Knowledgebase of Interatomic Models Application Programming Interface
(KIM API)

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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 iaiables 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 API concept and implementation:

1. The KIM API facilitates communication between **Models** and **Tests**
2. The most challenging technical requirement is the need for multi-language support
3. The KIM API is based on exchanging pointers to data and methods
4. 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
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   Each base data element can hold a pointer to any relevant data (scalar, array, method, etc.)

KIM overview

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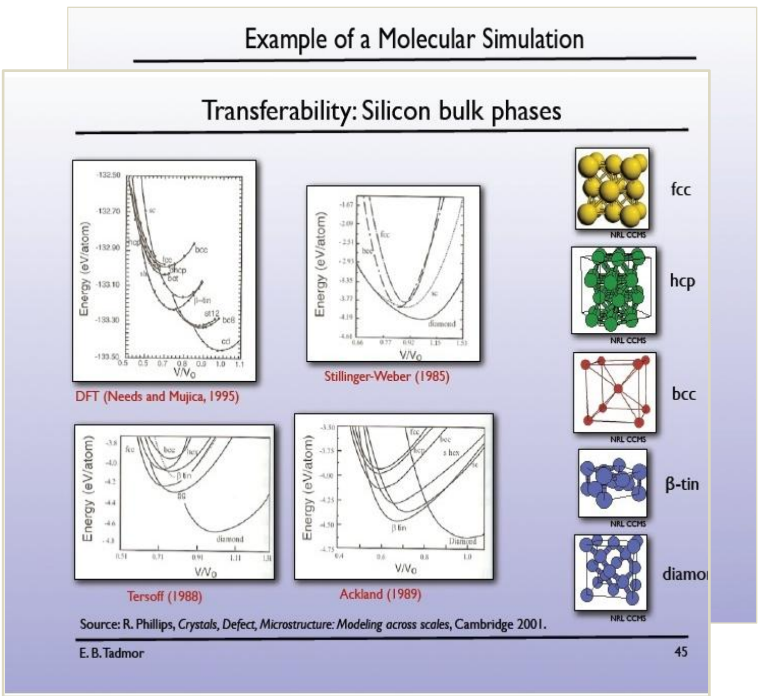
Molecular/atomistic simulations: tests and models

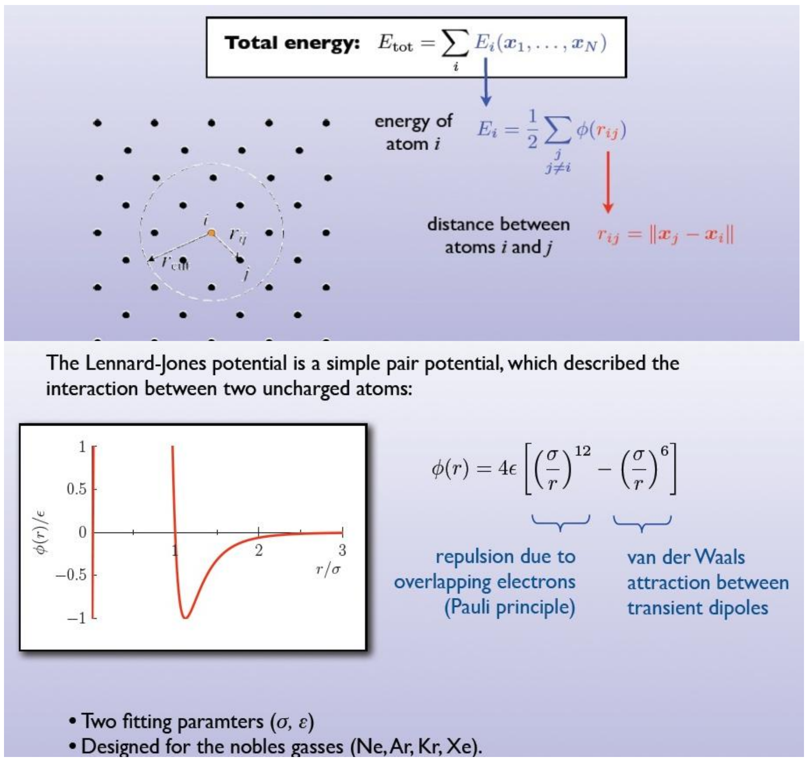
Tests

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).



