



# A Brief User's Guide and Developer's Introduction to OpenKIM

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Funding from NSF: CDI & CDS&E

LAMMPS Workshop and Symposium
Albuquerque, NM — Aug. 1–3, 2017

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# Outline



Start from the beginning (Linux setup)
Building KIM and LAMMPS
Test the setup with the KIM example in LAMMPS
Setup to execute an OpenKIM Test with the local LAMMPS
Prepare and run the Tests locally
Compare the results

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# Initial files

This version of Install.py will be included in the next stable release of LAMMPS

2. Ryans-MBP-6:~/lammps-kim (bash)

```
<516 Ryans-MBP-6:lammps-kim >ls -l
total 192544
-rw-r--r--  1 relliott  staff      8090 Jul 31 18:46 Install.py
-rw-r--r--  1 relliott  staff       249 Jul 31 18:33 Vagrantfile
-rw-r--r--@ 1 relliott  staff  98570047 Jul 31 18:48 lammps-24Jul17.tar.gz
<517 Ryans-MBP-6:lammps-kim >
```

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# Vagrant file

Vagrant (http://www.vagrantup.com) and Virtual Box (http://www.virtualbox.org) are not necessary.
This demonstration should work on most Linux systems.

2. Ryans-MBP-6:~/lammps-kim (bash)

```
<518 Ryans-MBP-6:lammps-kim >cat Vagrantfile
Vagrant.configure("2") do |config|
  config.vm.box = "ubuntu/trusty64"

  # increase the memory size
  config.vm.provider :virtualbox do |vb|
    # increase the memory size
    vb.customize ["modifyvm", :id, "--memory", 4096, "--cpus", 1]
  end
end
<519 Ryans-MBP-6:lammps-kim >
```

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# Boot the VM



2. Ryans-MBP-6:~/lammps-kim (bash)

```
<526 Ryans-MBP-6:lammps-kim >vagrant up
Bringing machine 'default' up with 'virtualbox' provider...
==> default: Importing base box 'ubuntu/trusty64'...
==> default: Matching MAC address for NAT networking...
==> default: Checking if box 'ubuntu/trusty64' is up to date...
==> default: Setting the name of the VM: lammps-kim_default_1501545214776_1526
==> default: Clearing any previously set forwarded ports...
==> default: Clearing any previously set network interfaces...
==> default: Preparing network interfaces based on configuration...
    default: Adapter 1: nat
==> default: Forwarding ports...
    default: 22 (guest) => 2222 (host) (adapter 1)
==> default: Running 'pre-boot' VM customizations...
==> default: Booting VM...
==> default: Waiting for machine to boot. This may take a few minutes...
    default: SSH address: 127.0.0.1:2222
    default: SSH username: vagrant
    default: SSH auth method: private key
    default:
    default: Vagrant insecure key detected. Vagrant will automatically replace
    default: this with a newly generated keypair for better security.
    default:
    default: Inserting generated public key within guest...
    default: Removing insecure key from the guest if it's present...
    default: Key inserted! Disconnecting and reconnecting using new SSH key...
==> default: Machine booted and ready!
==> default: Checking for guest additions in VM...
    default: The guest additions on this VM do not match the installed version of
    default: VirtualBox! In most cases this is fine, but in rare cases it can
    default: prevent things such as shared folders from working properly. If you see
    default: shared folder errors, please make sure the guest additions within the
    default: virtual machine match the version of VirtualBox you have installed on
    default: your host and reload your VM.
    default:
    default: Guest Additions Version: 4.3.36
    default: VirtualBox Version: 5.1
==> default: Mounting shared folders...
    default: /vagrant => /Users/relliott/lammps-kim
<527 Ryans-MBP-6:lammps-kim >
```

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# Login to the VM



2. vagrant@vagrant-ubuntu-trusty-64: /vagrant (ssh)

```
<528 Ryans-MBP-6:lammps-kim >vagrant ssh
Welcome to Ubuntu 14.04.5 LTS (GNU/Linux 3.13.0-125-generic x86_64)

 * Documentation:  https://help.ubuntu.com/

  System information as of Mon Jul 31 23:53:54 UTC 2017

  System load:  0.14              Processes:           82
  Usage of /:   3.6% of 39.34GB   Users logged in:     0
  Memory usage: 3%                IP address for eth0: 10.0.2.15
  Swap usage:   0%

  Graph this data and manage this system at:
    https://landscape.canonical.com/

  Get cloud support with Ubuntu Advantage Cloud Guest:
    http://www.ubuntu.com/business/services/cloud

0 packages can be updated.
0 updates are security updates.

New release '16.04.2 LTS' available.
Run 'do-release-upgrade' to upgrade to it.


vagrant@vagrant-ubuntu-trusty-64:~$
vagrant@vagrant-ubuntu-trusty-64:~$ cd /vagrant/
vagrant@vagrant-ubuntu-trusty-64:/vagrant$
vagrant@vagrant-ubuntu-trusty-64:/vagrant$ ls -l
total 96272
-rw-r--r-- 1 vagrant vagrant     8090 Jul 31 23:46 Install.py
-rw-r--r-- 1 vagrant vagrant 98570047 Jul 31 23:48 lammps-24Jul17.tar.gz
-rw-r--r-- 1 vagrant vagrant      249 Jul 31 23:33 Vagrantfile
vagrant@vagrant-ubuntu-trusty-64:/vagrant$
```

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# Install the compilers



2. vagrant@vagrant-ubuntu-trusty-64: /vagrant (vagrant)

```
vagrant@vagrant-ubuntu-trusty-64:/vagrant$ sudo apt-get update -qq
vagrant@vagrant-ubuntu-trusty-64:/vagrant$
vagrant@vagrant-ubuntu-trusty-64:/vagrant$ sudo apt-get install g++ gfortran -qq
Selecting previously unselected package libgfortran3:amd64.
(Reading database ... 63129 files and directories currently installed.)
Preparing to unpack .../libgfortran3_4.8.4-2ubuntu1~14.04.3_amd64.deb ...
Unpacking libgfortran3:amd64 (4.8.4-2ubuntu1~14.04.3) ...
Selecting previously unselected package libstdc++-4.8-dev:amd64.
Preparing to unpack .../libstdc++-4.8-dev_4.8.4-2ubuntu1~14.04.3_amd64.deb ...
Unpacking libstdc++-4.8-dev:amd64 (4.8.4-2ubuntu1~14.04.3) ...
Selecting previously unselected package g++-4.8.
Preparing to unpack .../g++-4.8_4.8.4-2ubuntu1~14.04.3_amd64.deb ...
Unpacking g++-4.8 (4.8.4-2ubuntu1~14.04.3) ...
Selecting previously unselected package g++.
Preparing to unpack .../g++_4%3a4.8.2-1ubuntu6_amd64.deb ...
Unpacking g++ (4:4.8.2-1ubuntu6) ...
Selecting previously unselected package libgfortran-4.8-dev:amd64.
Preparing to unpack .../libgfortran-4.8-dev_4.8.4-2ubuntu1~14.04.3_amd64.deb ...
Unpacking libgfortran-4.8-dev:amd64 (4.8.4-2ubuntu1~14.04.3) ...
Selecting previously unselected package gfortran-4.8.
Preparing to unpack .../gfortran-4.8_4.8.4-2ubuntu1~14.04.3_amd64.deb ...
Unpacking gfortran-4.8 (4.8.4-2ubuntu1~14.04.3) ...
Selecting previously unselected package gfortran.
Preparing to unpack .../gfortran_4%3a4.8.2-1ubuntu6_amd64.deb ...
Unpacking gfortran (4:4.8.2-1ubuntu6) ...
Processing triggers for man-db (2.6.7.1-1ubuntu1) ...
Setting up libgfortran3:amd64 (4.8.4-2ubuntu1~14.04.3) ...
Setting up libstdc++-4.8-dev:amd64 (4.8.4-2ubuntu1~14.04.3) ...
Setting up g++-4.8 (4.8.4-2ubuntu1~14.04.3) ...
Setting up g++ (4:4.8.2-1ubuntu6) ...
update-alternatives: using /usr/bin/g++ to provide /usr/bin/c++ (c++) in auto mode
Setting up libgfortran-4.8-dev:amd64 (4.8.4-2ubuntu1~14.04.3) ...
Setting up gfortran-4.8 (4.8.4-2ubuntu1~14.04.3) ...
Setting up gfortran (4:4.8.2-1ubuntu6) ...
update-alternatives: using /usr/bin/gfortran to provide /usr/bin/f95 (f95) in auto mode
Processing triggers for libc-bin (2.19-0ubuntu6.13) ...
vagrant@vagrant-ubuntu-trusty-64:/vagrant$
```

