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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- Knowledgebase of Interatomic Models (KIM) is proposed to overcome the barriers
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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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4. The KIM API object is an array of base data elements.
   Each base data element can hold a pointer to any relevant data (scalar, array, method, etc.)

KIM overview

KIM TEAM

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

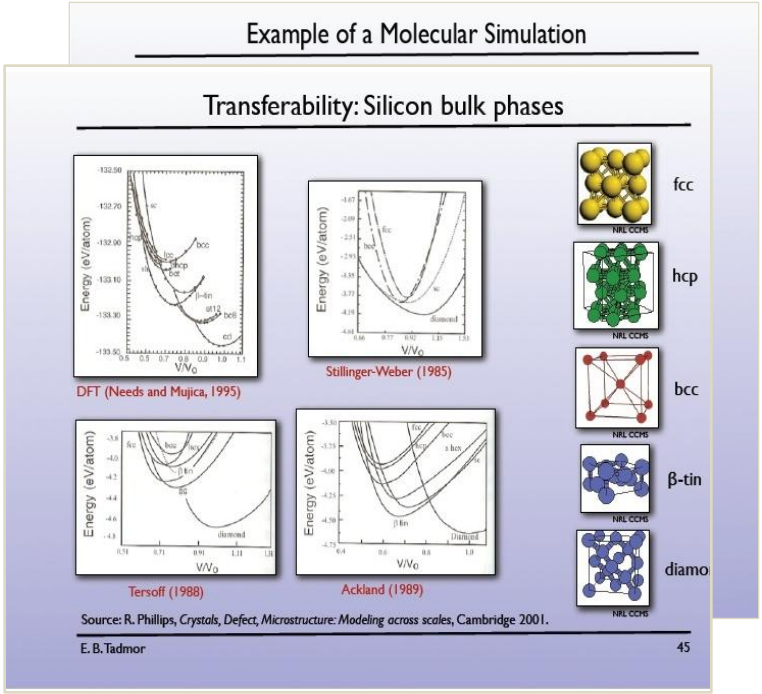
Developers
Valeriu Smirichinski (U. Minnesota)
Daniel Karls (U. Minnesota)
Mihir Khadilkar (Cornell)
Alex Alemi (Cornell)
John Crow (Silicon Life Sciences)
Trevor Wenblom (Silicon Life Sciences)

Advisory Board
Graeme Ackland (U. Edinburgh)
Michael Baskes (LANL)
Chandler Becker (NIST)
Noam Bernstein (NRL)
Ioana Cozmuta (NASA)
Karsten Jacobsen (Tech. U. Den.)
Ronald Miller (Carleton)
John Moriarty (LLNL)
Sadasivan Shankar (Intel)
Adri van Duin (Penn State)
Gabriel Wainer (Carleton)

Molecular/atomistic simulations: tests and models

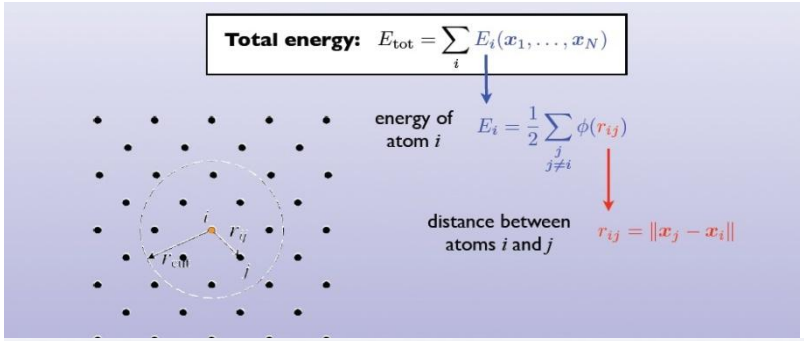
Tests

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).



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

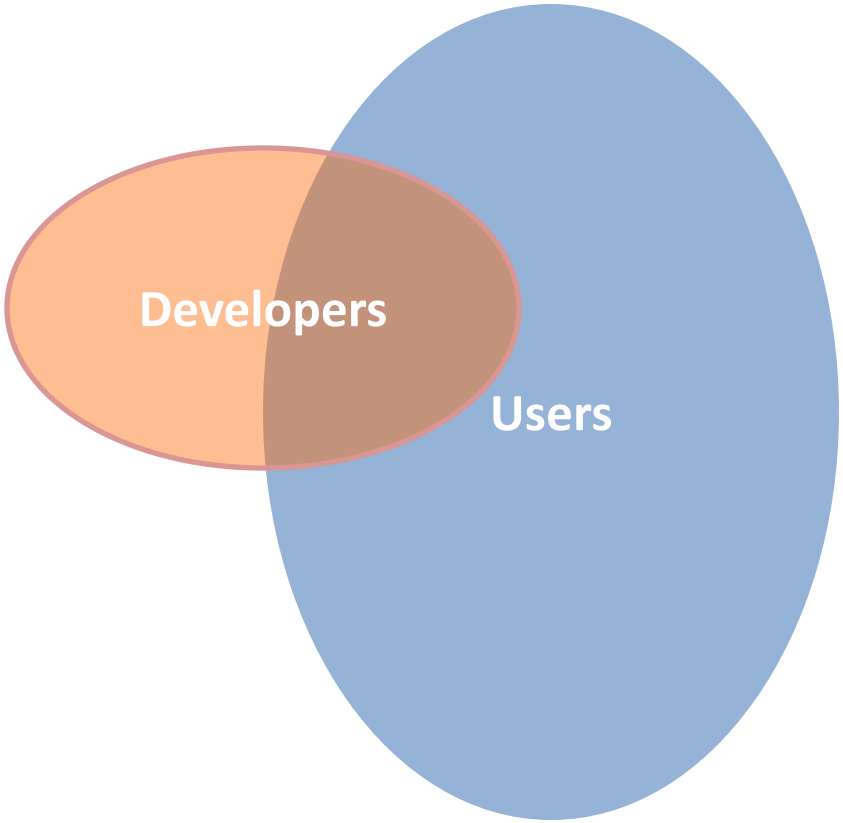
Very broadly speaking there are two types of *molecular modelers*:

