Knowledgebase of Interatomic Models Application Programming Interface
(KIM API)

Valeriu Smirichinski, Ryan S. Elliott and Ellad B. Tadmor
Dept. of Aerospace Engineering and Mechanics, University of Minnesota

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This document describes how KIM **Tests** and **Models** written in different languages work together. A unified interface, tuned for the specific needs of atomistic simulations, is presented. This interface is based on the concept of "descriptor files". A descriptor file specifies all variables and methods required for communication between a particular **Model** and a **Test**. A "KIM API object" is created, based on the descriptor files, that holds all arguments (variable/data and method pointers) needed for **Test**/**Model** interaction. A complete set of KIM API service routines are available for accessing the various pointers in the KIM API object.

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KIM TEAM

PIs
Ellad Tadmor (U. Minnesota)
Ryan Elliott (U. Minnesota)
James Sethna (Cornell)

Developers
Valeriu Smirichinski (U. Minnesota)
Daniel Karls (U. Minnesota)
Mihir Khadilkar (Cornell)
Alex Alemi (Cornell)
John Crow (Silicon Life Sciences)
Trevor Wenblom (Silicon Life Sciences)

Advisory Board
Graeme Ackland (U. Edinburgh)
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Ioana Cozmuta (NASA)
Karsten Jacobsen (Tech. U. Den.)
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John Moriarty (LLNL)
Sadasivan Shankar (Intel)
Adri van Duin (Penn State)
Gabriel Wainer (Carleton)

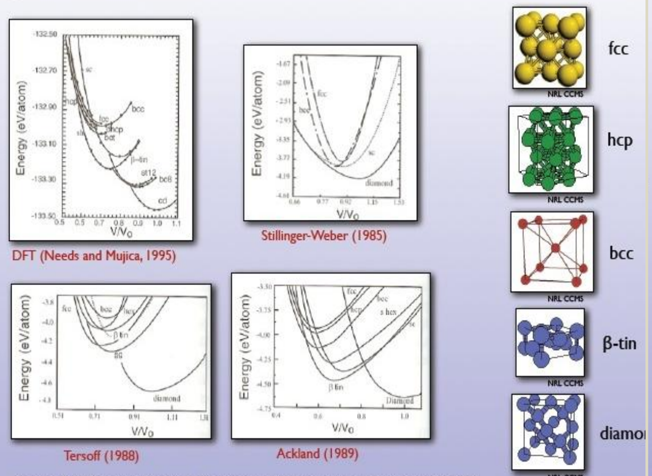
Molecular/atomistic simulations: tests and models

Tests

Test :a specific computer program which, when coupled with a suitable Model, calculates and returns a specific Prediction about a particular Configuration (or sequence of Configurations for dynamical properties).

Example of a Molecular Simulation

Transferability: Silicon bulk phases



Source: R. Phillips, *Crystals, Defect, Microstructure: Modeling across scales*, Cambridge 2001.

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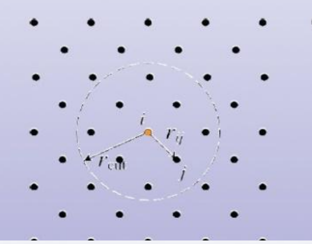
Models

Model : Computer implementation representing a specific interaction between atoms, e.g. an interatomic potential or force field

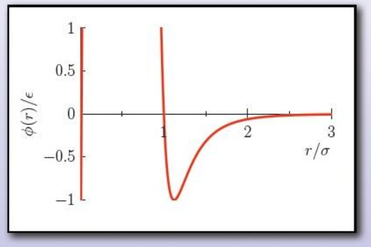
Total energy: $E_{\text{tot}} = \sum_i E_i(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N)$



energy of atom i $\quad E_i = \frac{1}{2}\sum_{\substack{j \\ j \neq i}} \phi(r_{ij})$

distance between atoms i and j $\quad r_{ij} = \|\boldsymbol{x}_j - \boldsymbol{x}_i\|$

The Lennard-Jones potential is a simple pair potential, which described the interaction between two uncharged atoms:



$$\phi(r) = 4\epsilon\left[\underbrace{\left(\frac{\sigma}{r}\right)^{12}}_{\text{repulsion due to overlapping electrons (Pauli principle)}} - \underbrace{\left(\frac{\sigma}{r}\right)^{6}}_{\text{van der Waals attraction between transient dipoles}}\right]$$

- Two fitting paramters (σ, ε)
- Designed for the nobles gasses (Ne, Ar, Kr, Xe).

Source: openkim.org

Types of molecular modelers

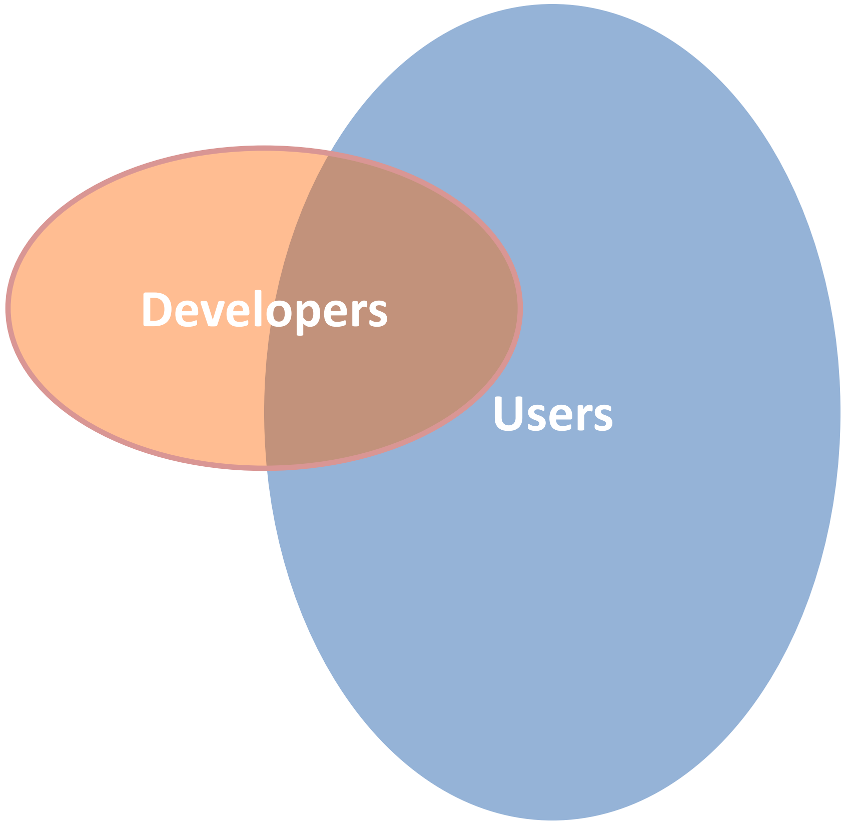
Very broadly speaking there are two types of *molecular modelers*:

Developers

- Create new models
- Study materials physics and applications
- Create new knowledge

Users

- Use models to study materials problems of scientific/technological importance
- Build sophisticated simulations to extract meaningful data
- Create new knowledge



Barriers faced by molecular modelers

The difficulties faced by developers and users of interatomic models include:

1. No easy access to an extensive list of reliable *reference data* from experiments and first principles calculations for fitting.
2. No easy access to implementations of existing models with known *provenance* and *cross-language capability*.
3. No *standardized tests* for evaluating properties of molecular systems.
4. No framework for evaluating the *precision and transferability* of models and therefore no *rigorous guidelines* for choosing an appropriate model for a given application.

Knowledgebase of Interatomic Models (KIM) is proposed to overcome the barriers

The *Knowledgebase of Interatomic Models (KIM)* project is based on a four-year NSF cyber-enabled discovery and innovation (CDI) grant. The KIM project is designed to overcome the barriers mentioned on the previous page. KIM has the following main objectives:

• Development of an *online open resource* for standardized testing and long-term warehousing of interatomic models (potentials and force fields) and data.

• Development of an *application programming interface* (*API*) standard for atomistic simulations, which will allow any interatomic model to work seamlessly with any atomistic simulation code.

• Fostering the development of a quantitative theory *of transferability* of interatomic models to provide guidance for selecting application-appropriate models based on rigorous criteria, and error bounds on results.

• Striving for the permanence of the KIM project, including development of a sustainability plan, and establishment of a long-term home for its content.