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# Unpack LAMMPS



2. vagrant@vagrant-ubuntu-trusty-64: /vagrant/lammps-24Jul17/lib/kim (ssh)

```
vagrant@vagrant-ubuntu-trusty-64:/vagrant$ tar xzf lammps-24Jul17.tar.gz
vagrant@vagrant-ubuntu-trusty-64:/vagrant$
vagrant@vagrant-ubuntu-trusty-64:/vagrant$
vagrant@vagrant-ubuntu-trusty-64:/vagrant$ mv Install.py lammps-24Jul17/lib/kim/
vagrant@vagrant-ubuntu-trusty-64:/vagrant$
vagrant@vagrant-ubuntu-trusty-64:/vagrant$
vagrant@vagrant-ubuntu-trusty-64:/vagrant$ ls -l
total 96264
drwxr-xr-x 1 vagrant vagrant      408 Jul 24 15:01 lammps-24Jul17
-rw-r--r-- 1 vagrant vagrant 98570047 Jul 31 23:48 lammps-24Jul17.tar.gz
-rw-r--r-- 1 vagrant vagrant      249 Jul 31 23:33 Vagrantfile
vagrant@vagrant-ubuntu-trusty-64:/vagrant$
vagrant@vagrant-ubuntu-trusty-64:/vagrant$
vagrant@vagrant-ubuntu-trusty-64:/vagrant$ cd lammps-24Jul17/lib/kim/
vagrant@vagrant-ubuntu-trusty-64:/vagrant/lammps-24Jul17/lib/kim$
vagrant@vagrant-ubuntu-trusty-64:/vagrant/lammps-24Jul17/lib/kim$
vagrant@vagrant-ubuntu-trusty-64:/vagrant/lammps-24Jul17/lib/kim$ ls -l
total 20
-rw-r--r-- 1 vagrant vagrant 8090 Jul 31 23:46 Install.py
-rw-r--r-- 1 vagrant vagrant 1319 Jul 13 17:28 Makefile.lammps
-rw-r--r-- 1 vagrant vagrant  198 Apr 13  2016 pair-kim.release.info
-rw-r--r-- 1 vagrant vagrant 2273 Jul 20 18:06 README
vagrant@vagrant-ubuntu-trusty-64:/vagrant/lammps-24Jul17/lib/kim$
```

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# The KIM Install.py script

2. vagrant@vagrant-ubuntu-trusty-64: /vagrant/lammps-24Jul17/lib/kim (vagrant)

```
vagrant@vagrant-ubuntu-trusty-64:/vagrant/lammps-24Jul17/lib/kim$ python Install.py

Syntax from src dir: make lib-kim args="-v version -b -a kim-name"
Syntax from lib dir: python Install.py -v version -b -a kim-name

specify one or more options, order does not matter

  -v = version of KIM API library to use
       default = kim-api-v1.8.2 (current as of June 2017)
  -b = download and build KIM API library with example Models
  -a = add single KIM model or model driver with kim-name
       to existing KIM API lib (see example below).
       If kim-name = everything, then rebuild KIM API library with
       all available OpenKIM Models (this implies -b).
  -vv = be more verbose about what is happening while the script runs

Examples:

make lib-kim args="-b"   # install KIM API lib with only example models
make lib-kim args="-b -a Glue_Ercolessi_Adams_Al__MO_324507536345_001"  # Ditto plus one
 model
make lib-kim args="-b -a everything"   # install KIM API lib with all models
make lib-kim args="-a EAM_Dynamo_Ackland_W__MO_141627196590_002"   # add one model or mo
del driver

See the list of KIM model drivers here:
https://openkim.org/kim-items/model-drivers/alphabetical

See the list of all KIM models here:
https://openkim.org/kim-items/models/by-model-drivers

See the list of example KIM models included by default here:
https://openkim.org/kim-api
in the "What is in the KIM API source package?" section

vagrant@vagrant-ubuntu-trusty-64:/vagrant/lammps-24Jul17/lib/kim$
```

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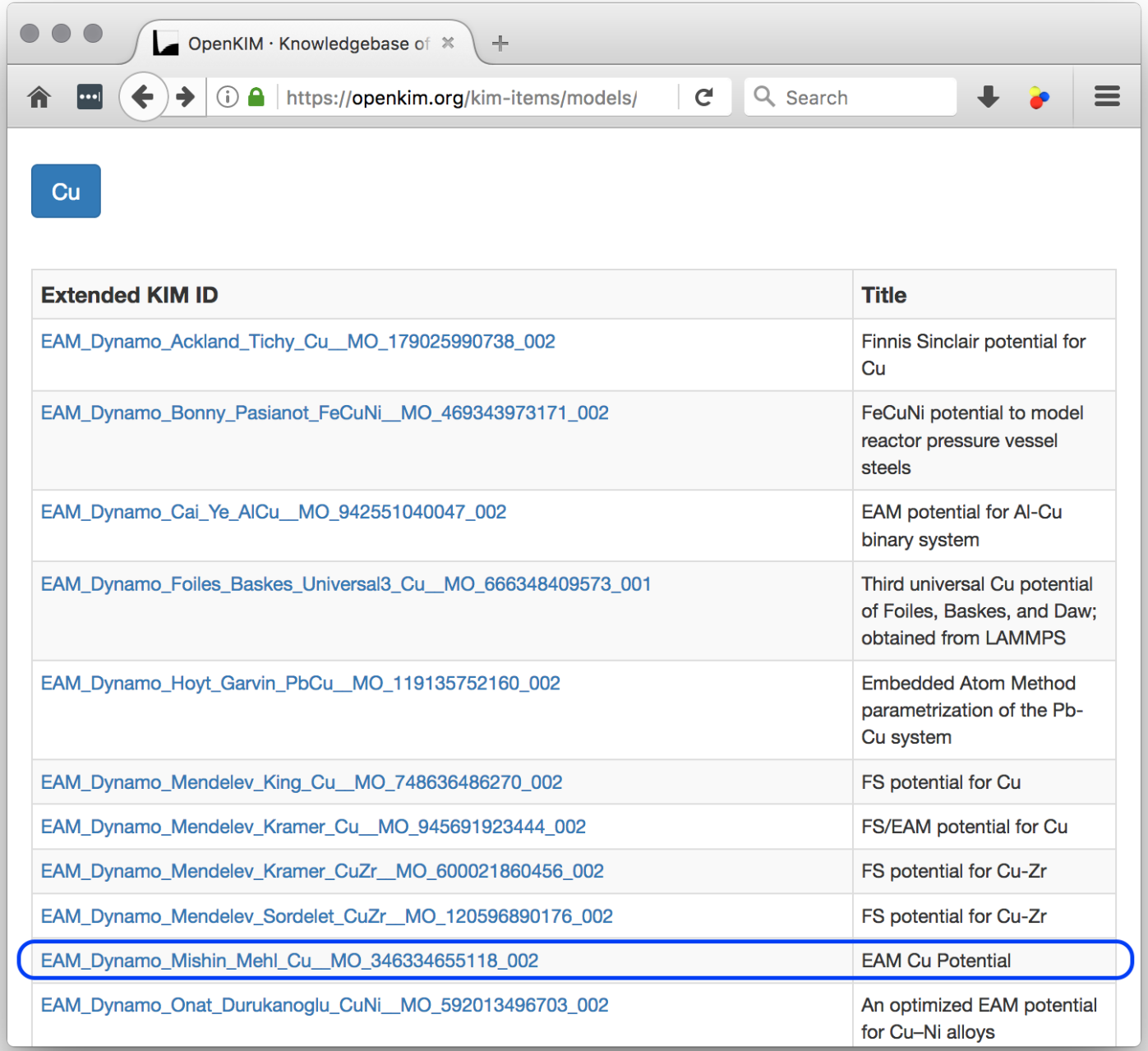
# OpenKIM Cu Models