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

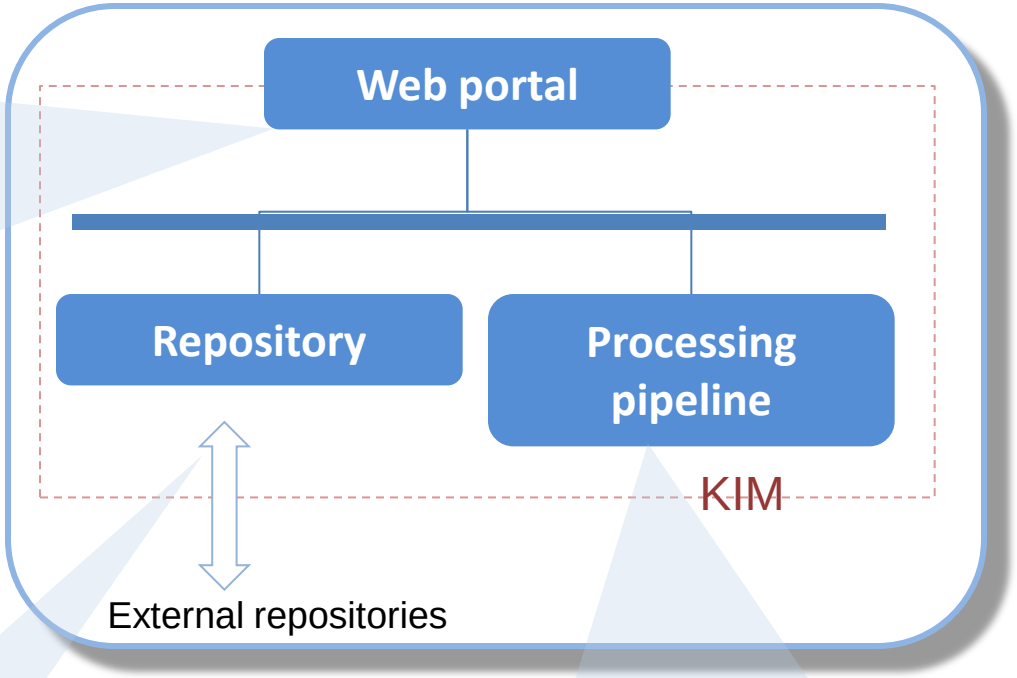
KIM framework

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

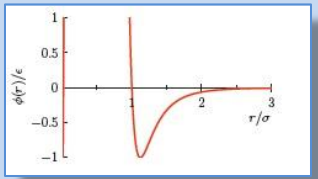
KIM repository: Models

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
- lattice constants
- cohesive energy
- vacancy formation energy
- surface energy
- grain boundary energy
- vacancy migration barrier
- dislocation mobility
- peierls stress
- melting temperature
-...

Tensors
- stress
- elastic constants
-...

Configurations
- dislocation core structure
- surface structure
- grain boundary structure
- nanocluster structure
-...

Graph
- phonon spectrum
- cohesive energy vs volume
- energy along transition path
- radial distribution functions
-...

Fields
- simulated TEM hi-res image
- 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