More information on KIM is available at the project website: http://openKIM.org

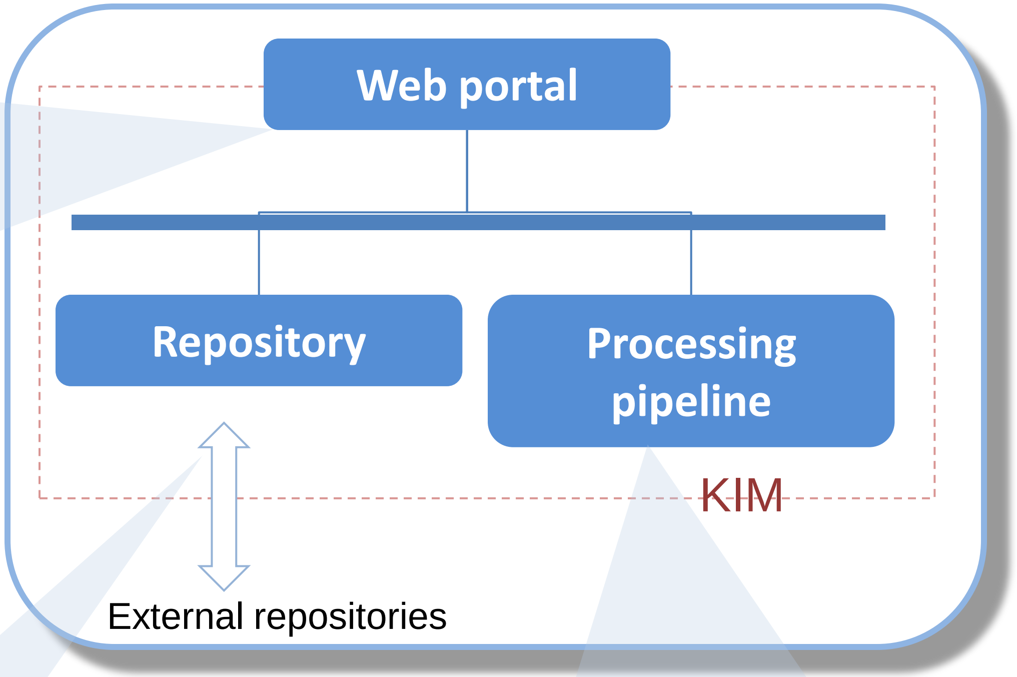
KIM framework

A web interface that will facilitate:

- user upload and download of Tests, Models and Reference Data
- searching and querying the repository
- comparing and visualizing Predictions and Reference Data
- recording user feedback (ranking and discussion forums)

A user-extendible database of

- interatomic Models
- standardized Tests (simulation codes)
- Predictions (results from Model-Test couplings)
- Reference Data (obtained from experiments and first principles calculations)



Processing Pipeline:
An automatic system for generating Predictions due to new Test or Model upload or changes:

- detect viable Test-Model couplings
- assign computational resources based on priority and dependencies
- store results in Repository
- requires an application programming interface (API) to be defined

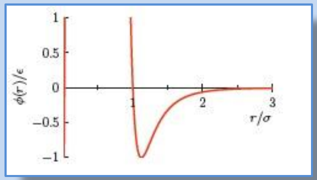
KIM repository: Models

Models | Tests | Predictions | Reference Data | KIM API

Model: Computer implementation representing a specific interaction between atoms, e.g. an interatomic potential or force field.

- Model Format
  - Stand-alone Model (black box)
  - Model Driver (e.g. Lennard-Jones)
    + Parameter Set (e.g. $\varepsilon_{\mathrm{Ar}}$ =10.4 meV, σ_{Ar} =0.34 nm)

$$\phi(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$



Lennard-Jones (pair)	⋮	⋮	**EDIP**
• Ar parameterization	**Stillinger-Weber (3-bdy)**	**CHARMM/AMBER**	**Brenner**
• ...	• Si parameterization	⋮	⋮
⋮	• ...	**EAM/Finnis-Sinclair/glue**	**Bond-order potentials**
Morse (pair)	⋮	⋮	⋮
• Cu parameterization	**MGPT (4-body)**	**MEAM**	**ReaxFF**
• ...	• Mo parameterization	⋮	⋮
⋮	• Ta parameterization	**Tersoff**	**GAP**
Born-Mayer (ionic pair)	• ...	⋮	⋮

• Every model will have a unique KIM ID for referencing in papers.

KIM repository: Tests

Models | **Tests** | Predictions | Reference Data | KIM API

Test: a specific computer program which when coupled with a suitable Model, possible including additional input, calculates and returns a specific Prediction about a particular Configuration (or sequence of Configurations for dynamical properties).

- *Prediction* of a Test will be a logical, scalar, tensor, graph, configuration or field, computed from a *Test-Model coupling*

Scalars	**Tensors**	**Graph**
- lattice constants	- stress	- phonon spectrum
- cohesive energy	- elastic constants	- cohesive energy vs volume
- vacancy formation energy	-...	- energy along transition path
- surface energy		- radial distribution functions
- grain boundary energy	**Configurations**	-...
- vacancy migration barrier	- dislocation core structure	
- dislocation mobility	- surface structure	**Fields**
- peierls stress	- grain boundary structure	- simulated TEM hi-res image
- melting temperature	- nanocluster structure	- gamma surface
-...	-...	-…

- Popular codes (ddcMD, DL_POLY, GROMACS, GULP, iMD, LAMMPS, NAMD, SPaSM, etc.) can be included in a library of tools for writing *Tests.*
- Automatic test generation by linking to external repositories of first principles results.

KIM repository: KIM Data

Models Tests **Predictions Reference Data** KIM API

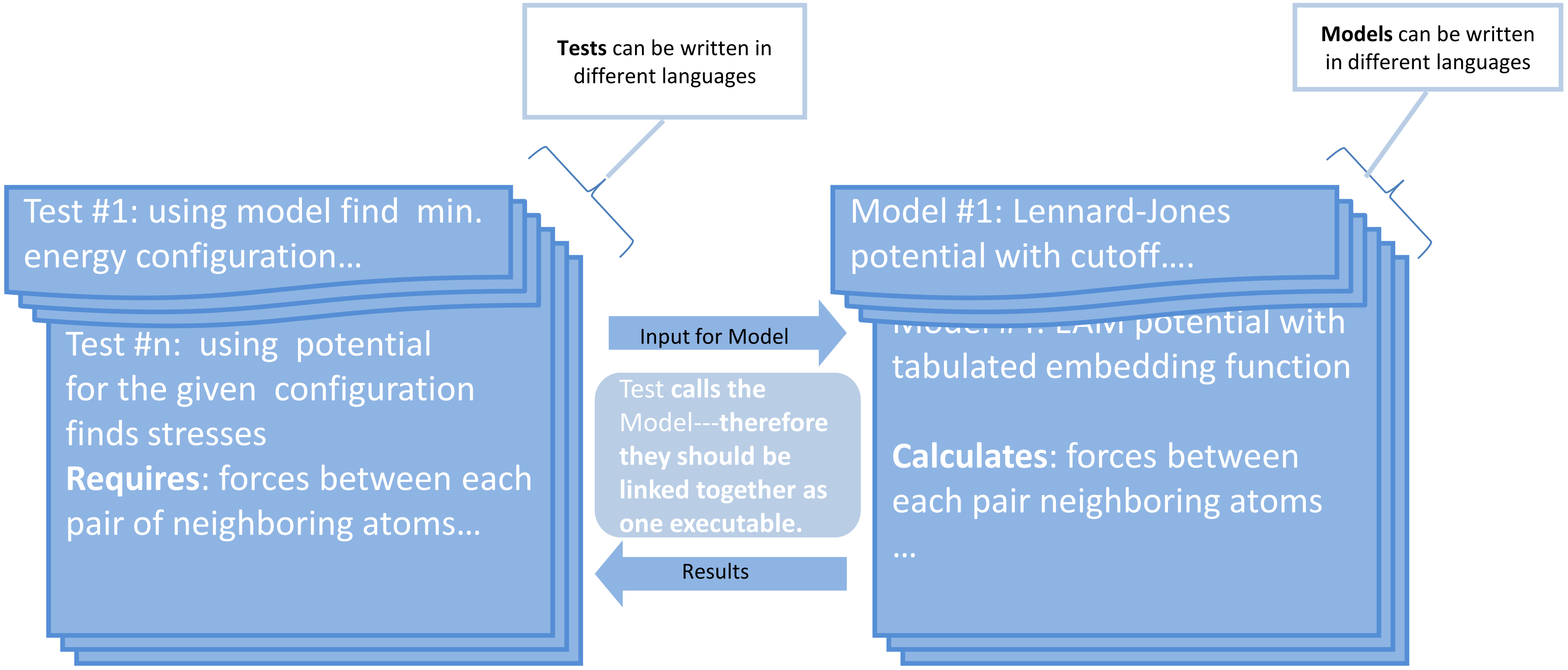
Data in KIM can either be

- a *Prediction* computed from a Test-Model coupling, or
- *Reference Data* computed by first principles or measured experimentally.