| Extended KIM ID | Title |
|---|---|
| EAM_Dynamo_Ackland_Tichy_Cu__MO_179025990738_002 | Finnis Sinclair potential for Cu |
| EAM_Dynamo_Bonny_Pasianot_FeCuNi__MO_469343973171_002 | FeCuNi potential to model reactor pressure vessel steels |
| EAM_Dynamo_Cai_Ye_AlCu__MO_942551040047_002 | EAM potential for Al-Cu binary system |
| EAM_Dynamo_Foiles_Baskes_Universal3_Cu__MO_666348409573_001 | Third universal Cu potential of Foiles, Baskes, and Daw; obtained from LAMMPS |
| EAM_Dynamo_Hoyt_Garvin_PbCu__MO_119135752160_002 | Embedded Atom Method parametrization of the Pb-Cu system |
| EAM_Dynamo_Mendelev_King_Cu__MO_748636486270_002 | FS potential for Cu |
| EAM_Dynamo_Mendelev_Kramer_Cu__MO_945691923444_002 | FS/EAM potential for Cu |
| EAM_Dynamo_Mendelev_Kramer_CuZr__MO_600021860456_002 | FS potential for Cu-Zr |
| EAM_Dynamo_Mendelev_Sordelet_CuZr__MO_120596890176_002 | FS potential for Cu-Zr |
| EAM_Dynamo_Mishin_Mehl_Cu__MO_346334655118_002 | EAM Cu Potential |
| EAM_Dynamo_Onat_Durukanoglu_CuNi__MO_592013496703_002 | An optimized EAM potential for Cu–Ni alloys |

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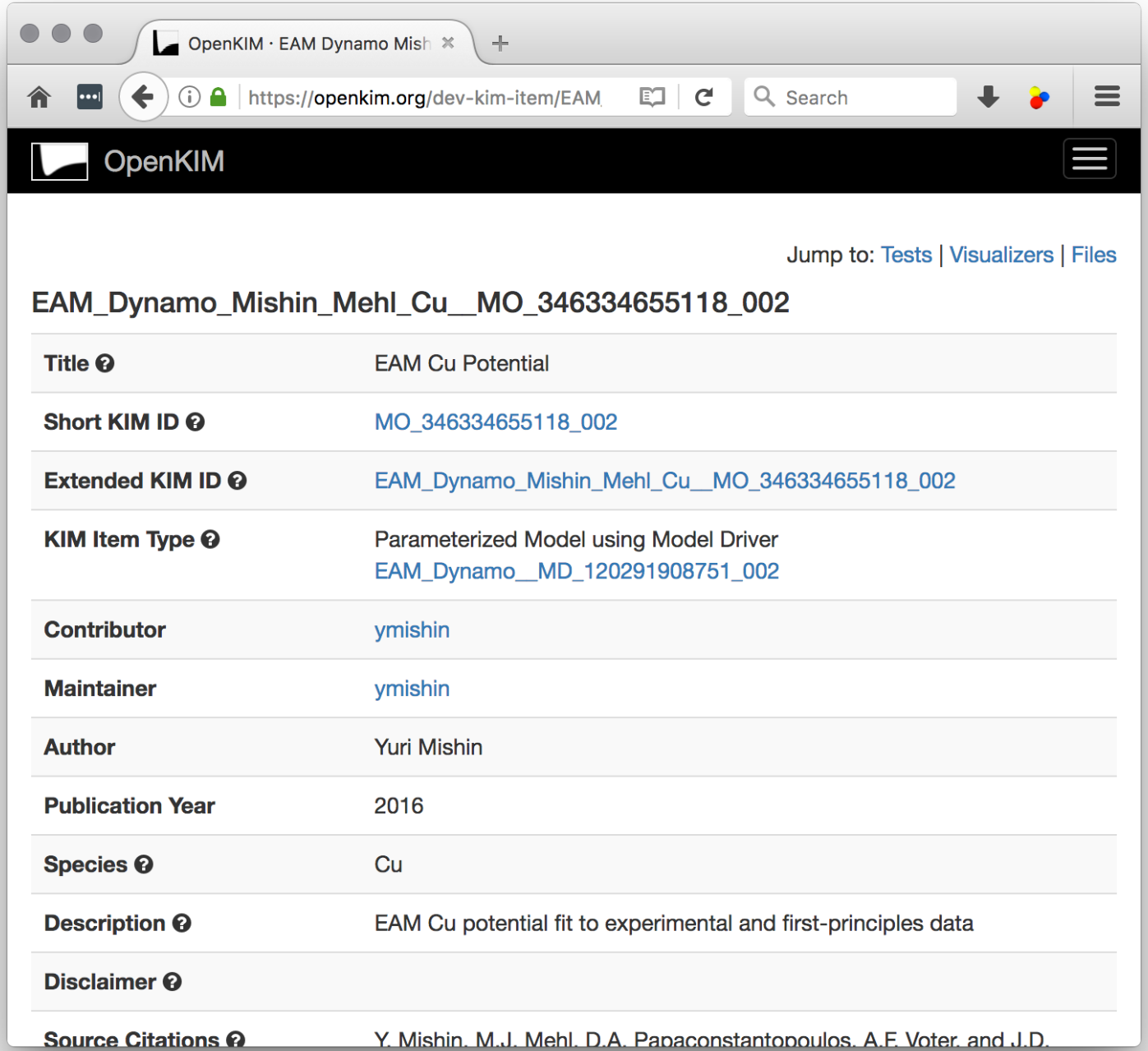
# The Mishin–Mehl EAM Model



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# Build KIM with example Models and Mishin–Mehl



2. vagrant@vagrant-ubuntu-trusty-64: /vagrant/lammps-24Jul17/lib/kim (vagrant)

```
vagrant@vagrant-ubuntu-trusty-64:/vagrant/lammps-24Jul17/lib/kim$ \
> python Install.py -b -a EAM_Dynamo_Mishin_Mehl_Cu__MO_346334655118_002
Created /vagrant/lammps-24Jul17/lib/kim/Makefile.KIM_DIR : using /vagrant/lammps-24Jul17
/lib/kim/installed-kim-api-v1.8.2
Downloading kim-api tarball ...
Unpacking kim-api tarball ...
Configuring kim-api ...
Configuring example Models
Building kim-api ...
Installing kim-api ...
Removing kim-api source and build files ...
Downloading tarball for EAM_Dynamo_Mishin_Mehl_Cu__MO_346334655118_002...
Unpacking item tarball ...
Building item ...
First installing model driver: EAM_Dynamo__MD_120291908751_002...
Now installing model : EAM_Dynamo_Mishin_Mehl_Cu__MO_346334655118_002
Downloading tarball for EAM_Dynamo_Mishin_Mehl_Cu__MO_346334655118_002...
Unpacking item tarball ...
Building item ...
Removing kim item source and build files ...

vagrant@vagrant-ubuntu-trusty-64:/vagrant/lammps-24Jul17/lib/kim$
vagrant@vagrant-ubuntu-trusty-64:/vagrant/lammps-24Jul17/lib/kim$ ls -l
total 28
drwxr-xr-x 1 vagrant vagrant  170 Aug  1 00:22 installed-kim-api-v1.8.2
-rw-r--r-- 1 vagrant vagrant 8090 Jul 31 23:46 Install.py
-rw-r--r-- 1 vagrant vagrant   96 Aug  1 00:22 Makefile.KIM_Config
-rw-r--r-- 1 vagrant vagrant  132 Aug  1 00:22 Makefile.KIM_DIR
-rw-r--r-- 1 vagrant vagrant 1319 Jul 13 17:28 Makefile.lammps
-rw-r--r-- 1 vagrant vagrant  198 Apr 13  2016 pair-kim.release.info
-rw-r--r-- 1 vagrant vagrant 2273 Jul 20 18:06 README
vagrant@vagrant-ubuntu-trusty-64:/vagrant/lammps-24Jul17/lib/kim$
```

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# Locally available Model listing