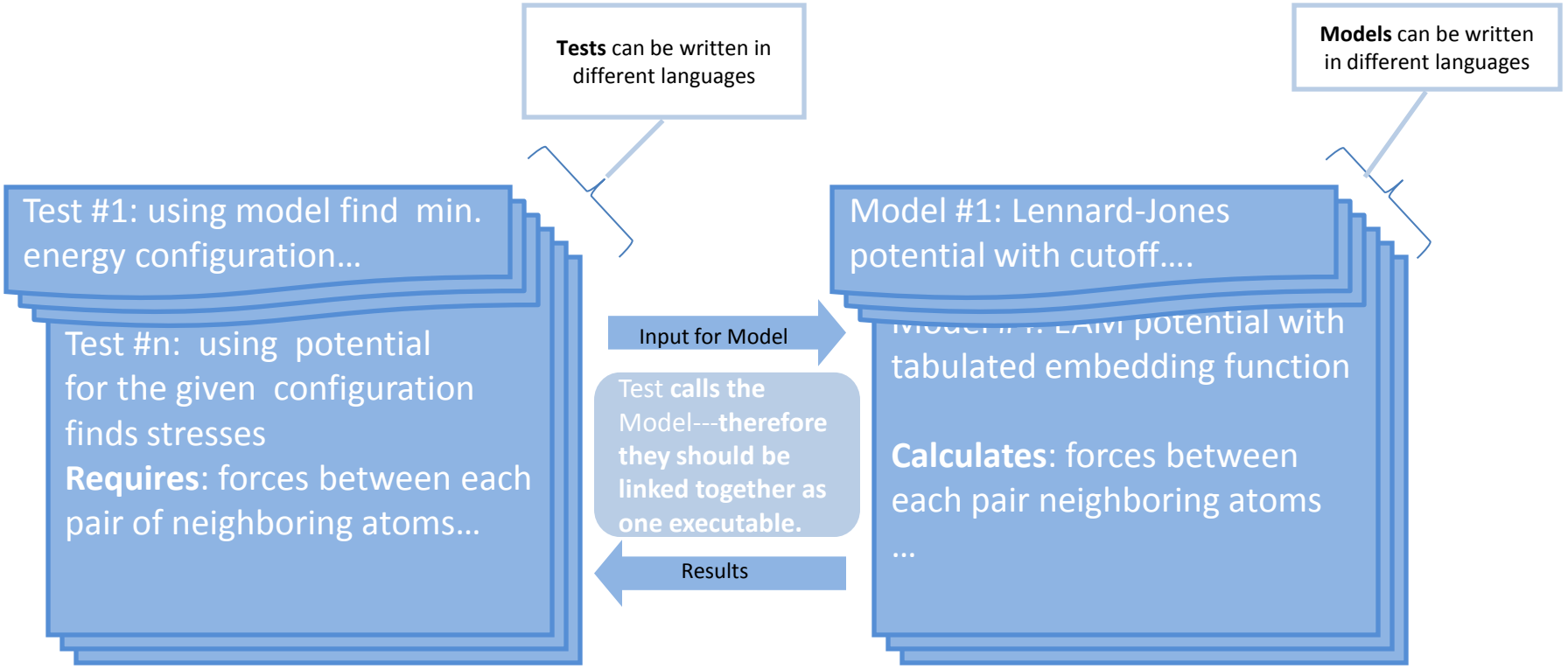
Data in KIM can either be

- 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

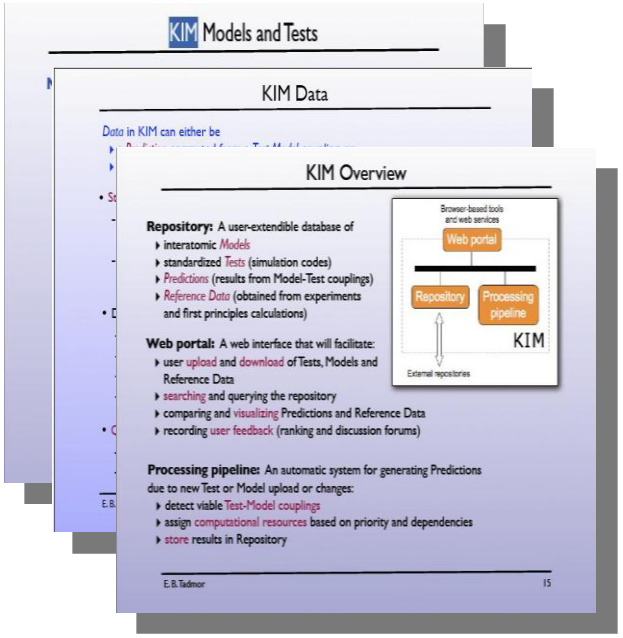
The KIM API facilitates communication between Models **and** Tests



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

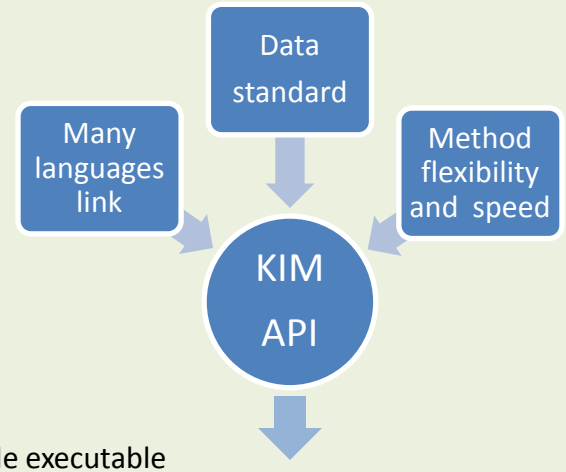
- detect a viable **Model/Test** coupling
- **build (compile and link)** Tests **against** Model
- **run probe-tests**
- assign computational resources
- run full-scale **Test** against **Model**
- analyze results …
- store results in the repository