- Standardization of Data
  - Identified in terms of a set of "descriptors" drawn from a standardized "dictionary" (similar to that used in the Protein Data Bank project)
  - Descriptors will be automatically generated when possible (for example, the "Space Group" descriptor will be automatically generated for a given crystal structure).
- Data classes
  - *Logical (true/false result for a test, e.g. a given crystal phase is stable)*
  - *Scalar or Tensor (lattice constant, cohesive energy, elastic constants...)*
  - *Graphs (transition pathway energy, phonon spectrum, ...)*
  - *Configurations (relaxed defect core, surface structure, ...)*
  - *Fields (simulated hires TEM image, ...)*
- Quality assurance
  - Acceptance of only "publication quality" data enforced by KIM Editor
  - "Data Provenance"

KIM API concept and implementation

The KIM API facilitates communication between Models and Tests


Tests can be written in different languages
Models can be written in different languages
Test #1: using model find min. energy configuration…
Test #n: using potential for the given configuration finds stresses
Requires: forces between each pair of neighboring atoms…
Input for Model
Test **calls the** Model---**therefore they should be linked together as one executable.**
Results
Model #1: Lennard-Jones potential with cutoff….
Model # 1: EAM potential with tabulated embedding function
Calculates: forces between each pair neighboring atoms
…

Users and developers will be able to download **Tests** and **Models** (from openkim.org) , then compile, link and run the resulting programs to produce new results.

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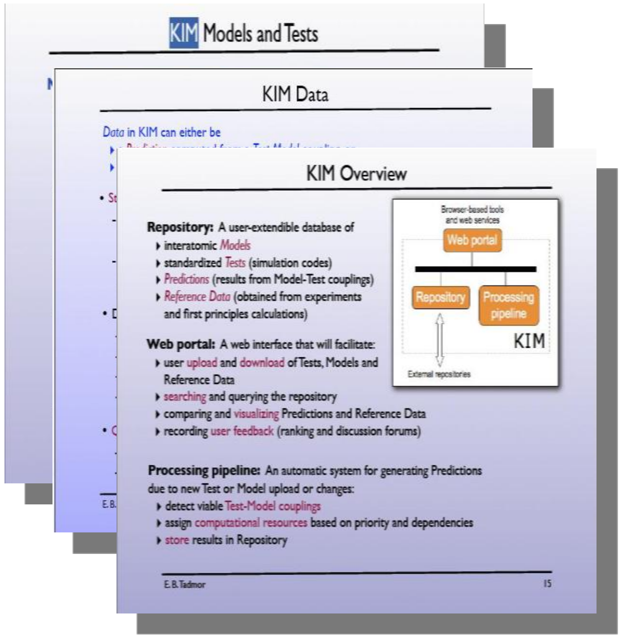
The most challenging technical requirement is the need for multi-language support

openKIM.org framework



KIM Models and Tests

KIM Data

Data in KIM can either be

KIM Overview

Repository: A user-extendible database of
- interatomic *Models*
- standardized *Tests* (simulation codes)
- *Predictions* (results from Model-Test couplings)
- *Reference Data* (obtained from experiments and first principles calculations)

Web portal: A web interface that will facilitate:
- user upload and download of Tests, Models and Reference Data
- searching and querying the repository
- comparing and visualizing Predictions and Reference Data
- recording user feedback (ranking and discussion forums)

Processing pipeline: An automatic system for generating Predictions due to new Test or Model upload or changes:
- detect viable Test-Model couplings
- assign computational resources based on priority and dependencies
- store results in Repository

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Processing pipeline: an automatic system for generating predictions when Tests or Models are uploaded or changed.

Requirements:

- Multilanguage support (C, C++, F77, FORTRAN 90, Python …)
- A variety of data structures need to be accommodated: scalars, multidimensional arrays, variable size arrays, etc..
- Speed & performance are very important
- Standardized API, version tracking, etc…

Processing pipeline: sequence of actions

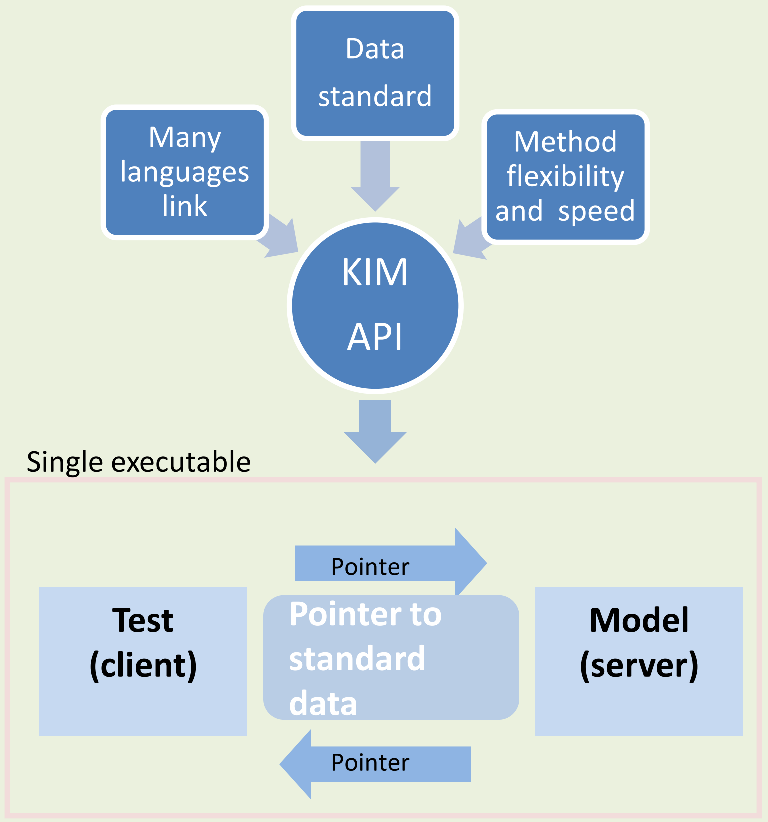
- detect a viable **Model/Test** coupling
- **build (compile and link)** Tests **against** Model
- **run probe-tests**
- assign computational resources
- run full-scale **Test** against **Model**
- analyze results …
- store results in the repository

Need a simple interface : ideally just one argument per call

Source: KIM kickoff presentation

The KIM API is based on exchanging pointers to data and methods

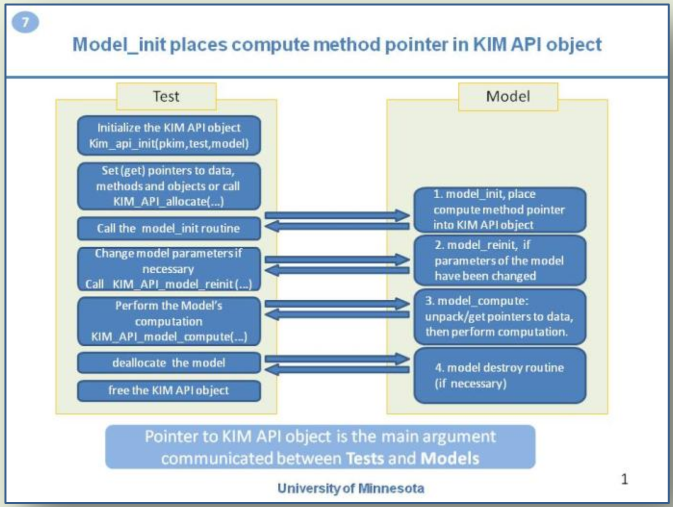
Concept



Data standard should accommodate every possible data set required for the model

Schematic of implementation

1. Data and method pointers are packed in one object. The Interface consists of exchanging one pointer to the KIM API object between a **Test** and a **Model**
2. All languages naturally support pointers:
   - FORTRAN (cray or 2003 standard)
   - C/C++
   - Java
   - Python



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Model_init places compute method pointer in KIM API object

Test

- Initialize the KIM API object Kim_api_init(pkim,test,model)
- Set (get) pointers to data, methods and objects or call KIM_API_allocate(...)
- Call the model_init routine
- Change model parameters if necessary Call KIM_API_model_reinit(...)
- Perform the Model's computation KIM_API_model_compute(...)
- deallocate the model
- free the KIM API object

Model

1. model_init, place compute method pointer into KIM API object
2. model_reinit, if parameters of the model have been changed
3. model_compute: unpack/get pointers to data, then perform computation.
4. model destroy routine (if necessary)

Pointer to KIM API object is the main argument communicated between **Tests** and **Models**

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Using C-style pointers in Fortran

In order to implement the KIM API concept in a cross-language environment, all languages have to work with C-style pointers.