Models

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



Source: openkim.org

Types of molecular modelers

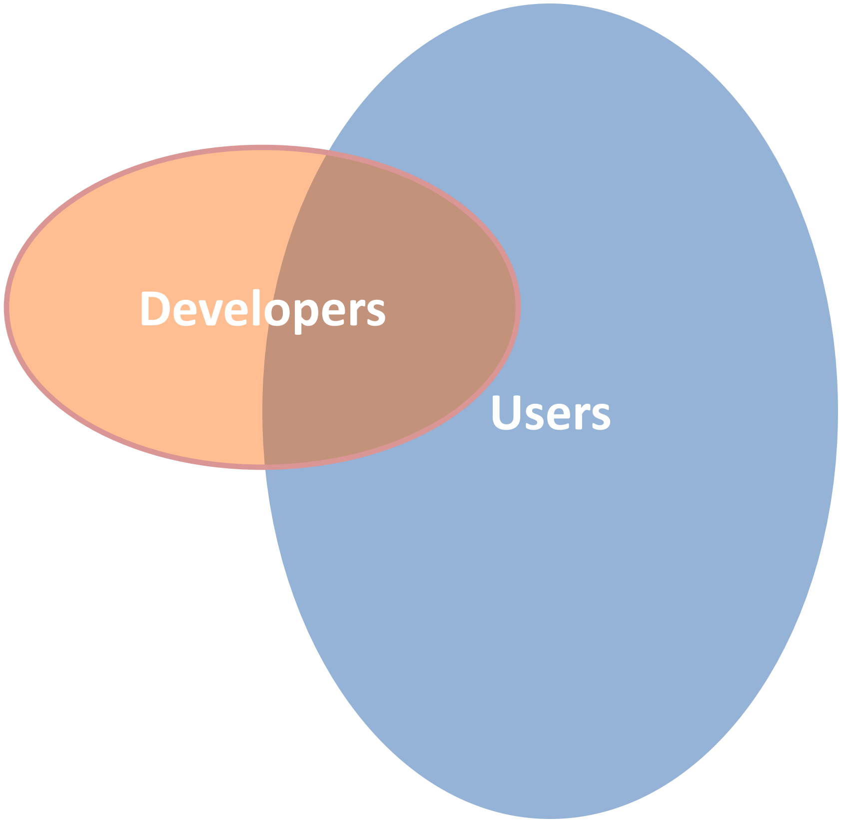
Very broadly speaking there are two types of *molecular modelers*:

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.

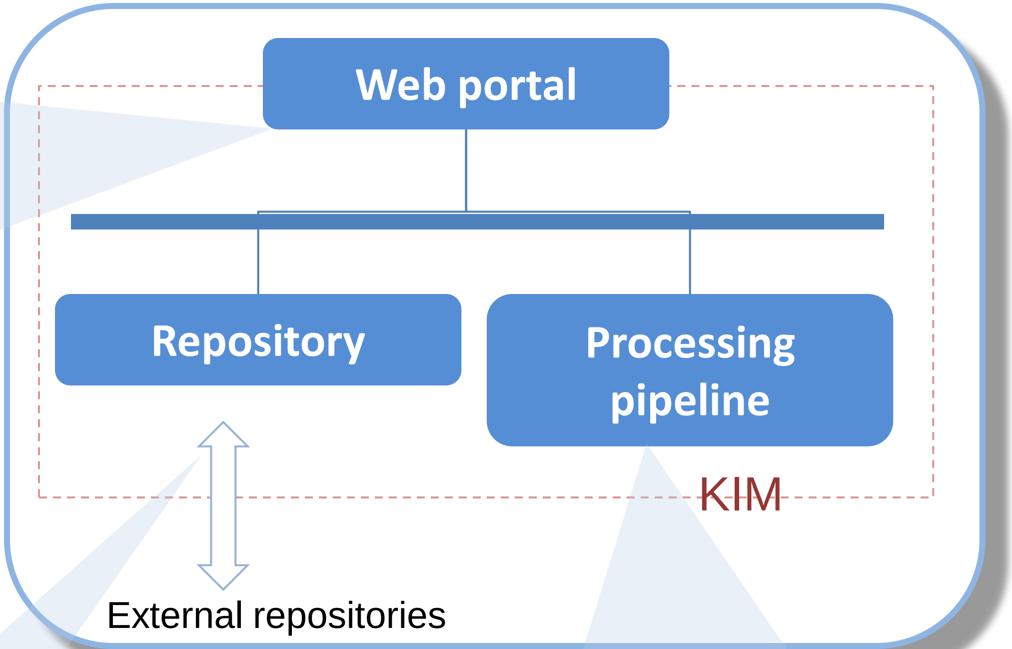
• Striving for the permanence of the KIM project, including development of a sustainability plan, and establishment of a long-term home for its content.