Need a simple interface : ideally just one argument per call

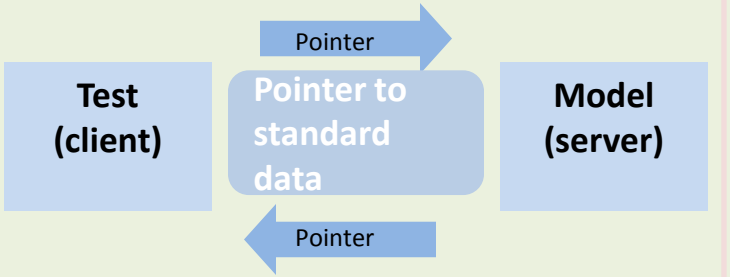
Source: KIM kickoff presentation

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

Concept



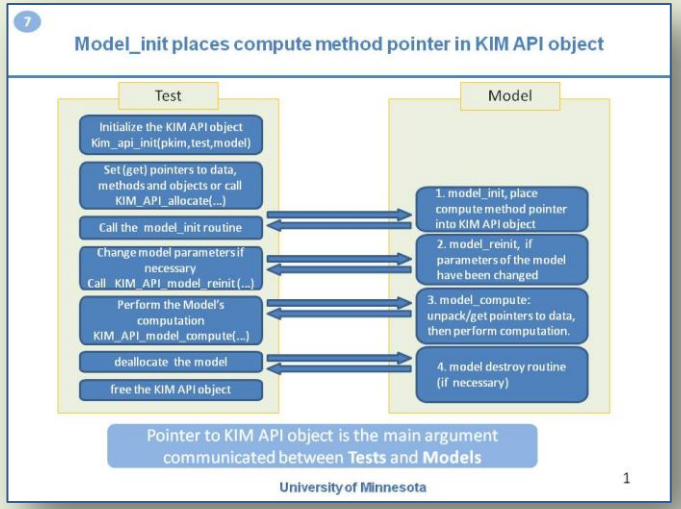
Single executable



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);
…
```

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

model_Ne_P_MLJ_NEIGH_PURE_H.kim

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

MODEL_NAME := model_Ne_P_MLJ_NEIGH_PURE_H
SystemOfUnitsFix := fixed

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

Ne                       spec                      1

...

MODEL_INPUT:
# Name                   Type         Unit       SystemU/Scale          Shape              Requirements

numberOfAtoms            integer*8    none       none                   []

numberAtomTypes          integer      none       none                   []

atomTypes                integer      none       none                   [numberOfAtoms]
...
```

KIM API descriptor file defines all variables that the model needs for computation including input and output variables. 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 variables that will be communicated using the KIM API

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

Structure of descriptor file

Model/Test name and system of units lines

```
MODEL_NAME:=model_Ar_P_Morse

SystemOfUnitsFix := fixed
```

Section lines

```
SUPPORTED_ATOM/PARTICLES_TYPES:

CONVENTIONS:

MODEL_INPUT:

MODEL_OUTPUT:

MODEL_PARAMETERS:
```

Data lines

* Species Data lines
* Dummy 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.
* Dummy 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 a variable and its properties

MODELs/model_Ar_P_MLJ_F90.kim

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

```
MODEL_NAME := model_Ar_P_MLJ_F90
SystemOfUnitsFix := fixed
….
compute             method      none       none                    []

MODEL_OUTPUT:
# Name              Type        Unit       SystemU/Scale           Shape               requirements
energy              real*8      energy     standard                 []

energyPerAtom       real*8      energy     standard                 [numberOfAtoms]     optional
….
```

Method means a subroutine or function pointer

The name of a variable 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

System of units: standard, SI, none

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

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

Note: detailed description of all Types value , Unit, SystemU/Scale can be found in the file KIM_API/standard.kim

Specifying atom types – species data lines

MODELs/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_listAtomTypes()** service routine allows one to obtain a list of all atom species used by the model during runtime. Also the **KIM_API_get_atypeCode()** service routine allows one to get the atom species integer code (see KIMserviceDescription.txt).

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

DOCs/TEMPLATEs/model_El_P_Template.f.kim

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

OneBasedLists             dummy

Neigh_IterAccess          dummy

Neigh_LocaAccess          dummy

NEIGH-RVEC-F              dummy

NEIGH-PURE-H              dummy

...
```

A dummy 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 `dummy'

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

For a detailed description of all dummy lines see the file KIM_API/standard.kim. Also see template files in DOCs/TEMPLATEs/.

5.4

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

model_Ar_P_MLJ_CLUSTER/model_Ar_P_MLJ_CLUSTER.kim

```
MODEL_PARAMETERS:

# Name                  Type        Unit      SystemU/Scale          Shape     requirements

PARAM_FREE_sigma        real*8      length    standard               []

PARAM_FREE_epsilon      real*8      energy    standard               []

PARAM_FIXED_cutsq       real*8      area      standard               []
 ...
```

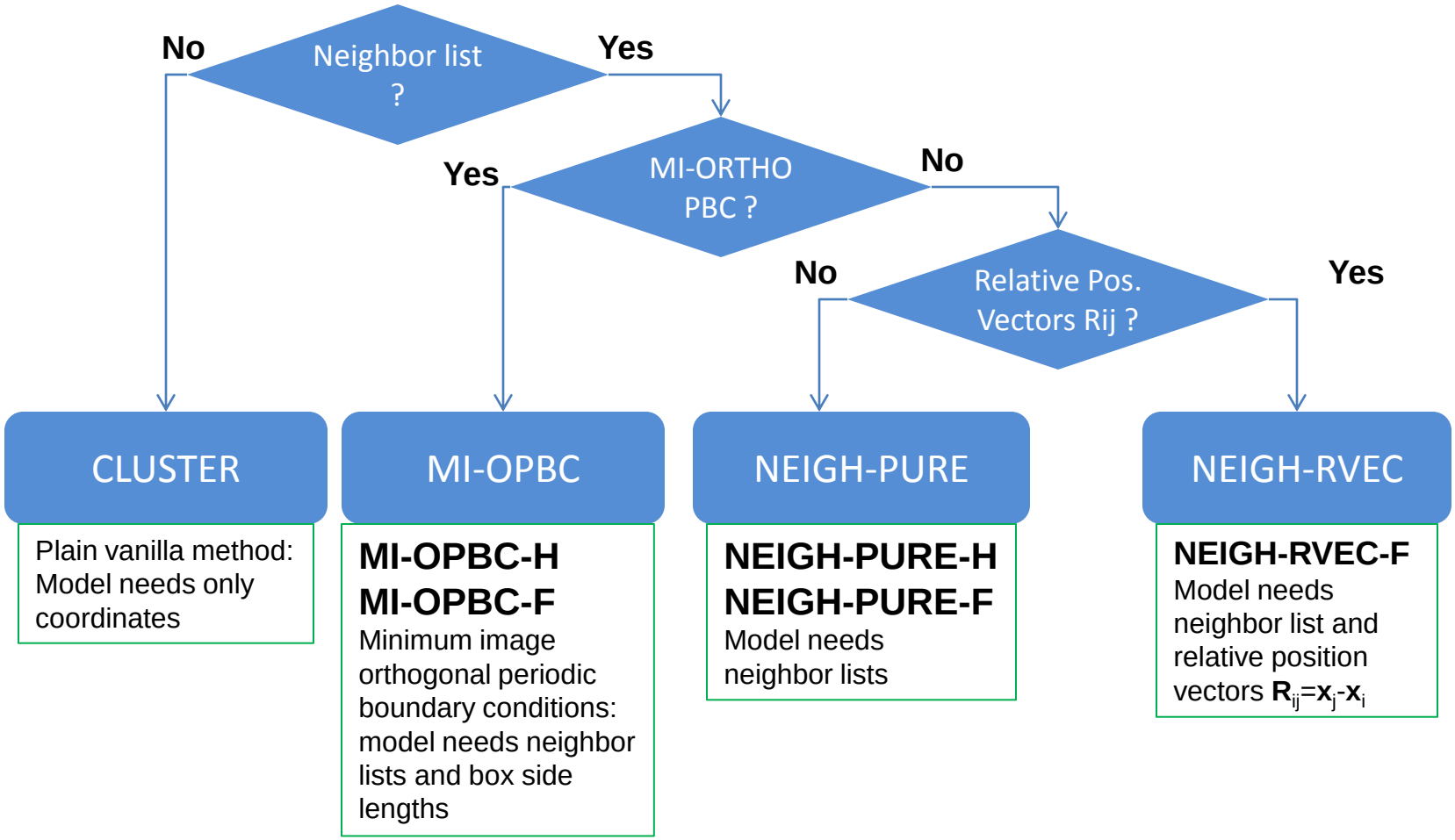
The format for parameter variables in a KIM descriptor file is the same as that for argument data types.

