get_model_supported_species()

```

subroutine 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 628 of file utility_forces_numer_deriv.F03.

11.77.1.6 neigh_pure_cluster_neighborlist()

```
subroutine 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 749 of file utility_forces_numer_deriv.F03.

11.77.1.7 update_neighborlist()

```
subroutine 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 674 of file utility_forces_numer_deriv.F03.

11.77.1.8 vc_forces_numer_deriv()

```
program vc_forces_numer_deriv ( )
```

Definition at line 152 of file utility_forces_numer_deriv.F03.

11.78 kim-api-v2.0.0-alpha.0/fortran/include/kim_argument_name_module.f90 File Reference

Modules

- module [kim_argument_name_module](#)

Variables

- type(kim_argument_name_type), public, protected [kim_argument_name_module::kim_argument_name_number_of_particles](#)
- type(kim_argument_name_type), public, protected [kim_argument_name_module::kim_argument_name_particle_species_code](#)
- type(kim_argument_name_type), public, protected [kim_argument_name_module::kim_argument_name_particle_contributing](#)
- type(kim_argument_name_type), public, protected [kim_argument_name_module::kim_argument_name_coordinates](#)
- type(kim_argument_name_type), public, protected [kim_argument_name_module::kim_argument_name_partial_energy](#)
- type(kim_argument_name_type), public, protected [kim_argument_name_module::kim_argument_name_partial_forces](#)
- type(kim_argument_name_type), public, protected [kim_argument_name_module::kim_argument_name_partial_particle_energy](#)
- type(kim_argument_name_type), public, protected [kim_argument_name_module::kim_argument_name_partial_virial](#)
- type(kim_argument_name_type), public, protected [kim_argument_name_module::kim_argument_name_partial_particle_virial](#)

11.79 kim-api-v2.0.0-alpha.0/fortran/include/kim_callback_name_module.f90 File Reference

Modules

- module [kim_callback_name_module](#)

Variables

- type(kim_callback_name_type), public, protected [kim_callback_name_module::kim_callback_name_get_neighbor_list](#)
- type(kim_callback_name_type), public, protected [kim_callback_name_module::kim_callback_name_process_dedr_term](#)
- type(kim_callback_name_type), public, protected [kim_callback_name_module::kim_callback_name_process_d2edr2_term](#)

11.80 kim-api-v2.0.0-alpha.0/fortran/include/kim_charge_unit_module.f90 File Reference

Modules

- module [kim_charge_unit_module](#)

Variables

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

11.81 kim-api-v2.0.0-alpha.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](#)

11.82 kim-api-v2.0.0-alpha.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](#)

11.83 kim-api-v2.0.0-alpha.0/fortran/include/kim_language_name_module.f90 File Reference

Modules

- module [kim_language_name_module](#)

Variables

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