FORTRAN 77 and Fortran 90/95 do not support C-style pointers directly, however essentially all compilers support the `cray pointers' extension which provides this capability. A cray pointer is an integer that can store a memory address. An example below shows the general syntax and usage of a cray pointer in Fortran compared with C.

FORTRAN code

```
…
double precision :: y=10.0d0
double precision :: x
pointer (px,x)
…
px = loc(y)
print*,”x=“,x
…
```

Keyword pointer, followed by two arguments

px - is a pointer (analog double *x in C)
x - is a pointee

As soon as px holds an address, access to that address is done by pointee x

C code

```
…
double y=10.0;

double *x;

x = &y;
printf(“*x=%f \n”, *x);
…
```

How can a Test know what type of input/output data is required by a Model? We have solved this problem by introducing the KIM API descriptor file

ex_model_Ne_P_MLJ_NEIGH_PURE_H.kim

```
#######################################################################################

MODEL_NAME := ex_model_Ne_P_LJ_NEIGH_PURE_H
Unit_Handling     := fixed
...
#######################################################################################
SUPPORTED_ATOM/PARTICLES_TYPES:
# Symbol/name               Type                        code

Ne                          spec                        1
...

MODEL_INPUT:
# Name                       Type         Unit                  Shape                 Requirements

numberOfParticles            integer      none                  []
...
numberParticleTypes          integer      none                  []

particleTypes                integer      none                  [numberOfParticles]

...
```

KIM API descriptor file defines all arguments that the model needs for computation including input and output arguments. Also on the test side, the .kim file defines what the Test can provide as input for the Model and what it expects from the Model as a result.

Tests and Models expose the required input/output arguments that will be communicated using the KIM API

Note: full .kim file shown here can be found in EXAMPLEs/MODELs/ex_model_Ne_P_MLJ_NEIGH_PURE_H/

5

Structure of descriptor file

Model/Test name and system of units lines

```
MODEL_NAME   := ex_model_Ar_P_Morse

Unit_Handling    := flexible
```

Section lines

```
SUPPORTED_ATOM/PARTICLES_TYPES:

CONVENTIONS:

MODEL_INPUT:

MODEL_OUTPUT:

MODEL_PARAMETERS:
```

Data lines

```
* Species Data lines

* Flag Data lines

* Argument Data lines
```

Brief description of Section lines

```
   These lines identify logically distinct sections within
the KIM descriptor file.
   All lines following a Section line, up to the next
Section line or end of the file, will be assigned to the
indicated section.
   These sections may occur in any order within a KIM
descriptor file, however the order given here is
recommended. A section line may only occur once within a KIM
descriptor file.
```

Brief description of Data lines

```
   These lines are used to specify the information that a
Model (Test) will provide to and require from a Test
(Model), as well as the conventions that the Model(Test)
uses.
 * Species Data lines - allow for the definition of atomic
species by providing a symbol and an integer code. These
lines are located in section SUPPORTED_ATOM/PARTICLES_TYPES.
 * Flag Data lines - this line type defines a convention
that can be used to ensure that Models and Tests are able to
work together, and should only be used within the
CONVENTIONS section of the KIM descriptor file.
  * Argument Data lines -  the main KIM descriptor file line
format, used within the MODEL_INPUT, MODEL_OUTPUT, and
MODEL_PARAMETERS sections.
```

5.1

Each argument line in the descriptor file describes an argument and its properties

EXAMPLEs/MODELs/ex_model_Ar_P_MLJ_F90.kim

```
MODEL_NAME := ex_model_Ar_P_MLJ_F90
Unit_Handling     := fixed
….
compute              method     none                   []


MODEL_OUTPUT:
# Name               Type         Unit                  Shape                        Requirements

energy               real*8       energy                []                           optional

force                real*8       force                 [numberOfParticles,3]        optional
```

All characters after a '#' are ignored (a comment field)

Method means a subroutine or function pointer

The name of an argument is its "key word". By using key words, the KIM service routines can pack/unpack data pointers from the KIM API object. Key words are standardized as part of the KIM API.

Type of data in computer representation

Physical dimensions

The shape of an argument describes its array properties. It specifies the number (rank) and size (range or extent) of indices. For example, [] means a scalar (zero-dimensional array), [numberOfParticles] means a one-dimensional array and [numberOfParticles,3] means a two-dimensional array of size numberOfParticles x 3.

The "requirements" field is only used in **Model** descriptor files. An empty field indicates that the argument is required. A value of "optional" indicates that the associated data will be computed only if the argument is in the **Test**'s descriptor file and if the **Test** explicitly requests it.

Note: a detailed description of all Type values and Units can be found in the file DOCs/standard.kim

Specifying particle types – species data lines

EXAMPLEs/MODELs/ex_model_Ar_P_MLJ_F90.kim

```
...
###############################################
SUPPORTED_ATOM/PARTICLES_TYPES:
# Symbol/name               Type                   code

Ar                          spec                      1

###############################################
...
```

Species data lines define the atom/particle types supported by the Test/Model and should only be used within the SUPPORTED_ATOM/PARTICLES_TYPES section of the KIM descriptor file. Each line consists of three white-space separated (case sensitive) strings The three strings are as follows:

code: This is the integer that the Model uses internally to identify the atom/particle type. The value specified by a Test is ignored.

Type: This must be `spec'.

Name: This string gives a unique name to the atom/particle type. This name is checked against the standard list in `standard.kim'.

The **KIM_API_get_partcl_types()** service routine allows one to obtain a list of all particle types used by the model during runtime. Also the **KIM_API_get_partcl_type_code()** service routine allows one to get the particle type integer code (see DOCs/KIM_API_Description.txt).

5.3

In order to define “conventions” of test/model behavior, flag data lines are reserved

EXAMPLEs/MODELs/ex_model_Ar_P_MLJ_F90.kim

```
##############################################
CONVENTIONS:
# Name                       Type


OneBasedLists                    flag

Neigh_IterAccess                 flag

Neigh_LocaAccess                 flag

NEIGH_PURE_H                     flag

NEIGH_PURE_F                     flag

NEIGH_RVEC_F                     flag

...
```

A flag data line defines a convention, that can be used to ensure that **Models** and **Tests** are able to work together, and should only be used within the CONVENTIONS section of the KIM descriptor file. The line consists of two white-space separated (case sensitive) strings. The two strings, in order, are as follows:

Name: This string gives a unique name to the convention. This name is checked against the standard list in `standard.kim‘

Type: This must be `flag'

KIM_API_allocate() has **no effect** on “flag“ type arguments, because they are not “data pointer holders“.

For a detailed description of all flag lines see the file DOCs/standard.kim. Also see the files in DOCs/.

5.4

Parameter arguments are used to publish/access internal parameters of a Model

EXAMPLEs/MODELs/ex_model_Ar_P_MLJ_CLUSTER_F90/ex_model_Ar_P_MLJ_CLUSTER_F90.kim

```
MODEL_PARAMETERS:

# Name                         Type          Unit                 Shape                Requirements

PARAM_FREE_sigma               real*8        length               []

PARAM_FREE_epsilon             real*8        energy               []

PARAM_FREE_cutoff              real*8        length               []
...
```

The format for parameter arguments in a KIM descriptor file is the same as that for argument data types.

```
Two types of model parameters are allowed
 1) PARAM_FIXED_XXXXXX  - these should not be changed by the Test
 2) PARAM_FREE_XXXXXX   - these may be changed by the Test (which must then call the
    Model's reinit() function to inform the model that its parameters have changed)


KIM_API_get_params() service routine will return a list of all parameters in the object during
runtime (as an array of text strings).
KIM_API_get_free_params() service routine will return a list of FREE parameters and
KIM_API_get_fixed_params() will return a list of FIXED parameters (see KIM_API_Description.txt)
```

Names of parameter arguments are not checked against standard.kim

5.5

Specifying units that model can handle: Units Handling and base units

EXAMPLEs/MODELs/ex_model_Ar_P_MLJ_F90/ex_model_Ar_P_MLJ_F90.kim

```
...
#########################################

MODEL_NAME := ex_model_Ar_P_MLJ_F90
Unit_Handling     := fixed

Unit_length       := A
Unit_energy       := eV
Unit_charge       := e
Unit_temperature  := K
Unit_time         := fs

#########################################
...
```

For Models, a variable `Unit_Handling' specifies whether the Model can adjust its input and output to match a Test (`flexible') or can only work with one set of units (`fixed'). This information is ignored for Tests.