```
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_listParams() service routine will return a list of all parameters in the object during
runtime (as an array of text strings).
KIM_API_get_listFreeParams() service routine will return a list of FREE parameters and
KIM_API_get_listFixedParams() will return a list of FIXED parameters (see
KIMserviceDescription.txt)
```

Names of parameter variables are not checked against standard.kim

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.

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 ghost atoms are treated as regular atoms by the model, and it is up to the calling code to discard some information such as the forces on the ghost atoms and to compute the appropriate total energy from per-atom energies of the physical atoms, or to use a modified neighbor list to obtain the desired values.

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

DOCs/TEMPLATEs/model_El_P_Template.f.kim

```
…
CONVENTIONS:
# Name                      Type
OneBasedLists               dummy

NEIGH-RVEC-F

NEIGH-PURE-H                dummy

NEIGH-PURE-F                dummy

  ...

CLUSTER                     dummy
  ..
```

NBC Methods

The template example in model_El_P_Template.f.kim is designed to work with five 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            dummy     # presence of this line indicates that indexes
                                    # for atoms are from 0 to numberOfAtoms-1 (C-style)
OneBasedLists             dummy     # presence of this line indicates that indexes for
                                    # atoms are from 1 to numberOfAtoms   (Fortran-style)
Neigh_IterAccess          dummy     # works with iterator mode
Neigh_LocaAccess          dummy     # works with locator mode
Neigh_BothAccess          dummy     # needs both locator and iterator modes

MI-OPBC-H                 dummy
MI-OPBC-F                 dummy
NEIGH-RVEC-F              dummy
NEIGH-PURE-H              dummy
NEIGH-PURE-F              dummy

MODEL_INPUT:
# Name                    Type        Unit        SystemU/Scale     Shape       requirements
get_full_neigh            method      none        none                []
get_half_neigh            method      none        none                []
neighObject               pointer     none        none                []

boxlength                 real*8      length      unspecified         [3]
```

