Using LAMMPS with the Knowledgebase of Interatomic Models (KIM – http://openKIM.org)

Ryan S. Elliott, Ellad B. Tadmor, and Valeriu Smirichinski

Dept. of Aerospace Engineering and Mechanics, University of Minnesota

News item:
— Version 0.1.0 of the openKIM API was released yesterday, Aug. 8, 2011. (see http://openKIM.org/resources to download the source code.)

Funding:
National Science Foundation, Cyber-enabled Discovery and Innovation (CDI) grant
Program Manager: Beverly K. Berger
Knowledgebase of Interatomic Models (KIM)

The *Knowledgebase of Interatomic Models (KIM)* project is based on a four-year NSF cyber-enabled discovery and innovation (CDI) grant.

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](http://openKIM.org)
## The 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)
The 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
Model and Test examples available in the current version of the openKIM 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.
Using the openKIM API with LAMMPS


Download LAMMPS

There are 2 ways to get the LAMMPS software. You can follow the download instructions on this page to grab a tarball. Or if you have Subversion (SVN) or Git installed on your machine, you can use SVN or Git checkout and update commands to get the current version. Instructions on this are below for SVN and Git. Either way, once you have the code, follow the instructions in the LAMMPS documentation to build it.

To determine what version of LAMMPS you already have, or to stay up-to-date as features or bug-fixes are made to LAMMPS, see this page.

You can download older versions of LAMMPS, by going to this page and selecting the version you want, based on the date in the tarball filename. Not every version is available, because LAMMPS is updated frequently, and we have limited space on our WWW server.

Older parallel MD codes (ParaDyn, LJ) and the Python-based Pizza.py package, which provides pre- and post-processing and viz tools for LAMMPS, are available for download from this page.

- Download a tarball
- SVN checkout and update
- Git checkout and update
- Applying patches

Download a tarball

Select the code you want, click the "Download Now" button, and your browser should download a gzipped tar file. Unpack it with the following commands, and look for a README to get you started.
Using the openKIM API with LAMMPS

2. Get the openkim-api package:
Using the openKIM API with LAMMPS

2. Get the openkim-api package:
Using the openKIM API with LAMMPS

3. Get the lammps/kim interface and example files:
Using the openKIM API with LAMMPS

Go to command line window…
Using the openKIM API with LAMMPS

4. Don’t forget to sign up for updates!

Thanks for your attention!
The end