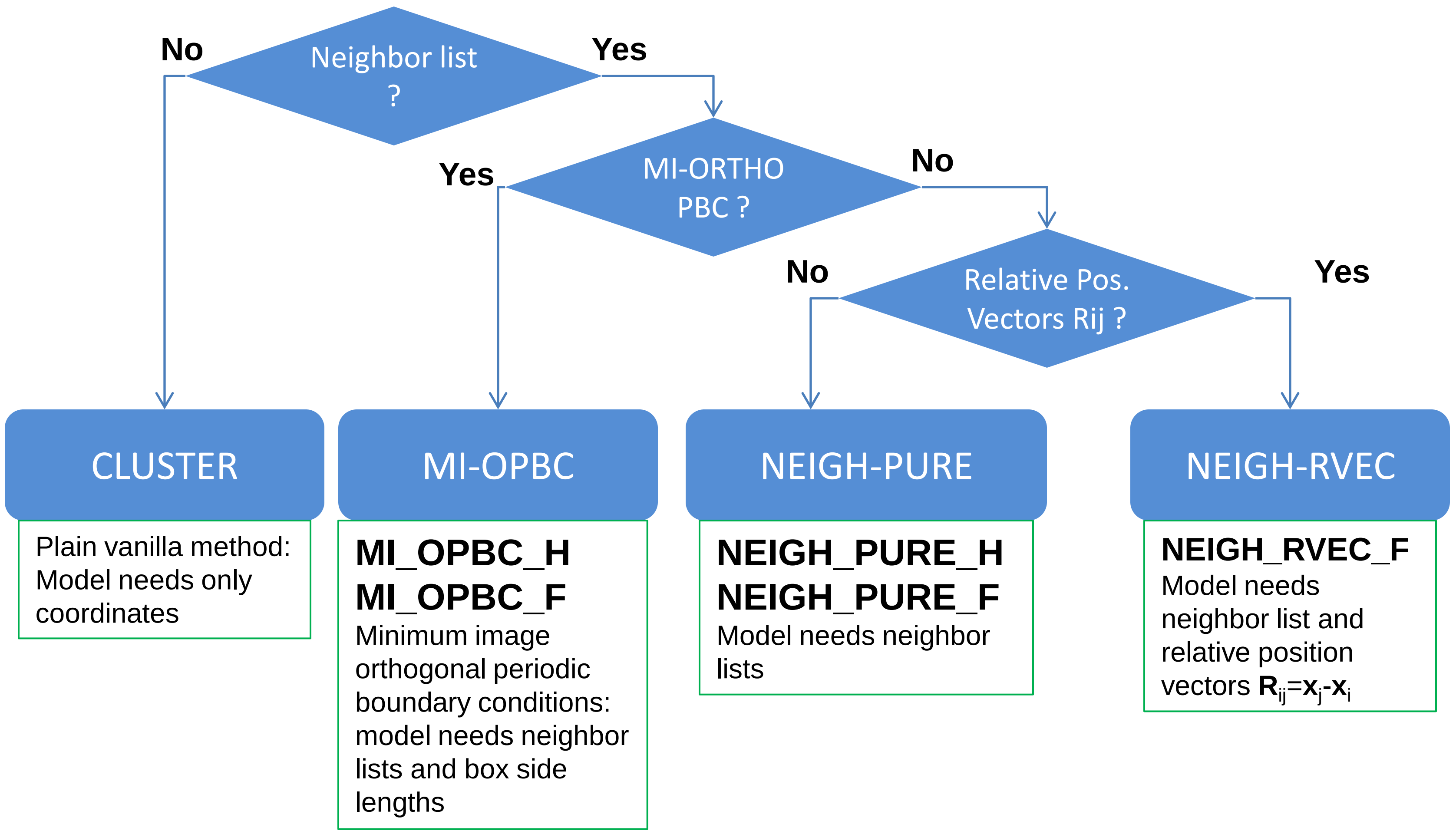
Base unit lines:
Five lines that describe a set of five base units from which all other units are derived in a consistent way:

Unit_length	:= `A' | `Bohr' | `cm' | `m' | `nm'
Unit_energy	:= `amu*A^2/(ps)^2' | `erg' | `eV' | `Hartree' | `J' |`kcal/mol' | kJ/mol'
Unit_charge	:= `C' | `e' | `statC'
Unit_temperature	:= `K'
Unit_time	:= `fs' | `ps' | `ns' | `s'

The list of recognized units above may be extended in the future.

There are several service routines related to units and units handling in KIM API:
KIM_API_get_unit_handling(), KIM_API_convert_to_act_unit(), KIM_API_get_unit_length(), KIM_API_get_unit_energy(), etc...(see DOCs/KIM_API_Description.txt).

Handling of Neighbor lists and Boundary Conditions – NBC methods



Plain vanilla method: Model needs only coordinates

MI_OPBC_H
MI_OPBC_F
Minimum image orthogonal periodic boundary conditions: model needs neighbor lists and box side lengths

NEIGH_PURE_H
NEIGH_PURE_F
Model needs neighbor lists

NEIGH_RVEC_F
Model needs neighbor list and relative position vectors $\mathbf{R}_{ij}=\mathbf{x}_j-\mathbf{x}_i$

Note: NBC stands for Neighbor lists and Boundary Conditions

Descriptions of the NBC methods

CLUSTER:
In the CLUSTER method, the Model receives the number of particles and coordinates without additional information (such as neighbor lists or other boundary condition specifiers) and computes requested quantities under the assumption that the particles form an isolated cluster. For example, if energy and forces are requested, it will compute the total energy of all the particles based on the supplied particle coordinates and the derivative of the total energy with respect to the positions of the particles.

NEIGH_PURE_[F|H]:
In the NEIGH_PURE methods (NEIGH_PURE_H and NEIGH_PURE_F), the Model receives the number of particles, coordinates and a full or half neighbor list. The neighbor list defines the environment of each particle, from which the particles's energy is defined. In the case of a half list, the value of the argument `numberContributingParticles' indicates that the first `numberContributingParticles' contribute their energy to the total and the remaining particles do not contribute to the energy (they are "ghost" particles). When `numberContributingParticles' is equal to `numberParticles' the half list is called "symmetric", otherwise it is called "unsymmetric." In the case of a full list, any particle that has one or more neighbors contributes its energy to the total and those particles with zero neighbors do not contribute to the total energy. The model computes the requested quantities using the supplied information. For example, if energy and forces are requested, it will compute the total energy of all the particles based on their neighbor lists and the derivative of the total energy with respect to the positions of the particles. This method can be used with codes that use ghost particles to apply boundary conditions. The ghost particles are treated as regular particles by the Model, and it is up to the calling code to discard some information such as the forces on the ghost particles and to compute the appropriate total energy from per-particle energies of the physical particles, or to use a modified neighbor list to obtain the desired values.
NEIGH_PURE_H:
This is the Pure Half neighbor list method. The model needs `coordinates', a half neighbor list (with data stored in the `neighObject' argument), the `numberContributingParticles', and the `get_neigh' method supplied by the Test.
NEIGH_PURE_F:
This is the Pure Full neighbor list method. The model needs `coordinates', a full neighbor list (with data stored in the `neighObject' argument), and the `get_neigh' method supplied by the Test.