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

Interface to methods: get_half_neigh & get_full_neigh

get_half_neigh and get _full_neigh functions both have the same interface 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_half_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_half_neigh
```

FORTRAN style

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

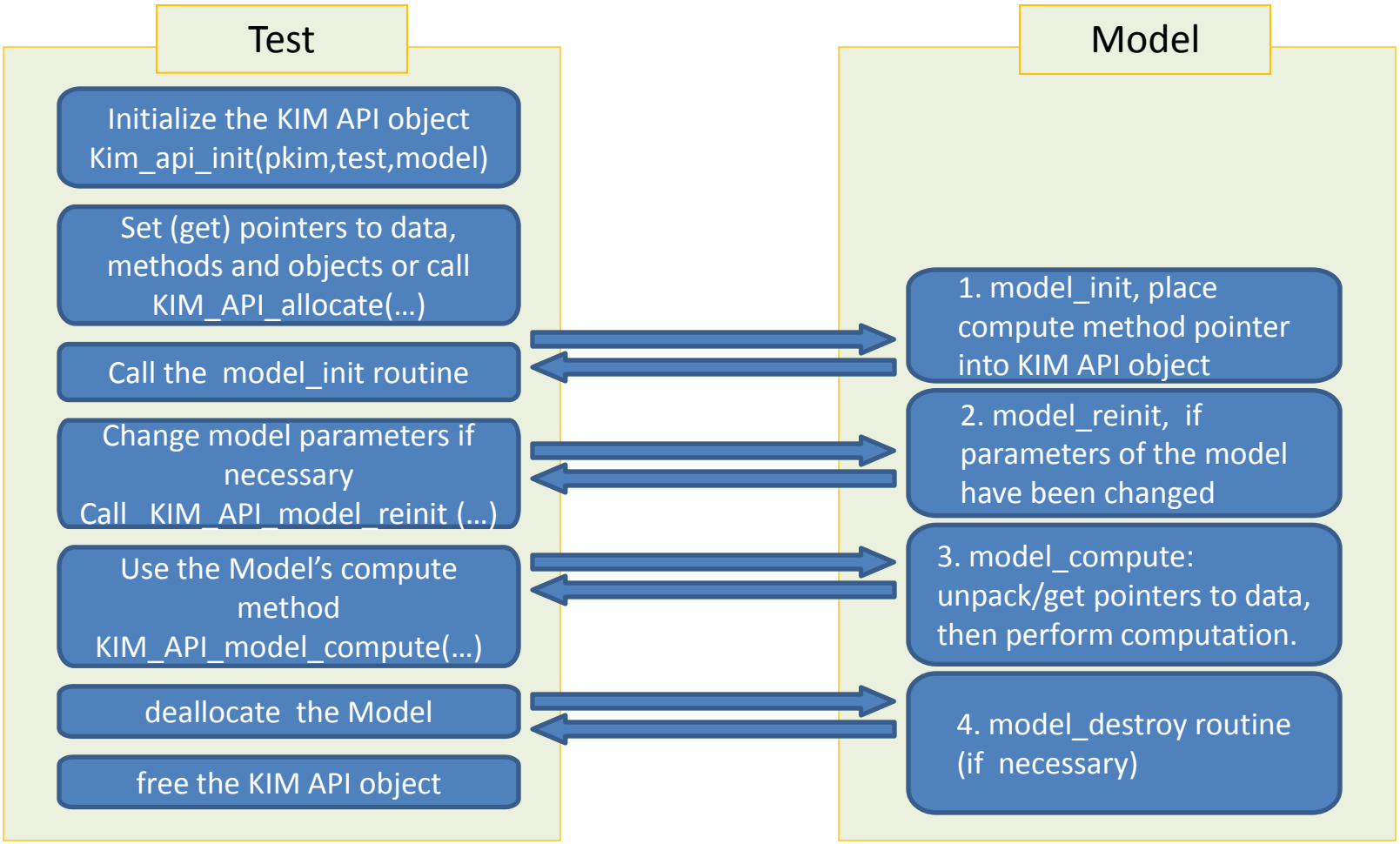
C style

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:
2 -- iterator has been successfully initialized
1 -- successful operation
0 -- iterator has been incremented past end of list
-1 -- or any negative value means unsuccessful operation (see KIM_API/KIMserviceDescription.txt)

Test must supply the get_half/full_neigh method and store a pointer to it in the KIM API object

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

KIMserviceC.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);

…
```

Initialization is done by analyzing test and model descriptor files

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

Call model_compute routine by address stored in KIM API object

Directly place data pointer into the KIM API object

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

Examples of using KIM_API_init and KIM_API_allocate service routines

test_Ar_free_cluster_CLUSTER/test_Ar_free_cluster_CLUSTER.F90

```
...
 ! Initialize the KIM object
  ier = kim_api_init_f(pkim, testname, modelname)
  if (ier.le.0) then
     call report_error(__LINE__, "kim_api_init_f", ier)
     stop
  endif
  ! Allocate memory via the KIM system
  call kim_api_allocate_f(pkim, N, ATypes, ier)
  if (ier.le.0) then
     call report_error(__LINE__, "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

test_Ar_multiple_models/test_Ar_multiple_models.c

```
...
if (1 != (status = KIM_API_init(&pkim_periodic_model_0,
testname, argv[1])))
      report_error(__LINE__,"KIM_API_init() for MODEL_ZERO
for periodic",status);
...
```

KIM_API_allocate will allocate memory for all arrays and variables 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 get/set data

test_Ar_free_cluster_CLUSTER/test_Ar_free_cluster_CLUSTER.F90

```
...
integer(kind=8) numberOfAtoms;
pointer(pnAtoms,numberOfAtoms)
...
! Unpack data from KIM object
!
pnAtoms = kim_api_get_data_f(pkim, "numberOfAtoms", ier);
if (ier.le.0) then
    call report_error(__LINE__, "kim_api_get_data_f", ier)
    stop
endif
...
```

KIM_API_get_data (or kim_api_get_data_f) will return address of data stored in the KIM API object.
ier will be equal 1 upon successful completion, otherwise it will be 0 or negative
(see **KIM_API/KIMserviceDescription.txt)**

KIM_API_set_data (or kim_api_set_data_f) will place the address of data into KIM API object and will return integer error code : 1– success, 0 or negative – unsuccessful completion

test_Ar_multiple_models/test_Ar_multiple_models.c

```
...
/* Register memory */
/* model inputs */
status = KIM_API_set_data(pkim_periodic_model_0, "numberOfAtoms", 1, &numberOfAtoms_periodic);
if (1 != status) report_error(__LINE__,"set data",status);
status = KIM_API_set_data(pkim_periodic_model_1, "numberOfAtoms", 1, &numberOfAtoms_periodic);
if (1 != status) report_error(__LINE__,"set data",status);
...
```

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

test_Ar_multiple_models/test_Ar_multiple_models.c

```
...
/* call model init routines */
if (1 != (status =
KIM_API_model_init(pkim_periodic_model_0)))
report_error(__LINE__,"KIM_API_model_init", status);
...
/* call compute functions */
KIM_API_model_compute(pkim_periodic_model_0, &status);
if (1 != status) report_error(__LINE__,"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:
model_ar_p_mlj_cluster_init_

model name

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

DOCs/TEMPLATEs/model_El_P_Template.F90

```
...
subroutine model_<FILL element name>_P_<FILL model name>_init(pkim)
...
! store pointer to compute function in KIM object
if (kim_api_set_data_f(pkim,"compute",one,loc(Compute_Energy_Forces)).ne.1)&
   stop '* ERROR: compute keyword not found in KIM object.'
...
```