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

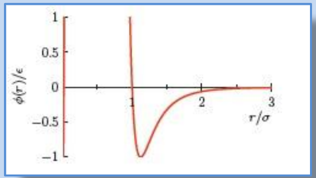
KIM repository: Models

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. ε_{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

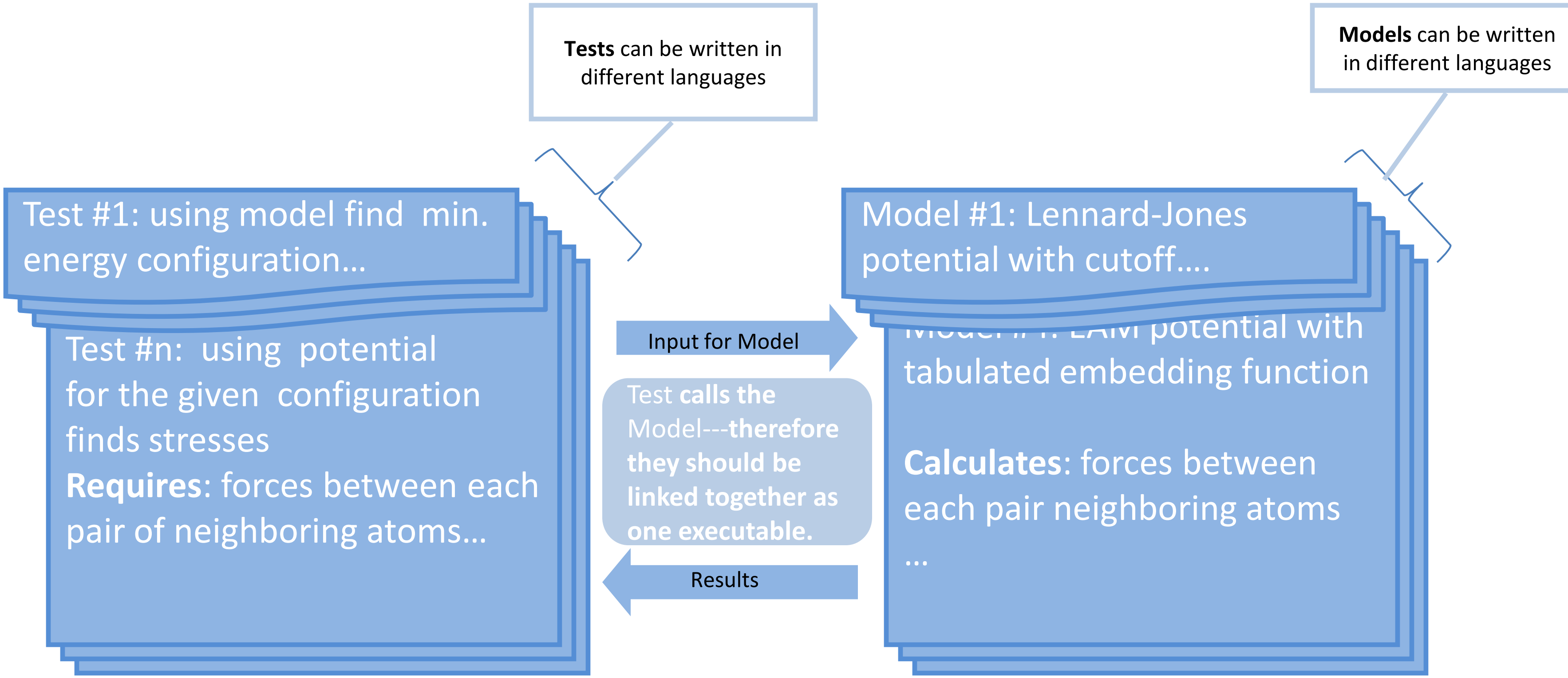
Data in KIM can either be

- 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

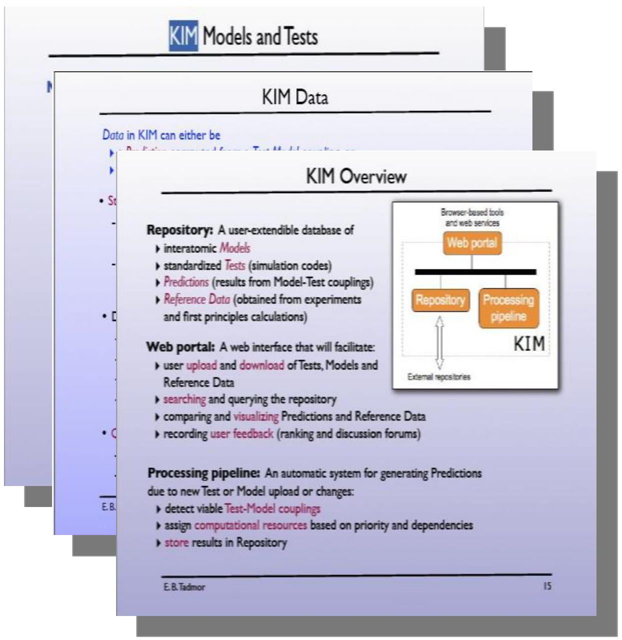
