

# 1. Downloading LAMMPS and aenet-lammps package from GitHub

This manual explains only clean install case using gnu g++, gfortran, and openmpi under linux OS.

If you make use of the aenet-LAMMPS interface, please cite the following references:

- [1] H. Mori and T. Ozaki, Phys. Rev. Materials 4 (2020) 040601.
- [2] M.S. Chen, T. Morawietz, H. Mori, T.E. Markland, N. Artrith, AENET-LAMMPS and AENET-TINKER: Interfaces for Accurate and Efficient Molecular Dynamics Simulations with Machine Learning Potentials, in preparation (2021).

Additional references:

- [3] ænet: N. Artrith and A. Urban, Comput. Mater. Sci. 114, 135 (2016).
- [4] LAMMPS: S. Plimpton, J. Comput. Phys. 117, 1 (1995).

Author & contact information

Author: Hideki Mori, College of Industrial Technology, Japan E-mail: morih@cit.sangitan.ac.jp or morih.cit.01@gmail.com

In [1]:

```
!wget https://github.com/lammps/lammps/archive/refs/tags/stable_290ct2020.tar
!wget https://github.com/HidekiMori-CIT/aenet-lammps/archive/refs/tags/2021Ma

--2021-07-17 14:34:32-- https://github.com/lammps/lammps/archive/refs/tags/s
table_290ct2020.tar.gz
Resolving github.com (github.com)... 140.82.114.4
Connecting to github.com (github.com)|140.82.114.4|:443... connected.
HTTP request sent, awaiting response... 302 Found
Location: https://codeload.github.com/lammps/lammps/tar.gz/refs/tags/stable_2
90ct2020 [following]
--2021-07-17 14:34:32-- https://codeload.github.com/lammps/lammps/tar.gz/ref
s/tags/stable_290ct2020
Resolving codeload.github.com (codeload.github.com)... 140.82.112.10
Connecting to codeload.github.com (codeload.github.com)|140.82.112.10|:443...
connected.
HTTP request sent, awaiting response... 200 OK
Length: unspecified [application/x-gzip]
Saving to: 'stable_290ct2020.tar.gz'

stable_290ct2020.ta      [          <=>  ] 121.19M  6.69MB/s   in 17s

2021-07-17 14:34:49 (7.19 MB/s) - 'stable_290ct2020.tar.gz' saved [127074024]

--2021-07-17 14:34:49-- https://github.com/HidekiMori-CIT/aenet-lammps/archi
ve/refs/tags/2021May04.tar.gz
Resolving github.com (github.com)... 140.82.114.4
Connecting to github.com (github.com)|140.82.114.4|:443... connected.
```

```

HTTP request sent, awaiting response... 302 Found
Location: https://codeload.github.com/HidekiMori-CIT/aenet-lammps/tar.gz/refs/
/tags/2021May04 [following]
--2021-07-17 14:34:49-- https://codeload.github.com/HidekiMori-CIT/aenet-lam
mps/tar.gz/refs/tags/2021May04
Resolving codeload.github.com (codeload.github.com)... 140.82.112.10
Connecting to codeload.github.com (codeload.github.com)|140.82.112.10|:443...
connected.
HTTP request sent, awaiting response... 200 OK
Length: unspecified [application/x-gzip]
Saving to: '2021May04.tar.gz'

```

```
2021May04.tar.gz          [ <=>          ] 37.48K --.-KB/s    in 0.006s
```

```
2021-07-17 14:34:50 (5.66 MB/s) - '2021May04.tar.gz' saved [38379]
```

## 2. Unpacking (and copy) LAMMPS and aenet-lammps package

Unpack the LAMMPS and aenet-lammps package. And copy USER-AENET/ and aenet/ in aenet-lammps/ to src/ and lib/ in lammps-29Oct20, respectively.

In [2]:

```

!tar xvzf stable_29oct2020.tar.gz
!tar xvzf 2021May04.tar.gz
%cp -r aenet-lammps-2021May04/USER-AENET/ lammps-stable_29oct2020/src/
%cp -r aenet-lammps-2021May04/aenet/ lammps-stable_29oct2020/lib/