2. vagrant@vagrant-ubuntu-trusty-64: /vagrant/lammps-24Jul17/lib/kim (vagrant)

```
vagrant@vagrant-ubuntu-trusty-64:/vagrant/lammps-24Jul17/lib/kim$ \
> ls -l installed-kim-api-v1.8.2/lib/kim-api/models/
total 0
drwxr-xr-x 1 vagrant vagrant 136 Aug  1 00:23 EAM_Dynamo_Mishin_Mehl_Cu__MO_346334655118
_002
drwxr-xr-x 1 vagrant vagrant 136 Aug  1 00:22 ex_model_Al_PF_ErcolessiAdams
drwxr-xr-x 1 vagrant vagrant 136 Aug  1 00:22 ex_model_ArNe_P_MLJ_NEIGH_RVEC_F
drwxr-xr-x 1 vagrant vagrant 136 Aug  1 00:22 ex_model_Ar_P_LJ
drwxr-xr-x 1 vagrant vagrant 136 Aug  1 00:22 ex_model_Ar_P_MLJ_C
drwxr-xr-x 1 vagrant vagrant 136 Aug  1 00:22 ex_model_Ar_P_MLJ_CLUSTER_C
drwxr-xr-x 1 vagrant vagrant 136 Aug  1 00:22 ex_model_Ar_P_MLJ_CLUSTER_F03
drwxr-xr-x 1 vagrant vagrant 136 Aug  1 00:22 ex_model_Ar_P_MLJ_F03
drwxr-xr-x 1 vagrant vagrant 136 Aug  1 00:22 ex_model_Ar_P_MLJ_MI_OPBC_H_F
drwxr-xr-x 1 vagrant vagrant 136 Aug  1 00:22 ex_model_Ar_P_MLJ_NEIGH_PURE_H_F
drwxr-xr-x 1 vagrant vagrant 136 Aug  1 00:22 ex_model_Ar_P_MLJ_NEIGH_RVEC_F
drwxr-xr-x 1 vagrant vagrant 136 Aug  1 00:22 ex_model_Ar_P_Morse
drwxr-xr-x 1 vagrant vagrant 136 Aug  1 00:22 ex_model_Cu_PF_Johnson
drwxr-xr-x 1 vagrant vagrant 136 Aug  1 00:22 ex_model_Ne_P_fastLJ
drwxr-xr-x 1 vagrant vagrant 136 Aug  1 00:22 ex_model_Ne_P_LJ
drwxr-xr-x 1 vagrant vagrant 136 Aug  1 00:22 ex_model_Ne_P_LJ_NEIGH_PURE_H
drwxr-xr-x 1 vagrant vagrant 136 Aug  1 00:22 ex_model_Ne_P_MLJ_NEIGH_RVEC_H
drwxr-xr-x 1 vagrant vagrant 136 Aug  1 00:22 ex_model_Ne_P_Morse
vagrant@vagrant-ubuntu-trusty-64:/vagrant/lammps-24Jul17/lib/kim$
```

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# Build LAMMPS with KIM support



2. vagrant@vagrant-ubuntu-trusty-64: /vagrant/lammps-24Jul17/src (vagrant)

```
vagrant@vagrant-ubuntu-trusty-64:/vagrant/lammps-24Jul17/lib/kim$ cd ../../
vagrant@vagrant-ubuntu-trusty-64:/vagrant/lammps-24Jul17$
vagrant@vagrant-ubuntu-trusty-64:/vagrant/lammps-24Jul17$ cd src/STUBS
vagrant@vagrant-ubuntu-trusty-64:/vagrant/lammps-24Jul17/src/STUBS$
vagrant@vagrant-ubuntu-trusty-64:/vagrant/lammps-24Jul17/src/STUBS$ make
g++ -O -fPIC -I.  -c mpi.c
ar rs libmpi_stubs.a mpi.o
ar: creating libmpi_stubs.a
vagrant@vagrant-ubuntu-trusty-64:/vagrant/lammps-24Jul17/src/STUBS$
vagrant@vagrant-ubuntu-trusty-64:/vagrant/lammps-24Jul17/src/STUBS$ cd ../
vagrant@vagrant-ubuntu-trusty-64:/vagrant/lammps-24Jul17/src$
vagrant@vagrant-ubuntu-trusty-64:/vagrant/lammps-24Jul17/src$ make yes-kim
Installing package kim
vagrant@vagrant-ubuntu-trusty-64:/vagrant/lammps-24Jul17/src$
vagrant@vagrant-ubuntu-trusty-64:/vagrant/lammps-24Jul17/src$ \
> make serial > make.log 2>&1
vagrant@vagrant-ubuntu-trusty-64:/vagrant/lammps-24Jul17/src$
vagrant@vagrant-ubuntu-trusty-64:/vagrant/lammps-24Jul17/src$ \
> tail make.log | cut -b 1-80
         fgets(str,256,one);
                            ^
g++ -g -O3  -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64  -I../STUBS    -I/vagrant/lammps-
g++ -g -O3  -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64  -I../STUBS    -I/vagrant/lammps-
g++ -g -O3  -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64  -I../STUBS    -I/vagrant/lammps-
g++ -g -O  -L../STUBS   -m64 -L/vagrant/lammps-24Jul17/lib/kim/installed-kim-api
size ../lmp_serial
   text    data     bss     dec     hex filename
5358029    8032     936 5366997  51e4d5 ../lmp_serial
make[1]: Leaving directory `/vagrant/lammps-24Jul17/src/Obj_serial'
vagrant@vagrant-ubuntu-trusty-64:/vagrant/lammps-24Jul17/src$
```

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# Find the KIM example provided with LAMMPS



2. vagrant@vagrant-ubuntu-trusty-64: /vagrant/lammps-24Jul17/examples/kim (vagrant)

```
vagrant@vagrant-ubuntu-trusty-64:/vagrant/lammps-24Jul17/src$ cd ../examples/kim/
vagrant@vagrant-ubuntu-trusty-64:/vagrant/lammps-24Jul17/examples/kim$
vagrant@vagrant-ubuntu-trusty-64:/vagrant/lammps-24Jul17/examples/kim$ ls -l
total 32
-rw-r--r-- 1 vagrant vagrant  636 Jul 26  2013 in.kim.lj
-rw-r--r-- 1 vagrant vagrant  635 Jul 26  2013 in.kim.lj.lmp
-rw-r--r-- 1 vagrant vagrant  567 Aug  1 00:49 kim.log
-rw-r--r-- 1 vagrant vagrant 1146 Oct  6  2016 log.28Jun15.kim.lj.lmp.ubuntu.1
-rw-r--r-- 1 vagrant vagrant 1120 Oct  6  2016 log.28Jun15.kim.lj.lmp.ubuntu.4
-rw-r--r-- 1 vagrant vagrant 1145 Oct  6  2016 log.28Jun15.kim.lj.ubuntu.1
-rw-r--r-- 1 vagrant vagrant 1121 Oct  6  2016 log.28Jun15.kim.lj.ubuntu.4
-rw-r--r-- 1 vagrant vagrant 2743 Aug  1 00:49 log.lammps
vagrant@vagrant-ubuntu-trusty-64:/vagrant/lammps-24Jul17/examples/kim$
```

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# Run the KIM example in LAMMPS



2. vagrant@vagrant-ubuntu-trusty-64: /vagrant/lammps-24Jul17/examples/kim (vagrant)

```
vagrant@vagrant-ubuntu-trusty-64:/vagrant/lammps-24Jul17/examples/kim$ \
> ../../src/lmp_serial -in in.kim.lj > output 2>&1
vagrant@vagrant-ubuntu-trusty-64:/vagrant/lammps-24Jul17/examples/kim$
vagrant@vagrant-ubuntu-trusty-64:/vagrant/lammps-24Jul17/examples/kim$ \
> tail -20 output | cut -b 1-80
---------------------------------------------------------------
Pair    | 2.6345     | 2.6345     | 2.6345     |   0.0 | 82.46
Neigh   | 0.47449    | 0.47449    | 0.47449    |   0.0 | 14.85
Comm    | 0.028606   | 0.028606   | 0.028606   |   0.0 |  0.90
Output  | 9.1791e-05 | 9.1791e-05 | 9.1791e-05 |   0.0 |  0.00
Modify  | 0.034564   | 0.034564   | 0.034564   |   0.0 |  1.08
Other   |            | 0.0226     |            |       |  0.71

Nlocal:    32000 ave 32000 max 32000 min
Histogram: 1 0 0 0 0 0 0 0 0 0
Nghost:    20131 ave 20131 max 20131 min
Histogram: 1 0 0 0 0 0 0 0 0 0
Neighs:    2.09236e+06 ave 2.09236e+06 max 2.09236e+06 min
Histogram: 1 0 0 0 0 0 0 0 0 0

Total # of neighbors = 2092355
Ave neighs/atom = 65.3861
Neighbor list builds = 5
Dangerous builds = 0
Total wall time: 0:00:03
vagrant@vagrant-ubuntu-trusty-64:/vagrant/lammps-24Jul17/examples/kim$
```