Place address of actual compute routine into the KIM API object

An example of using get_half/full_neigh methods through KIM API service routines

MODELs/ model_Ar_P_MLJ_NEIGH_PURE_H_F/ model_Ar_P_MLJ_NEIGH_PURE_H_F.F90

```
...
do i = 1,numberOfAtoms
       ! Get neighbors for atom i
       !
       atom = i ! request neighbors for atom i
       if (HalfOrFull.eq.1) then
          ier kim_api_get_half_neigh_f(pkim,1,atom,atom_ret,numnei, &
                                       pnei1atom,pRij_dummy)
       else
          ier = kim_api_get_full_neigh_f(pkim,1,atom,atom_ret,numnei, &
                                         pnei1atom,pRij_dummy)
       endif
       if (ier.le.0) then
          call report_error(__LINE__, "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_half/full_neigh will call the method using the address stored in the KIM API object (“get_half_neigh” or “get_full_neigh”). These methods are supplied by the Test.

KIM_API_get_half/full_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/KIMserviceDescription.txt**

Summary

1. KIM project aims to overcome the barriers faced by molecular modelers by creating an online resource for standardized testing, long-term warehousing and easy retrieval of interatomic models and data.

2. Tests and Models written by different researcher/developer teams, in different programming languages and programming styles, must be able to couple and work together.

3. To address the challenge, KIM API has been created. KIM API is based on descriptor files where the models and tests provide all variables and methods needed for their interactions. Using the descriptor files KIM API routines create an intermediate object that holds all pointers to the data variables, needed for test-model communications. Access to the data in that object is done also through service routines.

Appendix

A1

Every variable 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 variables 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 variables/methods can be identified as optional. Optional variables/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:

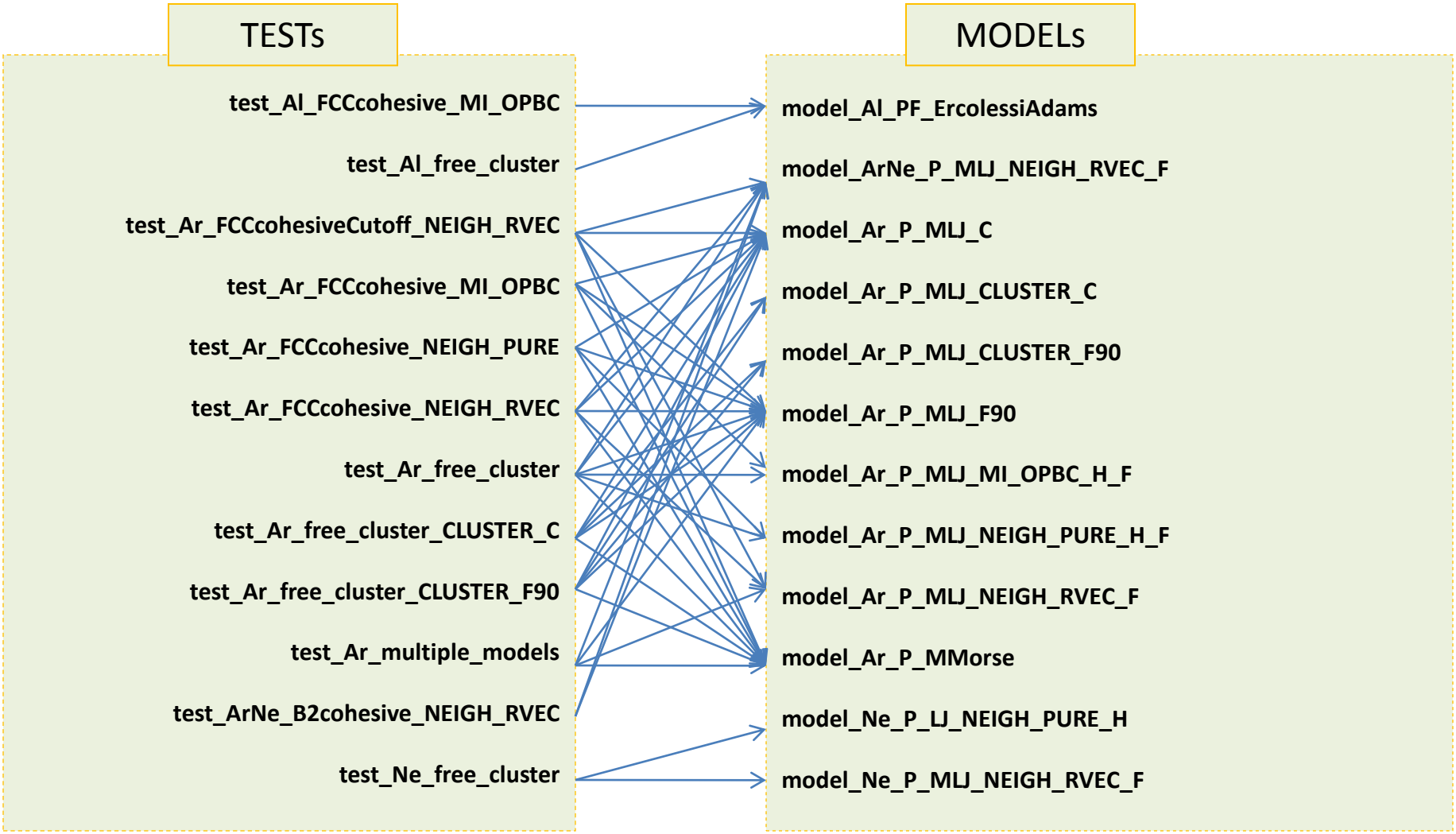