Descriptions of the NBC methods (2)

NEIGH_RVEC_F:
In the NEIGH_RVEC_F method, the Model receives the number of particles and coordinates, a full neighbor list and the relative position vectors r_ij (r_ij = x_j-x_i). The neighbor list and Rij vectors define the environment of each particle, from which the particles's energy is defined. The Model computes the requested quantities using the supplied information. For example, if energy and forces are requested, it will compute the total energy of all the
# particles based on their neighbor lists and relative position vectors and the derivative of the total energy with respect to the positions of the particles. This method enables the application of general periodic boundary conditions, including multiple images. (This approach can fail with half neighbor lists and therefore the _H variant of the method does not exist.) A possible future extension to this method is to allow the Test to provide a ForceTransformation() function for each neighbor, which would enable the application of complex boundary conditions such as torsion and objective boundary conditions. This is the Relative Vector BoundaryCondition Full neighbor list method. The Model needs `coordinates' and a full neighbor list (with data stored in the `neighObject' argument), and the `get_neigh' method supplied by the Test. The `neighObject' argument must also contain the relative position vectors (RVEC) (which are returned by the `get_neigh' function).

MI_OPBC_[F|H]:
In the MI_OPBC methods (MI_OPBC_H and MI_OPBC_F), the Model receives the number of particles and coordinates, the side lengths for the periodic orthogonal box and a neighbor list. It assumes all particles lie inside the periodic box. Side lengths of the box must be at least twice the cutoff range. This method computes the requested quantities under the assumption that the particles are subjected to the minimum image, orthogonal, periodic boundary conditions.
MI_OPBC_H:
This is the Minimum Image Orthogonal Periodic Boundary Condition Half neighbor list method. The Model needs `coordinates', a half neighbor list (with data stored in the `neighObject' argument), `numberContributingParticles', the`get_neigh' method supplied by theTest, and the `boxSideLengths' argument (which specifies the three side-lengths of the orthogonal simulation box).
MI_OPBC_H:
This is the Minimum Image Orthogonal Periodic Boundary Condition Full neighbor list method. The Model needs `coordinates', a full neighbor list (with data stored in the `neighObject' argument), the `get_neigh' method supplied by the Test, and the `boxSideLengths' argument (which specifies the three side-lengths of the orthogonal simulation box).

Example of using NBC methods in KIM file

EXAMPLEs/MODELs/ex_model_Ne_P_LJ/ ex_model_Ne_P_LJ.kim

```
…
CONVENTIONS:
#  Name                         Type
OneBasedLists                   flag

Neigh_IterAccess                flag

Neigh_LocaAccess                flag

NEIGH_PURE_H                    flag

NEIGH_PURE_F                    flag

NEIGH_RVEC_F                    flag

MI_OPBC_H                       flag

MI_OPBC_F                       flag

CLUSTER                         flag
 .
```

The example in ex_model_Ne_P_LJ.kim
is designed to work with six different NBC methods.

If the Test can also work with multiple NBC methods and there are several matches, the first matched method listed in the Model's KIM file will have precedence.

The KIM_API_init () routine will check that all needed data lines for the chosen method are in the KIM descriptor file.

NBC Methods

Neighbor list access methods: all related lines in the KIM descriptor files

DOCs/standard.kim (only related to Neighbor list access are shown here)

```
…
CONVENTIONS:
#  Name                    Type
…
ZeroBasedLists             flag    # presence of this line indicates that indexes
                                   # for particles are from 0 to numberOfParticles-1 (C-style)
OneBasedLists              flag    # presence of this line indicates that indexes for
                                   # atoms are from 1 to numberOfParticles   (Fortran-style)
Neigh_IterAccess           flag    # works with iterator mode
Neigh_LocaAccess           flag    # works with locator mode
Neigh_BothAccess           flag    # needs both locator and iterator modes

MI_OPBC_H                  flag
MI_OPBC_F                  flag
NEIGH_RVEC_F               flag
NEIGH_PURE_H               flag
NEIGH_PURE_F               flag

MODEL_INPUT:
#  Name                    Type         Unit          Shape        requirements
get_neigh                  method       none          []

neighObject                pointer      none          []

boxSideLengths             real*8       length        [3]
```

neighObject stores completely encapsulated neighbor list object Access to the object is done through method **get_neigh**. The neighbor list object and the method to access it are supplied by the Test.

Interface to get_neigh method

get_neigh function for access to the neighbor list object
here :

```
mode    -   operate in iterator or locator mode
            mode = 0  : iterator mode
            mode = 1  : locator mode

request -  Requested operation
            If mode = 0
               request = 0  : reset iterator
               request = 1  : increment iterator
            If mode = 1
               request = #  : number of the
                              particle whose
                              neighbor list
                              is requested
```

FORTRAN style

```
integer function  get_neigh(pkim,mode,request,particle,numnei,pnei1particle,prij)
     implicit none
     integer(kind=kim_intptr),   intent(in)    :: pkim
     integer,                    intent(in)    :: mode
     integer,                    intent(in)    :: request
     integer,                    intent(out)   :: particle
     integer,                    intent(out)   :: numnei
     integer,                    intent(out)   :: pnei1particle
     integer,                                  :: nei1particle(1);
                                                  pointer(pnei1particle,nei1particle)
     double precision,           intent(out)   :: prij
     double precision,                         :: rij(3,*);     pointer(prij,rij)
end function  get_neigh
```

C style

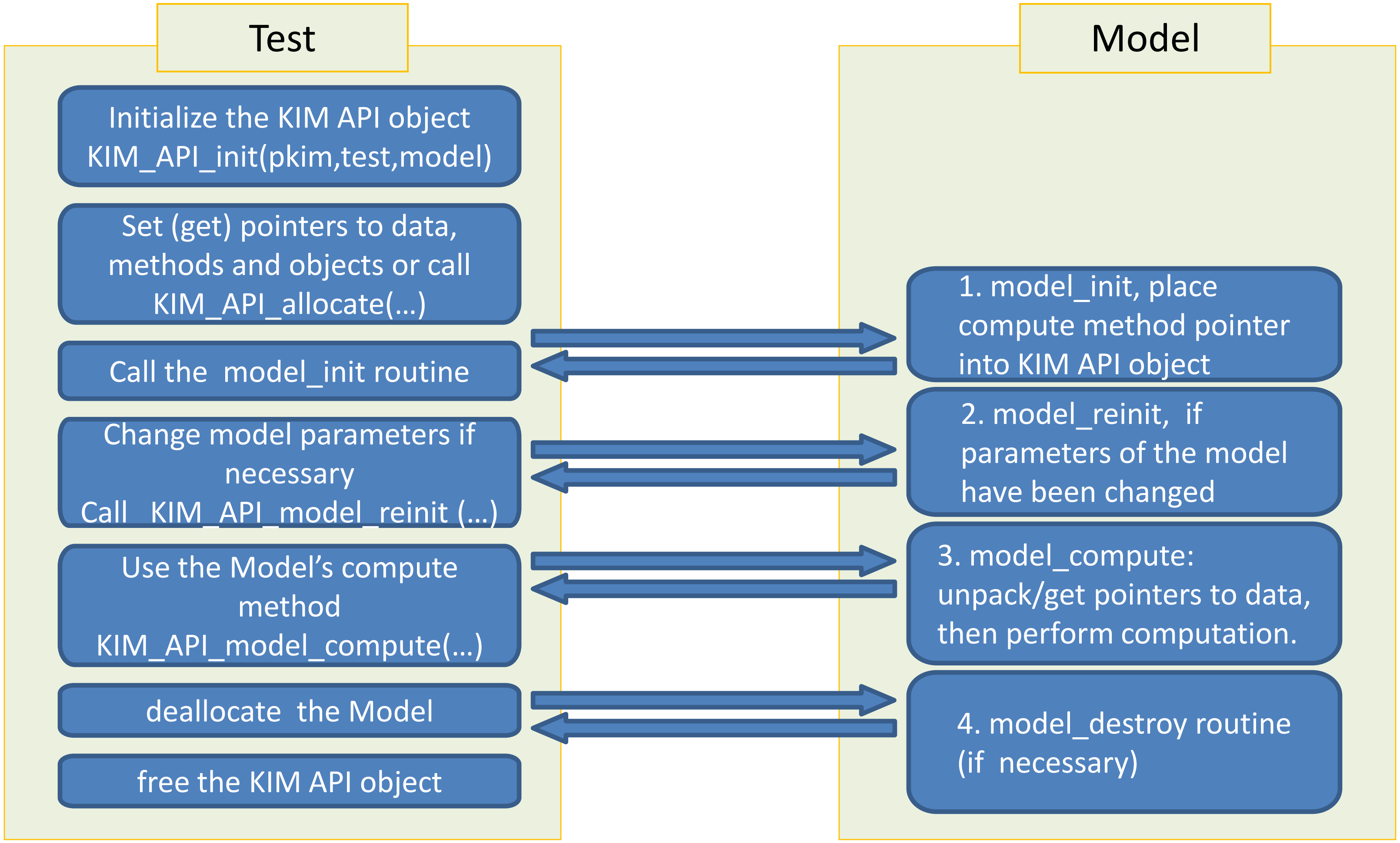
```
int get_neigh(void ** pkim, int * mode, int * request, int * particle,
                    int * numnei, int ** pnei1particle, double ** prij) ;
```

```
particle     - the number of the particle whose neighbor list is returned
numnei       - number of neighbors returned
nei1particle  - integer array of neighbors of an particle which will point
               to the list of neighbors on exit.
rij           - array of relative position vectors of the neighbors of a
                particle (including boundary conditions if applied) if they
                have been computed (NBC scenario NEIGH_RVEC_F
                only).  Has NULL value otherwise (all other NBC
                scenarios).
```