R. S. Elliott

# Put LAMMPS (temporally) on the system PATH



2. vagrant@vagrant-ubuntu-trusty-64: /vagrant (vagrant)

```
vagrant@vagrant-ubuntu-trusty-64:/vagrant/lammps-24Jul17/examples/kim$ cd ../../../
vagrant@vagrant-ubuntu-trusty-64:/vagrant$
vagrant@vagrant-ubuntu-trusty-64:/vagrant$ ls -l
total 96264
drwxr-xr-x 1 vagrant vagrant      408 Jul 24 15:01 lammps-24Jul17
-rw-r--r-- 1 vagrant vagrant 98570047 Jul 31 23:48 lammps-24Jul17.tar.gz
-rw-r--r-- 1 vagrant vagrant      249 Jul 31 23:33 Vagrantfile
vagrant@vagrant-ubuntu-trusty-64:/vagrant$
vagrant@vagrant-ubuntu-trusty-64:/vagrant$
vagrant@vagrant-ubuntu-trusty-64:/vagrant$ ln -s lammps-24Jul17/src/lmp_serial lammps
vagrant@vagrant-ubuntu-trusty-64:/vagrant$
vagrant@vagrant-ubuntu-trusty-64:/vagrant$ ls -l
total 96268
lrwxr-xr-x 1 vagrant vagrant       29 Aug  1 00:59 lammps -> lammps-24Jul17/src/lmp_seri
al
drwxr-xr-x 1 vagrant vagrant      408 Jul 24 15:01 lammps-24Jul17
-rw-r--r-- 1 vagrant vagrant 98570047 Jul 31 23:48 lammps-24Jul17.tar.gz
-rw-r--r-- 1 vagrant vagrant      249 Jul 31 23:33 Vagrantfile
vagrant@vagrant-ubuntu-trusty-64:/vagrant$
vagrant@vagrant-ubuntu-trusty-64:/vagrant$ \
> export PATH=${PATH}:/vagrant
vagrant@vagrant-ubuntu-trusty-64:/vagrant$
vagrant@vagrant-ubuntu-trusty-64:/vagrant$ printf "\n\n${PATH}\n\n"


/usr/local/sbin:/usr/local/bin:/usr/sbin:/usr/bin:/sbin:/bin:/usr/games:/usr/local/games
:/vagrant

vagrant@vagrant-ubuntu-trusty-64:/vagrant$ lammps
LAMMPS (24 Jul 2017)
^C
vagrant@vagrant-ubuntu-trusty-64:/vagrant$
```

R. S. Elliott



# Find OpenKIM.org Test Drivers that use LAMMPS

Nearly all OpenKIM.org Test Drivers use either:

Atomic Simulation Environment (ASE) OR LAMMPS

The Test Drivers that use LAMMPS are:

- ClusterEnergyAndForces__TD_000043093022_001
- CohesiveEnergyVsLatticeConstant__TD_554653289799_001
- Grain_Boundary_Symmetric_Tilt_Relaxed_Energy_vs_Angle_Cubic_Crystal__TD_410381120771_000
- LammpsExample2__TD_887699523131_002
- LammpsExample__TD_567444853524_003
- LatticeConstant2DHexagonalEnergy__TD_034540307932_000
- LatticeConstantHexagonalEnergy__TD_942334626465_002
- LinearThermalExpansionCoeffCubic__TD_522633393614_000
- TriclinicPBCEnergyAndForces__TD_892847239811_001

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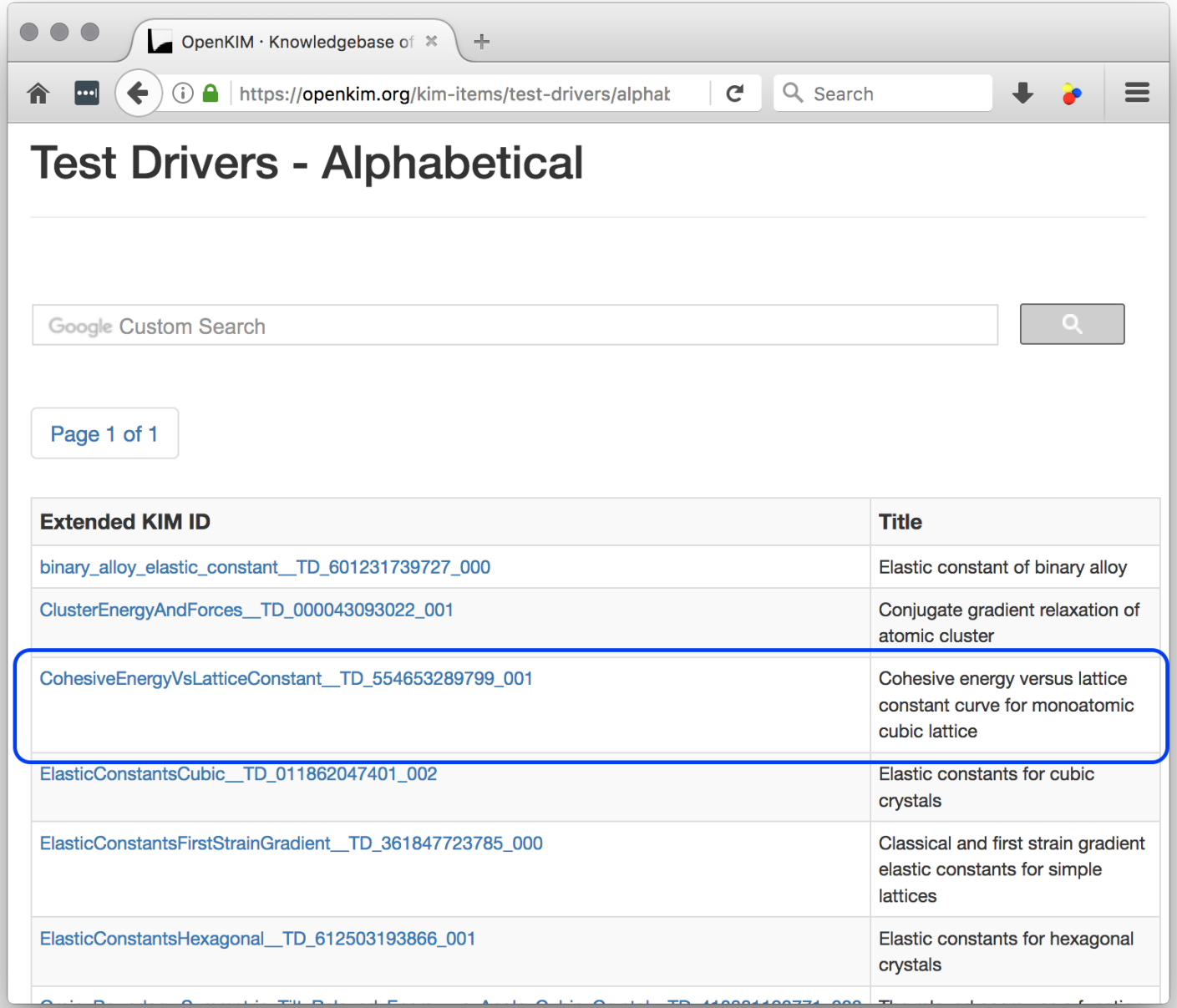
# OpenKIM.org Test Drivers