The KIM API facilitates communication between Models and Tests



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.

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

openKIM.org framework



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

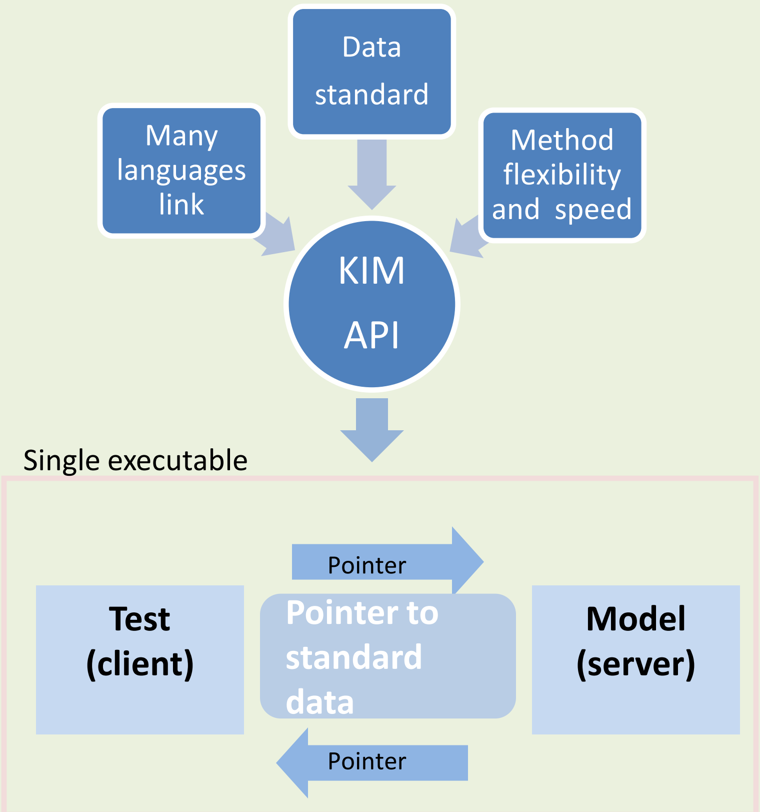
Need a simple interface : ideally just one argument per call