The return value depends on the results of execution.
(see DOCs/KIM_API_Description.txt for details)

Test must supply the get_neigh method and store a pointer to it in the KIM API object

Model_init places compute method pointer in KIM API object


Test
Initialize the KIM API object KIM_API_init(pkim,test,model)
Set (get) pointers to data, methods and objects or call KIM_API_allocate(…)
Call the model_init routine
Change model parameters if necessary Call KIM_API_model_reinit (…)
Use the Model's compute method KIM_API_model_compute(…)
deallocate the Model
free the KIM API object
Model
1. model_init, place compute method pointer into KIM API object
2. model_reinit, if parameters of the model have been changed
3. model_compute: unpack/get pointers to data, then perform computation.
4. model_destroy routine (if necessary)

Pointer to KIM API object is the main argument communicated between **Tests** and **Models**

8

Initialization of KIM API object, setting and getting data-pointers can be done through the KIM service routines

KIM_API/KIM_API_C.h

```
#include <stdint.h>
#ifdef  __cplusplus
extern "C" {
#endif
//global methods

int KIM_API_init(void * kimmdl, char * testname, char *mdlname);

void KIM_API_allocate(void *kimmdl, intptr_t natoms, int ntypes);

void KIM_API_free(void *kimmdl, int * kimerror);

void KIM_API_print(void *kimmdl, int *kimerror);

void KIM_API_model_compute(void * kimmdl,int *kimerror);
…
//element access methods
int  KIM_API_set_data(void *kimmdl,char *nm,  intptr_t size, void *dt);
void * KIM_API_get_data(void *kimmdl,char *nm, int * kimerror);
…
//multiple data set/get methods
//
void KIM_API_setm_data(void *kimmdl, int *error, int numargs, ... );
void KIM_API_getm_data(void *kimmdl, int *error, int numargs, ... );
```

Initialization is done by analyzing test and model descriptor files

One can use optional KIM service routine to allocate standard arguments and data

Call model_compute routine by address stored in KIM API object

Directly place data pointer into the KIM API object

"Multiple" version of set/get data

Description of all KIM API service routines are located in the file: **DOCs/KIM_API_Description.txt**

8.1

Examples of using KIM_API_init and KIM_API_allocate service routines

.../ex_test_Ar_free_cluster_CLUSTER_F90/ex_test_Ar_free_cluster_CLUSTER_F90.F90

```
...
! Initialize the KIM object
  ier = kim_api_init_f(pkim, testname, modelname)
  if (ier.lt.KIM_STATUS_OK) then
     idum = kim_api_report_error_f(__LINE__, __FILE__,
"kim_api_init_f", ier)
     stop
  endif
  ! Allocate memory via the KIM system
  call kim_api_allocate_f(pkim, N, ATypes, ier)
  if (ier.lt.KIM_STATUS_OK) then
     idum = kim_api_report_error_f(__LINE__, __FILE__,
"kim_api_allocate_f", ier)
     stop
  endif
...
```

KIM API init will check the consistency of KIM descriptor file (Test and Model) against standard.kim, after that will check if Test and Model match: NBC methods, particle species (if any) , conventions and argument data lines

If the match is successful, then the KIM API object is created. This object conforms to the Model descriptor KIM file and can store all described data as pointers

.../ex_test_Ar_multiple_models/ex_test_Ar_multiple_models.c

```
...
status = KIM_API_init(&pkim_periodic_model_0, testname,
modelname0);
   if (KIM_STATUS_OK > status)
      KIM_API_report_error(__LINE__,
__FILE__,"KIM_API_init() for MODEL_ZERO for period
...
```

KIM_API_allocate will allocate memory for all arguments with, fully specified shape, stored in the KIM API object

It is not mandatory to use KIM_ API_allocate. A Test can use its own memory and set address of the data in the KIM API object.

Examples of using KIM API getm/setm data
("multiple" version of get/set data)

.../ex_test_Ar_free_cluster_CLUSTER_F90/ex_test_Ar_free_cluster_CLUSTER_F90.F90

```
...
! Unpack data from KIM object
  call kim_api_getm_data_f(pkim, ier, &
       "numberOfParticles",    pnAtoms,           1, &
       "numberParticleTypes", pnparticleTypes,   1, &
       "particleTypes",        pparticleTypesdum, 1, &
       "coordinates",          pcoor,             1, &
       "cutoff",               pcutoff,           1, &
       "energy",               penergy,           1, &
       "virial",               pvirialglob,       1, &
       "forces",               pforces,           1)
  if (ier.lt.KIM_STATUS_OK) then
     idum = kim_api_report_error_f(__LINE__, __FILE__,&
                                "kim_api_getm_data_f", ier)
     stop
  endif
...
```

KIM_API_getm_data (or kim_api_getm_data_f) will return pointers stored in KIM_API object. "Multiple" version of get data routines allows to get several variable pointers from the KIM API object s at once.

KIM_API_setm_data (or kim_api_setm_data_f) allows to place (pack) several data pointers into KIM API objects See DOCs/KIM_API_Description.txt for the details

.../ex_test_Ar_multiple_models/ex_test_Ar_multiple_models.c.c

```
...
/* Register memory */
   KIM_API_setm_data(pkim_periodic_model_0, &status, 8*4,
                     "numberOfParticles",          1,   &numberOfParticles_periodic,     1,
                     "numberParticleTypes",        1,   &numberParticleTypes,            1,
                     ...
                     "energy",                     1,   &energy_periodic_model_0,        1);
   if (KIM_STATUS_OK > status) KIM_API_report_error(__LINE__,
__FILE__,"KIM_API_setm_data",status);...
```

KIM_API_model_init will call model initialize routine that, in turn, will place model compute into KIM object

.../ex_test_Ar_multiple_models/ex_test_Ar_multiple_models.c

```
...
/* call model init routines */
status = KIM_API_model_init(pkim_periodic_model_0);
if (KIM_STATUS_OK > status)
KIM_API_report_error(__LINE__,__FILE__,"KIM_API_model_i
...
/* call compute functions */
KIM_API_model_compute(pkim_periodic_model_0, &status);
if (KIM_STATUS_OK > status)
KIM_API_report_error(__LINE__, __FILE__,"compute",
status);
...
```

KIM_API_model_init will call the model_init routine . KIM_API_model_init utilizes the KIM standard naming convention in order to make the call. In C the name of the model init routine must have all lower case letters in the following format modelname_init_, for example:

$\underbrace{\textbf{model\_ar\_p\_mlj\_cluster}}_{\text{model name}}\textbf{\_init\_}$

KIM_API_model_compute calls the address of the model compute subroutine stored in KIM API object. By the time KIM_API_model_compute is called the address is placed in KIM API object by model_init_ routine

.../ex_model_Ar_P_MLJ_C/ex_model_Ar_P_MLJ_C.c

```
/* store pointer to compute function in KIM object */
ier = KIM_API_set_data(pkim, "compute", 1, (void*) &compute);
if (KIM_STATUS_OK > ier){
   KIM_API_report_error(__LINE__, __FILE__, "KIM_API_set_data", ier);
   exit(1);
}
...
```

Place address of actual compute routine into the KIM API object

8.4

An example of using get_neigh method through KIM API service routines

.../ex_model_Ar_P_MLJ_NEIGH_PURE_H_F/ex_model_Ar_P_MLJ_NEIGH_PURE_H_F.F90

```
...
do i = 1,numberOfParticles
    ! Get neighbors for atom i
    !
    atom = i ! request neighbors for atom i
    ier=  kim_api_get_neigh_f(pkim,1,atom,atom_ret,numnei,pnei1atom,&
                                pRij_dummy)
    if (ier.lt.KIM_STATUS_OK) then
          idum = kim_api_report_error_f(__LINE__, __FILE__,&
                                   "kim_api_get_neigh", ier)
          return
    endif

    ! Loop over the neighbors of atom i
    !
    do jj = 1, numnei
          j = nei1atom(jj)
          Rij(:) = coor(:,j) - coor(:,i)  ! distance vector between i j
          Rsqij = dot_product(Rij,Rij)    ! compute square distance
          if ( Rsqij < model_cutsq ) then ! particles are interacting?
             r = sqrt(Rsqij)                            ! compute distance
             call pair(model_epsilon,model_sigma,model_A,model_B,&
                     model_C, r,phi,dphi,d2phi)  ! compute pair potential
...
```

Locator mode -- get neighbors of a particle using half or full neighbor lists as requested.