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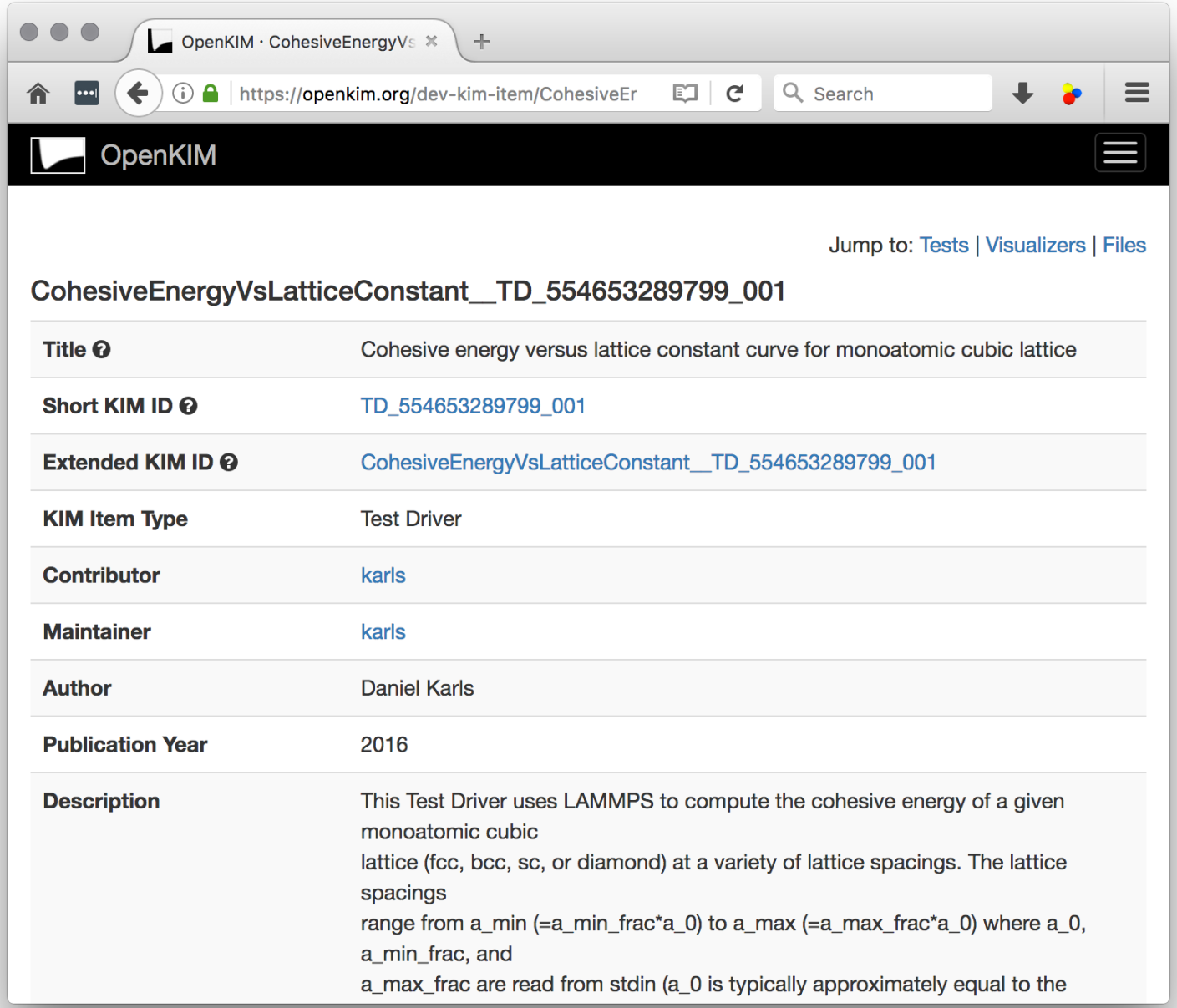
# OpenKIM.org LAMMPS Test Driver



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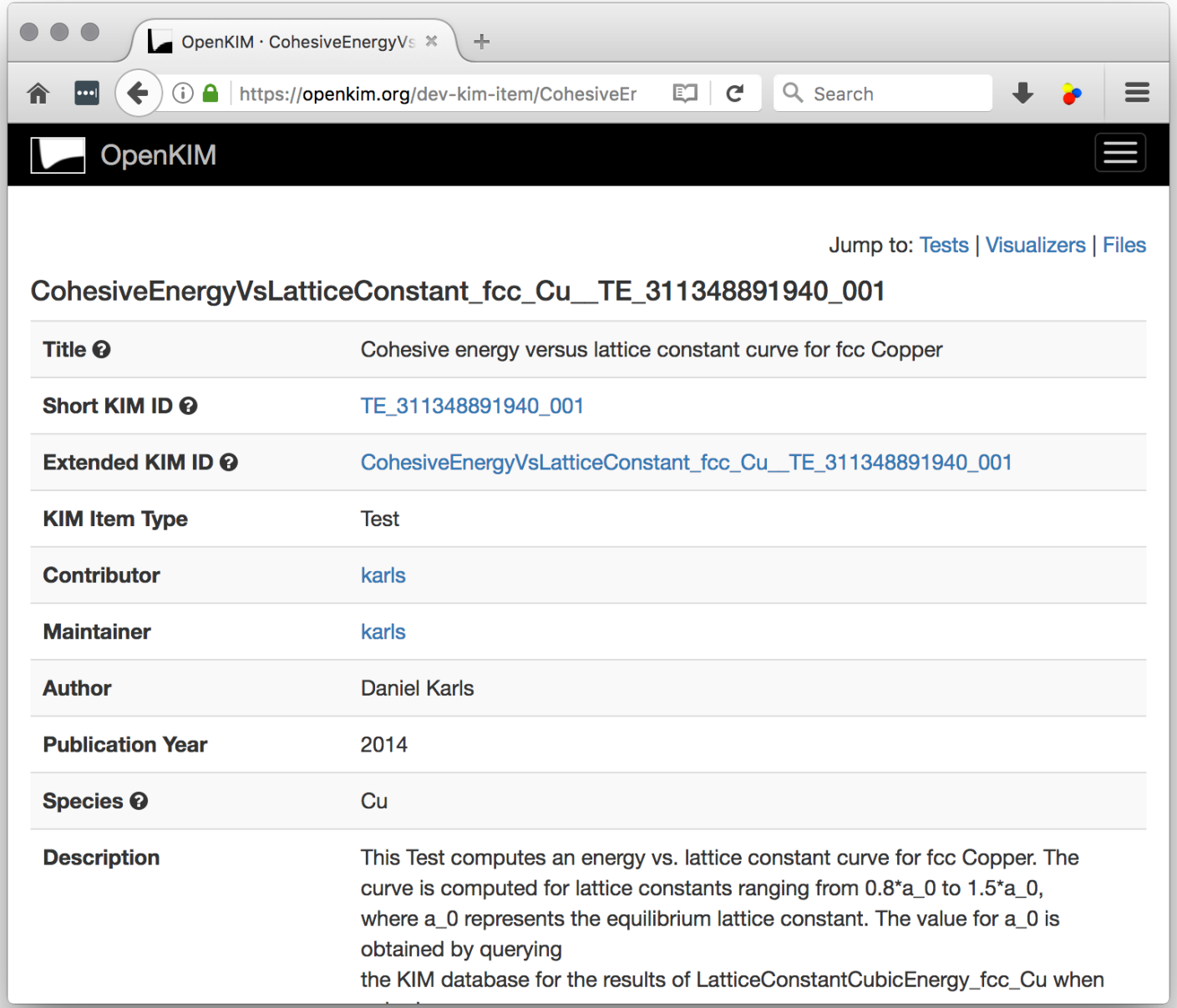
# Cu FCC Test from OpenKIM.org



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# Download the Test and Test Driver

OpenKIM · CohesiveEnergyVs

https://openkim.org/dev-kim-item/CohesiveEr

Search

## Download

| | | |
|---|---|---|
| CohesiveEnergyVsLatticeConstant_fcc_Cu__TE_311348891940_001.txz | Tar+XZ | Linux and OS X archive (modern compression) |
| CohesiveEnergyVsLatticeConstant_fcc_Cu__TE_311348891940_001.tgz | Tar+Gzip | Linux and OS X archive (legacy compression) |
| CohesiveEnergyVsLatticeConstant_fcc_Cu__TE_311348891940_001.zip | Zip | Windows archive |

## Download Dependency

This Test requires a Test Driver. Archives for the Test Driver CohesiveEnergyVsLatticeConstant__TD_554653289799_001 appear below.

| | | |
|---|---|---|
| CohesiveEnergyVsLatticeConstant__TD_554653289799_001.txz | Tar+XZ | Linux and OS X archive (modern compression) |
| CohesiveEnergyVsLatticeConstant__TD_554653289799_001.tgz | Tar+Gzip | Linux and OS X archive (legacy compression) |
| CohesiveEnergyVsLatticeConstant__TD_554653289799_001.zip | Zip | Windows archive |