Source: KIM kickoff presentation

3

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

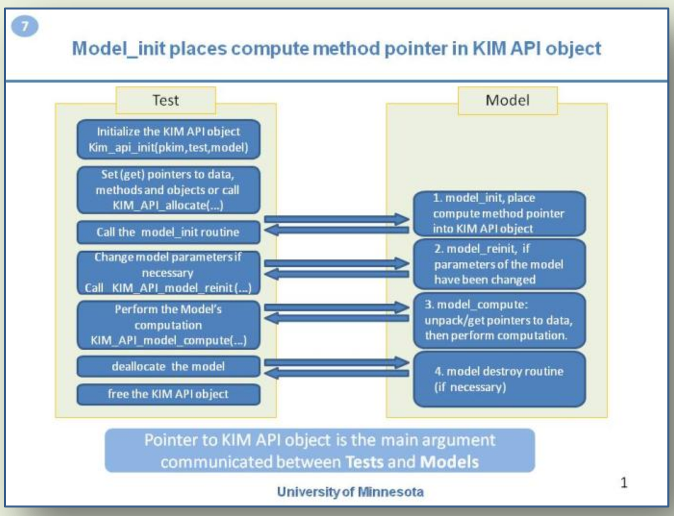
Concept



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



Using C-style pointer 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);
…
```

4

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 MODELs/ex_model_Ne_P_MLJ_NEIGH_PURE_H/

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

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.

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

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

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
```

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 and size (range) 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: detailed description of all Types value and Unit found in the file KIM_API/standard.kim

Specifying atom types – species data lines

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 atom species used by the model during runtime. Also the **KIM_API_get_partcl_type_code()** service routine allows one to get the atom species integer code (see KIM_API_Description.txt).

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

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 (or parameter), 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 KIM_API/standard.kim. Also see files in DOCs/.

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

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

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

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:

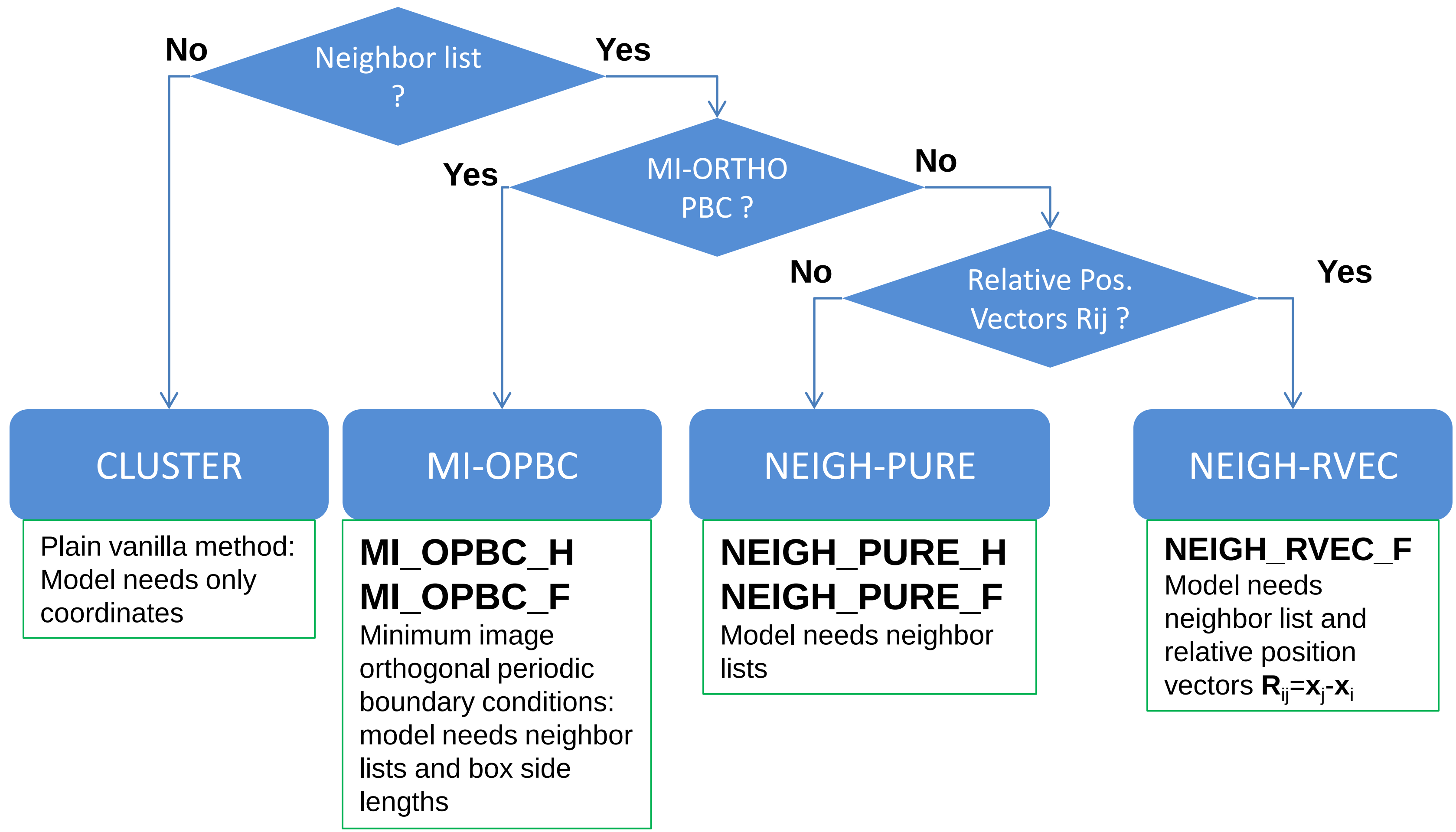
Unit_length := `A' | `Bohr' | `cm' | `m' | `nm'
Unit_energy := `amu*A^2/(ps)^2' | `erg' | `eV' | `Hartree' | `J' |`kcal/mol' | kJ/mol‘