- Check if the **Model** and **Test** match, also check if their descriptor files conform to the KIM API standard
- If they do -- create a KIM API object to store all variables described in the **Model**'s descriptor file
- Mark each optional variable that is not used by the **Test** "uncompute" (i.e.,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

Other service routines are used to:

- Set (get) variable 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 a variable in the KIM_API obejct (kim_api_isit_compute)
- Execute the Model's compute method (kim_api_model_compute)
- etc…

A3

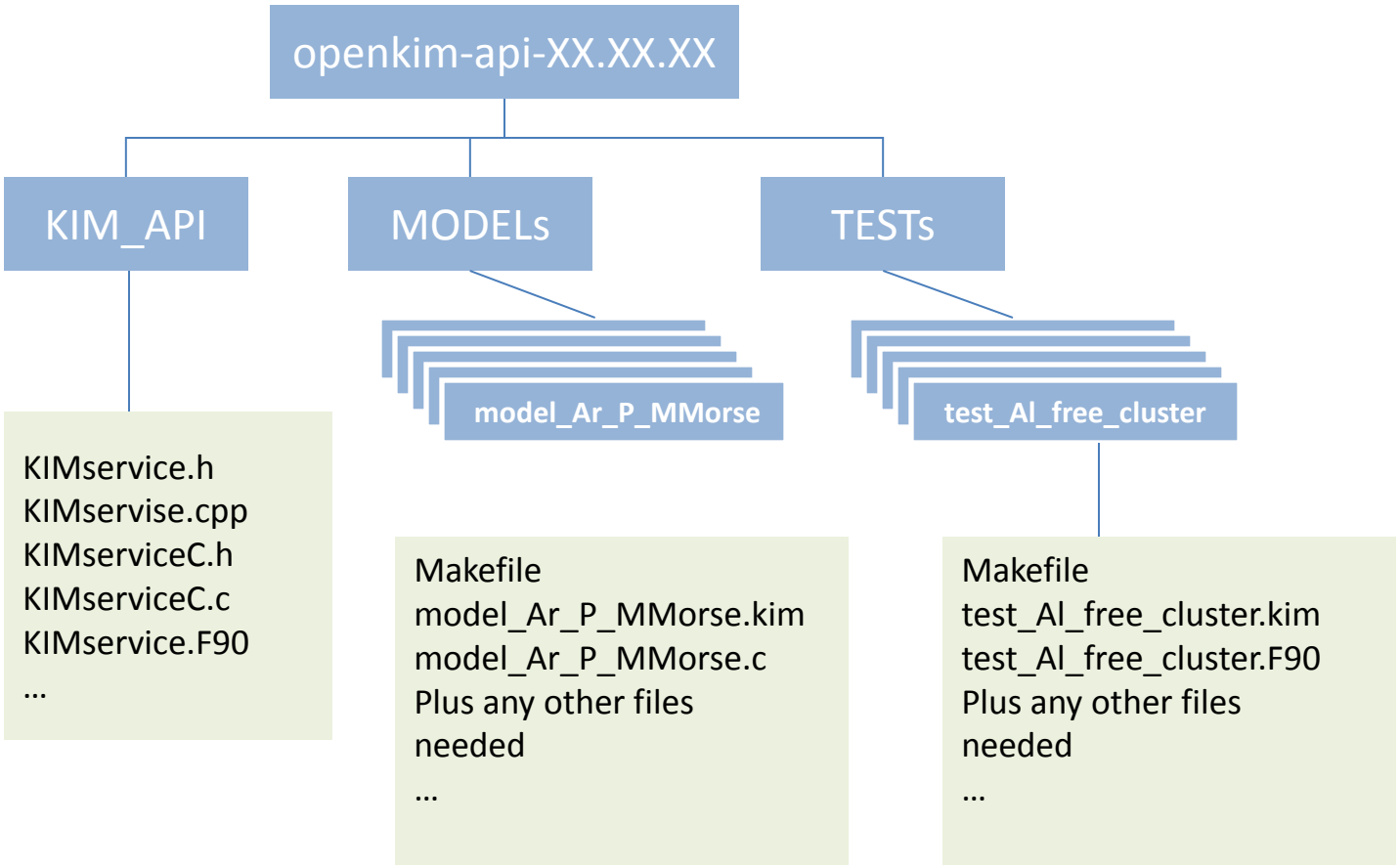
Model and Test examples available in the current version of KIM API



Indicates a **Test** can work (match) with a **Model** in the current KIM API version

Description of the Models and Tests provided with the KIM API package are given in the files MODELs/EXAMPLES.README and TESTs/EXAMPLES.README.

KIM API directory structure



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

A4

KIM API object is an array of Base data elements. Each Base data element can hold a pointer to any relevant data

Number of fields is fixed to 9

Base data:

- Can hold any type of array: real, integer, pointer…
- Stores enough information for a complete description of the data

pointer to contiguous array of data of size "size"

size of data in terms of underlying elements

auxiliary array: very useful for 2d arrays (variable and fixed dimensions)

name contains description information like "coordinates", "velocities", "forces", etc…

type tells the type for elements of array: "real", "real*8"integer", "integer*8", pointer

rank and shape:
- rank is the number of indices for the array: for 2D it is 2, for 3D it is 3 etc…
- shape is an integer array of size rank and holds the size (range) of each index.

Flag contains additional information (all fields are integers)

- **peratom**
- **freeable**
- **pointerchanged**
- **ID**

Every field in the Base data structure is a pointer or "pointer size" integer.

Base data type can be used to store all needed data for **Tests** and **Models**

The end