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# Unpack the Test and Test Driver





2. vagrant@vagrant-ubuntu-trusty-64: /vagrant (vagrant)

```
vagrant@vagrant-ubuntu-trusty-64:/vagrant$ ls -1
CohesiveEnergyVsLatticeConstant_fcc_Cu__TE_311348891940_001.tgz
CohesiveEnergyVsLatticeConstant__TD_554653289799_001.tgz
lammps
lammps-24Jul17
lammps-24Jul17.tar.gz
Vagrantfile
vagrant@vagrant-ubuntu-trusty-64:/vagrant$ \
> tar xzf CohesiveEnergyVsLatticeConstant__TD_554653289799_001.tgz
vagrant@vagrant-ubuntu-trusty-64:/vagrant$
vagrant@vagrant-ubuntu-trusty-64:/vagrant$ \
> tar xzf CohesiveEnergyVsLatticeConstant_fcc_Cu__TE_311348891940_001.tgz
vagrant@vagrant-ubuntu-trusty-64:/vagrant$
vagrant@vagrant-ubuntu-trusty-64:/vagrant$ ls -1
CohesiveEnergyVsLatticeConstant_fcc_Cu__TE_311348891940_001
CohesiveEnergyVsLatticeConstant_fcc_Cu__TE_311348891940_001.tgz
CohesiveEnergyVsLatticeConstant__TD_554653289799_001
CohesiveEnergyVsLatticeConstant__TD_554653289799_001.tgz
lammps
lammps-24Jul17
lammps-24Jul17.tar.gz
Vagrantfile
vagrant@vagrant-ubuntu-trusty-64:/vagrant$ \
> mv CohesiveEnergyVsLatticeConstant__TD_554653289799_001 test-driver
vagrant@vagrant-ubuntu-trusty-64:/vagrant$
vagrant@vagrant-ubuntu-trusty-64:/vagrant$ \
> mv CohesiveEnergyVsLatticeConstant_fcc_Cu__TE_311348891940_001 test
vagrant@vagrant-ubuntu-trusty-64:/vagrant$
vagrant@vagrant-ubuntu-trusty-64:/vagrant$ ls -1
CohesiveEnergyVsLatticeConstant_fcc_Cu__TE_311348891940_001.tgz
CohesiveEnergyVsLatticeConstant__TD_554653289799_001.tgz
lammps
lammps-24Jul17
lammps-24Jul17.tar.gz
test
test-driver
Vagrantfile
vagrant@vagrant-ubuntu-trusty-64:/vagrant$
```

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# Listing of Test files and `pipeline.stdin.tpl`



2. vagrant@vagrant-ubuntu-trusty-64: /vagrant/test (vagrant)

```
vagrant@vagrant-ubuntu-trusty-64:/vagrant$ cd test
vagrant@vagrant-ubuntu-trusty-64:/vagrant/test$
vagrant@vagrant-ubuntu-trusty-64:/vagrant/test$ ls -l
total 48
-rw-r--r-- 1 vagrant vagrant    21 Aug  1 01:11 dependencies.edn
-rw-r--r-- 1 vagrant vagrant   930 Aug  1 01:11 descriptor.kim
-rw-r--r-- 1 vagrant vagrant  2334 Aug  1 01:11 kimprovenance.edn
-rw-r--r-- 1 vagrant vagrant   877 Aug  1 01:11 kimspec.edn
-rw-r--r-- 1 vagrant vagrant 16373 Aug  1 01:11 LICENSE.CDDL
-rw-r--r-- 1 vagrant vagrant    71 Aug  1 01:11 Makefile
-rw-r--r-- 1 vagrant vagrant   363 Aug  1 01:11 pipeline.stdin.tpl
-rw-r--r-- 1 vagrant vagrant   562 Aug  1 01:11 README.txt
-rwxr-xr-x 1 vagrant vagrant   405 Aug  1 01:11 runner
vagrant@vagrant-ubuntu-trusty-64:/vagrant/test$
vagrant@vagrant-ubuntu-trusty-64:/vagrant/test$ cat pipeline.stdin.tpl | cut -b 1-80
@< path("CohesiveEnergyVsLatticeConstant__TD_554653289799_001") >@
@< MODELNAME >@
Cu
63.546
fcc
@< query({"flat": "on", "database": "data", "fields": {"_id": 0, "meta.runner._i
"TE_387272513402"
}, "meta.subject._id": MODELNAME},"project":["a.source-value"]}) >@
0.8
1.5
18
23
8
20
vagrant@vagrant-ubuntu-trusty-64:/vagrant/test$
```

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# Preparing the ex_model_Cu_PF_Johnson Test



2. vagrant@vagrant-ubuntu-trusty-64: /vagrant/test/output (vagrant)

```
vagrant@vagrant-ubuntu-trusty-64:/vagrant/test$ mkdir output
vagrant@vagrant-ubuntu-trusty-64:/vagrant/test$
vagrant@vagrant-ubuntu-trusty-64:/vagrant/test$ \
> cp pipeline.stdin.tpl output/pipeline.stdin
vagrant@vagrant-ubuntu-trusty-64:/vagrant/test$
vagrant@vagrant-ubuntu-trusty-64:/vagrant/test$ cd output/
vagrant@vagrant-ubuntu-trusty-64:/vagrant/test/output$
vagrant@vagrant-ubuntu-trusty-64:/vagrant/test/output$ ls -l
total 4
-rw-r--r-- 1 vagrant vagrant 363 Aug  1  2017 pipeline.stdin
vagrant@vagrant-ubuntu-trusty-64:/vagrant/test/output$
vagrant@vagrant-ubuntu-trusty-64:/vagrant/test/output$ vi pipeline.stdin
vagrant@vagrant-ubuntu-trusty-64:/vagrant/test/output$
vagrant@vagrant-ubuntu-trusty-64:/vagrant/test/output$ cat pipeline.stdin
../test-driver/runner
ex_model_Cu_PF_Johnson
Cu
63.546
fcc
3.615
0.8
1.5
18
23
8
20
vagrant@vagrant-ubuntu-trusty-64:/vagrant/test/output$
```

R. S. Elliott

# Running the ex_model_Cu_PF_Johnson Test



2. vagrant@vagrant-ubuntu-trusty-64: /vagrant/test (vagrant)

```
vagrant@vagrant-ubuntu-trusty-64:/vagrant/test/output$ cd ../
vagrant@vagrant-ubuntu-trusty-64:/vagrant/test$
vagrant@vagrant-ubuntu-trusty-64:/vagrant/test$ ls -l
total 48
-rw-r--r-- 1 vagrant vagrant    21 Aug  1 01:11 dependencies.edn
-rw-r--r-- 1 vagrant vagrant   930 Aug  1 01:11 descriptor.kim
-rw-r--r-- 1 vagrant vagrant  2334 Aug  1 01:11 kimprovenance.edn
-rw-r--r-- 1 vagrant vagrant   877 Aug  1 01:11 kimspec.edn
-rw-r--r-- 1 vagrant vagrant 16373 Aug  1 01:11 LICENSE.CDDL
-rw-r--r-- 1 vagrant vagrant    71 Aug  1 01:11 Makefile
drwxr-xr-x 1 vagrant vagrant   204 Aug  1  2017 output
-rw-r--r-- 1 vagrant vagrant   363 Aug  1 01:54 pipeline.stdin.tpl
-rw-r--r-- 1 vagrant vagrant   562 Aug  1 01:11 README.txt
-rwxr-xr-x 1 vagrant vagrant   405 Aug  1 01:11 runner
vagrant@vagrant-ubuntu-trusty-64:/vagrant/test$
vagrant@vagrant-ubuntu-trusty-64:/vagrant/test$
vagrant@vagrant-ubuntu-trusty-64:/vagrant/test$ \
> ./runner < output/pipeline.stdin > output/pipeline.stdout 2> output/pipeline.stderr
vagrant@vagrant-ubuntu-trusty-64:/vagrant/test$
vagrant@vagrant-ubuntu-trusty-64:/vagrant/test$
vagrant@vagrant-ubuntu-trusty-64:/vagrant/test$ ls -l output/
total 112
-rw-r--r-- 1 vagrant vagrant   669 Aug  1  2017 lammps.dump
-rw-r--r-- 1 vagrant vagrant  1991 Aug  1  2017 lammps.in
-rw-r--r-- 1 vagrant vagrant 90982 Aug  1  2017 lammps.log
-rw-r--r-- 1 vagrant vagrant     0 Aug  1  2017 pipeline.stderr
-rw-r--r-- 1 vagrant vagrant    84 Aug  1  2017 pipeline.stdin
-rw-r--r-- 1 vagrant vagrant  1409 Aug  1  2017 pipeline.stdout
-rw-r--r-- 1 vagrant vagrant  1343 Aug  1  2017 results.edn
vagrant@vagrant-ubuntu-trusty-64:/vagrant/test$
```