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 KIM_API_Description.txt).

Handling of Neighbor lists and Boundary Conditions – NBC methods



Note: NBC stands for Neighbor lists and Boundary Conditions

Descriptions of the NBC methods

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

MI-OPBC-[F|H]:
Receives the number of atoms and coordinates, the side lengths for the periodic orthogonal box and a neighbor list as detailed below. Assumes all atoms lie inside the periodic box. Side lengths of box must be at least twice the cutoff range. Computes the requested quantities under the assumption that the atoms are subjected to minimum image, orthogonal, periodic boundary conditions.

Neighbor list requirements for MI-OPBC-[F|H]:

1. The minimum image convention is applied during construction of the neighbor list consistent with the orthogonal box size.
2. The neighbor list can be supplied in either full or half mode.
   Full neighbor list: All neighbors of an atom are stored
   Half neighbor list: For an atom i only the neighbors j>i are stored. The \`numberContributingParticles' allows to distinguish image from real particles.

Calculated quantities for both –H and –F modes should be equivalent to those obtained were the model to compute its own neighbor list using the provided orthogonal periodic box side lengths.

Descriptions of the NBC methods (2)

NEIGH-PURE-[F|H]:
Receives the number of atoms, coordinates and a full or half neighbor list. The neighbor list defines the environment of each atom, from which the atom'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 atoms based on their neighbor lists and the derivative of the total energy with respect to the positions of the atoms. This method can be used with codes that use ghost atoms to apply boundary conditions. The `numberContributingParticles‘ allows to distinguish ghost from real particles.

NEIGH-RVEC-F:
Receives the number of atoms and coordinates, a full neighbor list and the relative position vectors $\mathbf{R}_{ij}$ ($\mathbf{R}_{ij} = \mathbf{x}_j - \mathbf{x}_i$). The neighbor list and $\mathbf{R}_{ij}$ vectors define the environment of each atom, from which the atom'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 atoms based on their neighbor lists and relative position vectors and the derivative of the total energy with respect to the positions of the atoms. 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.

Example of using NBC methods in KIM file

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
 .
```

NBC Methods

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 lines for the chosen method are in KIM descriptor file.

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

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

```
…
CONVENTIONS:
# Name                    Type
…
ZeroBasedLists            flag     # presence of this line indicates that indexes
                                    # for atoms 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 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 atom whose neighbor list is requested

```
integer function  get_neigh(pkim,mode,request,atom,numnei,pnei1atom,pRij)
      implicit none
      integer(kind=kim_intptr),    intent(in)     :: pkim
      integer,                     intent(in)     :: mode
      integer,                     intent(in)     :: request
      integer,                     intent(out)    :: atom
      integer,                     intent(out)    :: numnei
      integer,                     intent(out)    :: pnei1atom
      integer,                                    :: nei1atom(1);   pointer(pnei1atom,nei1atom)
      double precision,            intent(out)    :: pRij
      double precision,                           :: Rij(3,*);      pointer(pRij,Rij)
end function  get_neigh
```

FORTRAN style

```
int get_neigh(void ** pkim, int * mode, int * request, int * atom,
              int * numnei, int ** pnei1atom, double ** pRij) ;
```