KIM_API_get_neigh will call the method using the address stored in the KIM API object. These methods are supplied by the Test.

KIM_API_get_neigh will check if the arguments are set correctly. It will also convert the result from OneBaseLists to ZeroBaseLists (or vice versa) if necessary .

Details on the interface and a description of error codes are in **DOCs/KIM_API_Description.txt**

Computing quantities from the first derivative

MODELs/ ex_model_Ne_P_fastLJ/ex_model_Ne_P_fastLJ.c

```
...

while (KIM_STATUS_OK == *ier)
      {
         i = currentAtom + model_index_shift;;
         zi=i*DIM;

         /* loop over the neighbors of currentAtom */
         for (jj = 0; jj < numOfAtomNeigh; ++ jj)
         {
               ...

               /* process dEdr */
               if (comp_process_dEdr)
               {
                  R = sqrt(Rsqij);
                  double DE = fac*R;
                  KIM_API_process_dEdr(km, &DE, &R, &pdx, &i, &j, ier);
               }
               ...
...
```

This routine can be called by a Model to provide the Test with a contribution, dEdr, to the first derivative of the Model's energy with respect to the (scalar) distance r_ij between particle `i' and particle `j'. The Test can use this information to compute, via the chain-rule, many properties. Examples include forces, the virial, and other thermodynamic tensions. The KIM API performs automatic index conversion (based on ZeroBasedList and OneBasedList flag settings) before calling the Test‘s supplied process_dEdr function. If the Test does not provide its own process_dEdr routine, then the KIM API standard process_dEdr routine is used. If the standard process_dEdr routine is used, the KIM API ensures that any appropriate memory initializations are performed. This routine and currently supports the computation of `virial' and `particleVirial'.

int * I,j -- pointers to particle index I and j.

void **km -- pointer to KIM_API_model object

double *dE -- pointer to the contribution to the first derivative of the energy with respect to the pair-distance r_ij

double *r -- pointer to r_ij -- the distance between particles i and j

double **pdx -- pointer to the relative position vector of particle j relative to particle i (i.e., r_ij = x_j - x_i).

On details of interface using process_dEdr see documentation in KIM_API_Description.txt and standard.kim

Appendix

A1

Every argument that needs to be communicated between Tests and Models must be in the descriptor file

Each **Test** has its own descriptor file that describes the data it can supply to the **Model** and what data it expects the **Model** to compute. There are no optional arguments in a **Test**'s descriptor file (because the Test knows, a priori, what it will need to compute).

Each **Model** has its own descriptor file that describes the data it needs to perform its computations and what results it can compute. Some of the arguments/methods can be identified as optional. Optional arguments/methods are ones that the **Test** does not have to provide or are results that the **Model** will only compute if the **Test** explicitly requests it.

KIM service routines (such as KIM_API_init) use both **Test** and **Model** descriptor files to:

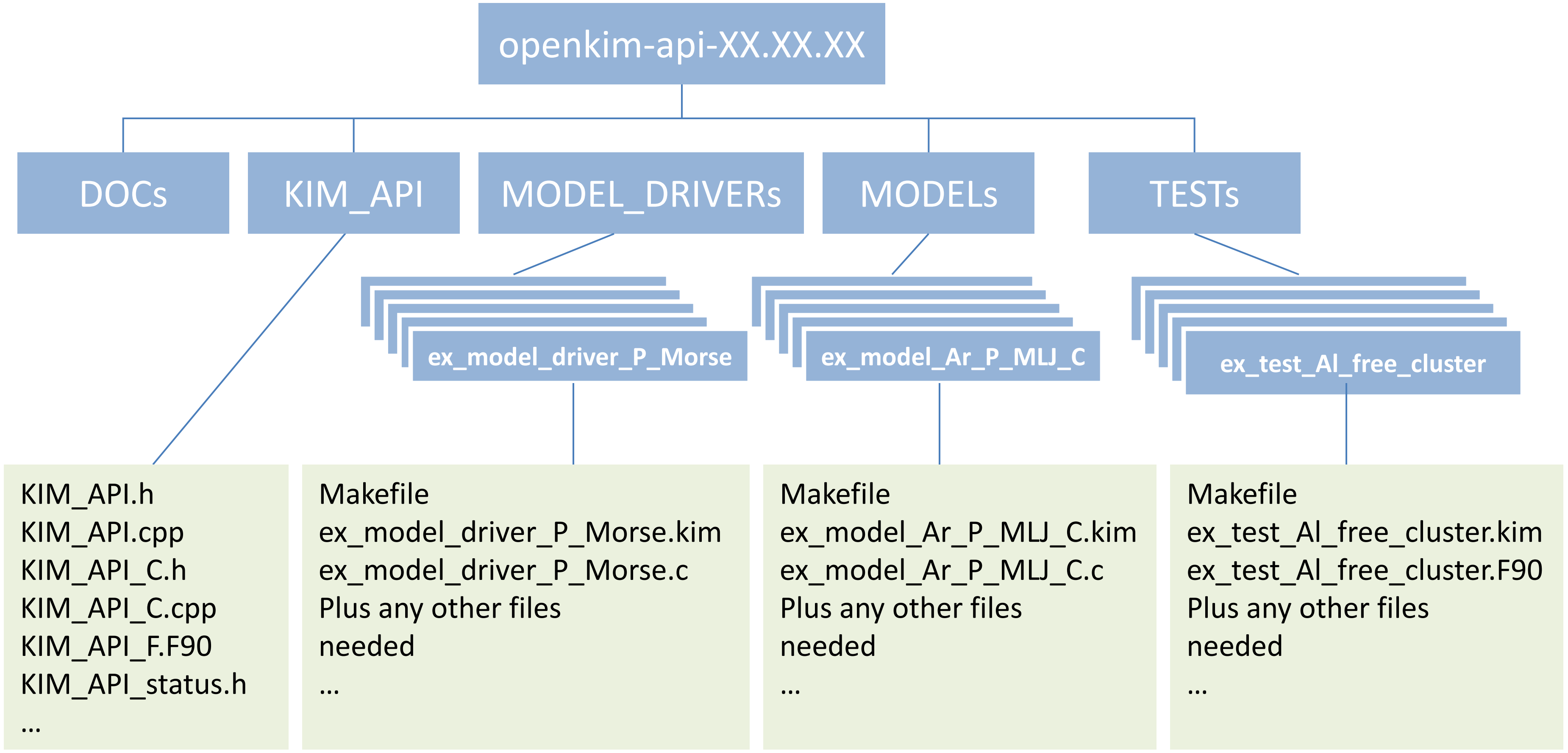
- Check if the **Model** and **Test** match, also check if their descriptor files conform to the KIM API standard
- If they do -- create a KIM API object to store all arguments described in the **Model**'s descriptor file
- Mark each optional argument that is not used by the **Test** "do not compute" (i.e., compute = false)
  The flag here is an integer value : 1 – compute, 0 – do not compute

Other service routines are used to:

- Set (get) argument or method pointers into (from) the KIM API object
  (e.g., KIM_API_set_data, KIM_API_get_data, etc.)
- Check if the "compute flag" is set to "compute" for an argument in the KIM API object
  (KIM_API_get_compute).
- Execute the Model's compute method (KIM_API_model_compute)
- etc…

A2

KIM API directory structure



Each **Test** and **Model** has its own descriptor file

The end