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# Results from the ex_model_Cu_PF_Johnson Test



2. vagrant@vagrant-ubuntu-trusty-64: /vagrant/test/output (vagrant)

```
vagrant@vagrant-ubuntu-trusty-64:/vagrant/test$ cd output/
vagrant@vagrant-ubuntu-trusty-64:/vagrant/test/output$
vagrant@vagrant-ubuntu-trusty-64:/vagrant/test/output$ cat results.edn | cut -b 1-80
{
  "property-id" "tag:staff@noreply.openkim.org,2014-04-15:property/cohesive-ener
  "instance-id" 1
  "short-name" {
    "source-value" [ "fcc" ]
  }
  "species" {
    "source-value" [
      "Cu"
      "Cu"
      "Cu"
      "Cu"
    ]
  }
  "a" {
    "source-value" [ 5.422500  5.059172  4.833997  4.670394  4.541823  4.435894
    "source-unit" "angstrom"
  }
  "basis-atom-coordinates" {
    "source-value" [
      [   0    0    0 ]
      [   0  0.5  0.5 ]
      [ 0.5    0  0.5 ]
      [ 0.5  0.5    0 ]
    ]
  }
  "cohesive-potential-energy" {
    "source-value" [ 0  0  1.72759  1.99072  2.2121  2.4018  2.56623  2.7098  2.
    "source-unit" "eV"
  }
}
vagrant@vagrant-ubuntu-trusty-64:/vagrant/test/output$
```

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# Preparing and running the Mishin–Mehl Test



2. vagrant@vagrant-ubuntu-trusty-64: /vagrant/test (vagrant)

```
vagrant@vagrant-ubuntu-trusty-64:/vagrant/test/output$ cd ..
vagrant@vagrant-ubuntu-trusty-64:/vagrant/test$
vagrant@vagrant-ubuntu-trusty-64:/vagrant/test$ mv output output-johnson
vagrant@vagrant-ubuntu-trusty-64:/vagrant/test$
vagrant@vagrant-ubuntu-trusty-64:/vagrant/test$ mkdir output
vagrant@vagrant-ubuntu-trusty-64:/vagrant/test$
vagrant@vagrant-ubuntu-trusty-64:/vagrant/test$ \
> cp pipeline.stdin.tpl output/pipeline.stdin
vagrant@vagrant-ubuntu-trusty-64:/vagrant/test$
vagrant@vagrant-ubuntu-trusty-64:/vagrant/test$ vi output/pipeline.stdin
vagrant@vagrant-ubuntu-trusty-64:/vagrant/test$
vagrant@vagrant-ubuntu-trusty-64:/vagrant/test$ cat output/pipeline.stdin
../test-driver/runner
EAM_Dynamo_Mishin_Mehl_Cu__MO_346334655118_002
Cu
63.546
fcc
3.615
0.8
1.5
18
23
8
20
vagrant@vagrant-ubuntu-trusty-64:/vagrant/test$
vagrant@vagrant-ubuntu-trusty-64:/vagrant/test$ \
> ./runner < output/pipeline.stdin > output/pipeline.stdout 2> output/pipeline.stderr
vagrant@vagrant-ubuntu-trusty-64:/vagrant/test$
vagrant@vagrant-ubuntu-trusty-64:/vagrant/test$ ls -l output
total 108
-rw-r--r-- 1 vagrant vagrant   669 Aug  1  2017 lammps.dump
-rw-r--r-- 1 vagrant vagrant  2015 Aug  1  2017 lammps.in
-rw-r--r-- 1 vagrant vagrant 87163 Aug  1  2017 lammps.log
-rw-r--r-- 1 vagrant vagrant     0 Aug  1  2017 pipeline.stderr
-rw-r--r-- 1 vagrant vagrant   108 Aug  1  2017 pipeline.stdin
-rw-r--r-- 1 vagrant vagrant  1409 Aug  1  2017 pipeline.stdout
-rw-r--r-- 1 vagrant vagrant  1361 Aug  1  2017 results.edn
vagrant@vagrant-ubuntu-trusty-64:/vagrant/test$
```

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# Results from the Mishin–Mehl Test



2. vagrant@vagrant-ubuntu-trusty-64: /vagrant/test/output (vagrant)

```
vagrant@vagrant-ubuntu-trusty-64:/vagrant/test$ cd output
vagrant@vagrant-ubuntu-trusty-64:/vagrant/test/output$
vagrant@vagrant-ubuntu-trusty-64:/vagrant/test/output$ cat results.edn | cut -b 1-80
{
  "property-id" "tag:staff@noreply.openkim.org,2014-04-15:property/cohesive-ener
  "instance-id" 1
  "short-name" {
    "source-value" [ "fcc" ]
  }
  "species" {
    "source-value" [
      "Cu"
      "Cu"
      "Cu"
      "Cu"
    ]
  }
  "a" {
    "source-value" [ 5.422500  5.059172  4.833997  4.670394  4.541823  4.435894
    "source-unit" "angstrom"
  }
  "basis-atom-coordinates" {
    "source-value" [
      [   0    0    0 ]
      [   0  0.5  0.5 ]
      [ 0.5    0  0.5 ]
      [ 0.5  0.5    0 ]
    ]
  }
  "cohesive-potential-energy" {
    "source-value" [ 0.905059  1.3868  1.74769  2.02858  2.25389  2.43959  2.595
    "source-unit" "eV"
  }
}
vagrant@vagrant-ubuntu-trusty-64:/vagrant/test/output$
```

R. S. Elliott

# Listing of results directories



2. vagrant@vagrant-ubuntu-trusty-64: /vagrant/test (vagrant)

```
vagrant@vagrant-ubuntu-trusty-64:/vagrant/test/output$ cd ../
vagrant@vagrant-ubuntu-trusty-64:/vagrant/test$
vagrant@vagrant-ubuntu-trusty-64:/vagrant/test$ mv output output-mishin-mehl
vagrant@vagrant-ubuntu-trusty-64:/vagrant/test$
vagrant@vagrant-ubuntu-trusty-64:/vagrant/test$ ls -l
total 220
-rw-r--r-- 1 vagrant vagrant     21 Aug  1 01:11 dependencies.edn
-rw-r--r-- 1 vagrant vagrant    930 Aug  1 01:11 descriptor.kim
-rw-r--r-- 1 vagrant vagrant    645 Aug  1  2017 kim.log
-rw-r--r-- 1 vagrant vagrant   2334 Aug  1 01:11 kimprovenance.edn
-rw-r--r-- 1 vagrant vagrant    877 Aug  1 01:11 kimspec.edn
-rw-r--r-- 1 vagrant vagrant  16373 Aug  1 01:11 LICENSE.CDDL
-rw-r--r-- 1 vagrant vagrant 168685 Aug  1  2017 log.lammps
-rw-r--r-- 1 vagrant vagrant     71 Aug  1 01:11 Makefile
drwxr-xr-x 1 vagrant vagrant    306 Aug  1 02:10 output-johnson
drwxr-xr-x 1 vagrant vagrant    306 Aug  1  2017 output-mishin-mehl
-rw-r--r-- 1 vagrant vagrant    363 Aug  1 01:54 pipeline.stdin.tpl
-rw-r--r-- 1 vagrant vagrant    562 Aug  1 01:11 README.txt
-rwxr-xr-x 1 vagrant vagrant    405 Aug  1 01:11 runner
vagrant@vagrant-ubuntu-trusty-64:/vagrant/test$
```

R. S. Elliott

# Plot of Energy vs. Lattice Constant results



Using your favorite edn parser and visualization packages,
we can visualize and compare the results