C style

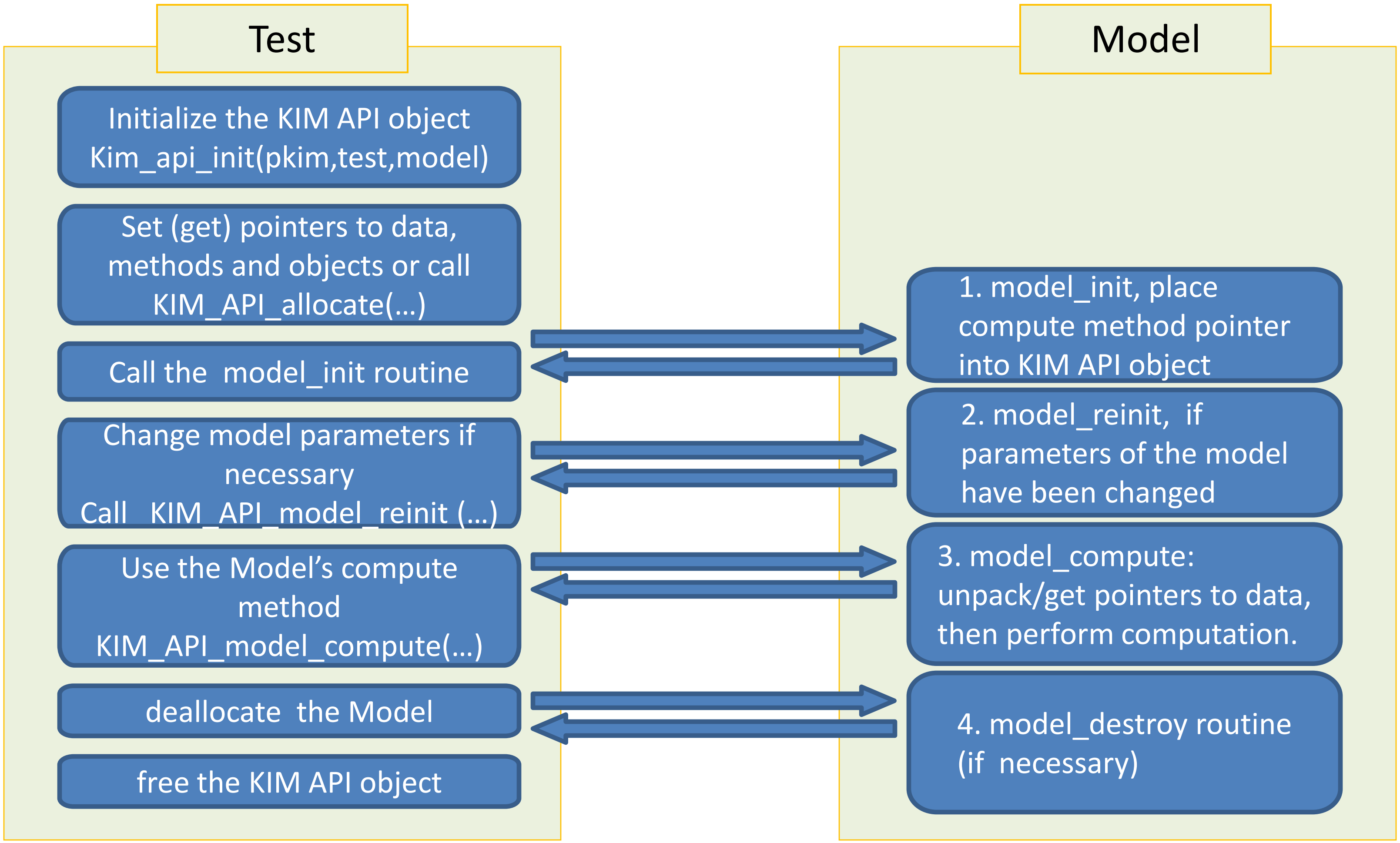
atom - the number of the atom whose neighbor list is returned
numnei - number of neighbors returned
nei1atom - integer array of neighbors of an atom which will point to the list of neighbors on exit.
Rij - array of relative position vectors of the neighbors of an atom (including boundary conditions if 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 KIM_API/KIM_API_Description.txt for details)

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

7

Model_init places compute method pointer in KIM API object



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

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

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: **KIM_API/KIM_API_Description.txt**

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, atom 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 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 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

MODELs/ 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

An example of using get_neigh method through KIM API service routines

MODELs/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 an atom 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 stangard.kim

Appendix

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:

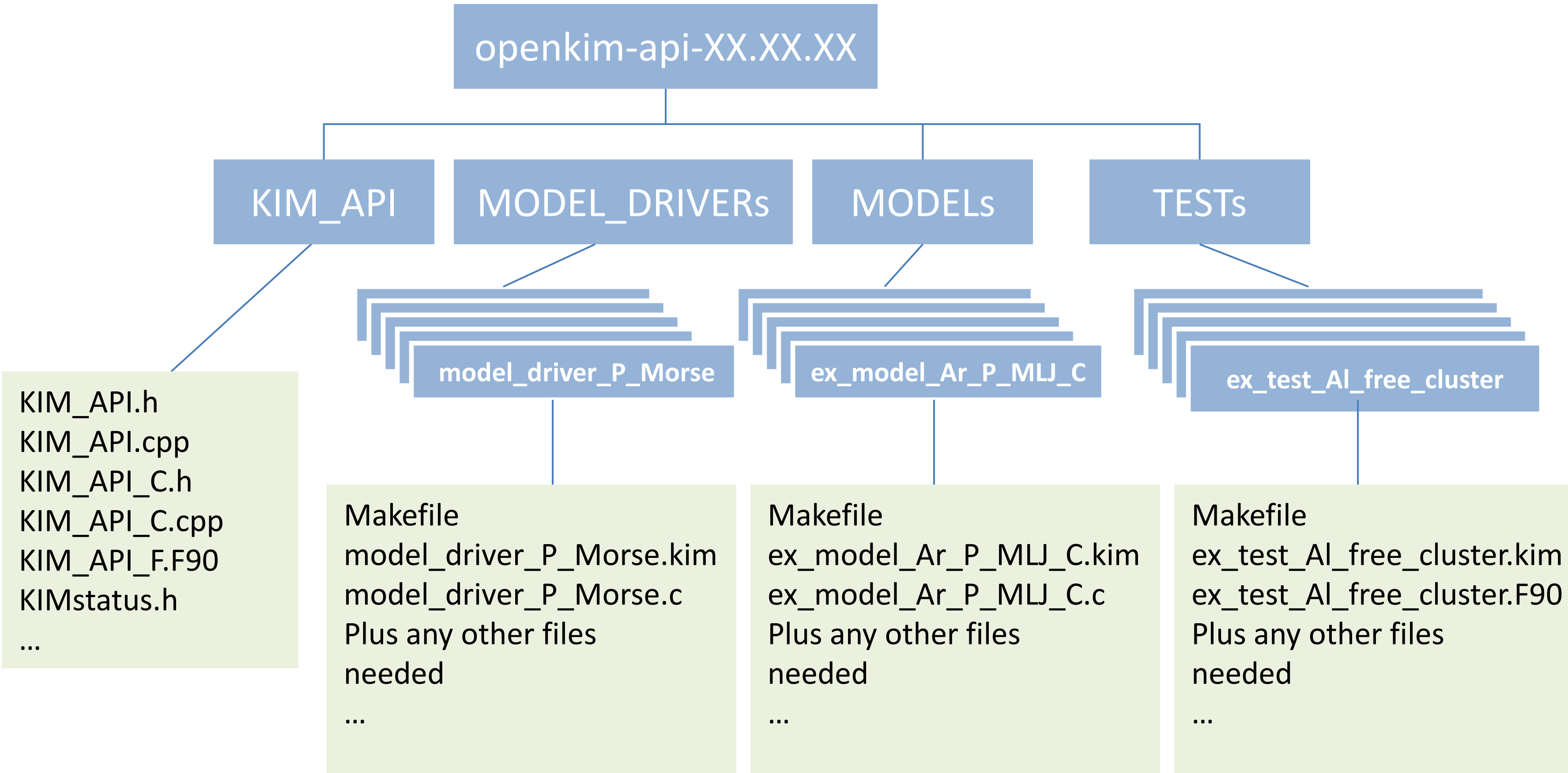
- Check if the **Model** and **Test** match, also check if their descriptor files conform to the KIM API standard
- If they do -- create a KIM API object to store all arguments described in the **Model**'s descriptor file
- Mark each optional argument that is not used by the **Test** "do not compute"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