```

```

lammps-stable_29oct2020/
lammps-stable_29oct2020/LICENSE
lammps-stable_29oct2020/README
lammps-stable_29oct2020/bench/
lammps-stable_29oct2020/bench/Cu_u3.eam
lammps-stable_29oct2020/bench/POTENTIALS/
lammps-stable_29oct2020/bench/POTENTIALS/CH.airebo
lammps-stable_29oct2020/bench/POTENTIALS/CH.rebo
lammps-stable_29oct2020/bench/POTENTIALS/CdTe.bop.table
lammps-stable_29oct2020/bench/POTENTIALS/Cu_u3.eam
lammps-stable_29oct2020/bench/POTENTIALS/Ni.adp
lammps-stable_29oct2020/bench/POTENTIALS/Ni.meam
lammps-stable_29oct2020/bench/POTENTIALS/README
lammps-stable_29oct2020/bench/POTENTIALS/Si.sw
lammps-stable_29oct2020/bench/POTENTIALS/Si.tersoff
lammps-stable_29oct2020/bench/POTENTIALS/data.airebo
lammps-stable_29oct2020/bench/POTENTIALS/data.comb
lammps-stable_29oct2020/bench/POTENTIALS/data.eff
lammps-stable_29oct2020/bench/POTENTIALS/data.eim
lammps-stable_29oct2020/bench/POTENTIALS/data.fene
lammps-stable_29oct2020/bench/POTENTIALS/data.gb
lammps-stable_29oct2020/bench/POTENTIALS/data.granular
lammps-stable_29oct2020/bench/POTENTIALS/data.protein
lammps-stable_29oct2020/bench/POTENTIALS/data.reax
lammps-stable_29oct2020/bench/POTENTIALS/data.rebo
lammps-stable_29oct2020/bench/POTENTIALS/data.spce
lammps-stable_29oct2020/bench/POTENTIALS/ffield.comb
lammps-stable_29oct2020/bench/POTENTIALS/ffield.eim

```

lammps-stable\_290ct2020/bench/POTENTIALS/ffield.reax  
lammps-stable\_290ct2020/bench/POTENTIALS/in.adp  
lammps-stable\_290ct2020/bench/POTENTIALS/in.airebo  
lammps-stable\_290ct2020/bench/POTENTIALS/in.bop  
lammps-stable\_290ct2020/bench/POTENTIALS/in.comb  
lammps-stable\_290ct2020/bench/POTENTIALS/in.dpd  
lammps-stable\_290ct2020/bench/POTENTIALS/in.eam  
lammps-stable\_290ct2020/bench/POTENTIALS/in.eff  
lammps-stable\_290ct2020/bench/POTENTIALS/in.eim  
lammps-stable\_290ct2020/bench/POTENTIALS/in.fene  
lammps-stable\_290ct2020/bench/POTENTIALS/in.gb  
lammps-stable\_290ct2020/bench/POTENTIALS/in.granular  
lammps-stable\_290ct2020/bench/POTENTIALS/in.lj  
lammps-stable\_290ct2020/bench/POTENTIALS/in.meamc  
lammps-stable\_290ct2020/bench/POTENTIALS/in.peri  
lammps-stable\_290ct2020/bench/POTENTIALS/in.protein  
lammps-stable\_290ct2020/bench/POTENTIALS/in.reaxc  
lammps-stable\_290ct2020/bench/POTENTIALS/in.rebo  
lammps-stable\_290ct2020/bench/POTENTIALS/in.spce  
lammps-stable\_290ct2020/bench/POTENTIALS/in.sw  
lammps-stable\_290ct2020/bench/POTENTIALS/in.tersoff  
lammps-stable\_290ct2020/bench/POTENTIALS/library.meam  
lammps-stable\_290ct2020/bench/POTENTIALS/log.90ct20.adp.1  
lammps-stable\_290ct2020/bench/POTENTIALS/log.90ct20.adp.4  
lammps-stable\_290ct2020/bench/POTENTIALS/log.90ct20.airebo.1  
lammps-stable\_290ct2020/bench/POTENTIALS/log.90ct20.airebo.4  
lammps-stable\_290ct2020/bench/POTENTIALS/log.90ct20.bop.1  
lammps-stable\_290ct2020/bench/POTENTIALS/log.90ct20.bop.4  
lammps-stable\_290ct2020/bench/POTENTIALS/log.90ct20.comb.1  
lammps-stable\_290ct2020/bench/POTENTIALS/log.90ct20.comb.4  
lammps-stable\_290ct2020/bench/POTENTIALS/log.90ct20.dpd.1  
lammps-stable\_290ct2020/bench/POTENTIALS/log.90ct20.dpd.4  
lammps-stable\_290ct2020/bench/POTENTIALS/log.90ct20.eam.1  
lammps-stable\_290ct2020/bench/POTENTIALS/log.90ct20.eam.4  
lammps-stable\_290ct2020/bench/POTENTIALS/log.90ct20.eff.1  
lammps-stable\_290ct2020/bench/POTENTIALS/log.90ct20.eff.4  
lammps-stable\_290ct2020/bench/POTENTIALS/log.90ct20.eim.1  
lammps-stable\_290ct2020/bench/POTENTIALS/log.90ct20.eim.4  
lammps-stable\_290ct2020/bench/POTENTIALS/log.90ct20.fene.1  
lammps-stable\_290ct2020/bench/POTENTIALS/log.90ct20.fene.4  
lammps-stable\_290ct2020/bench/POTENTIALS/log.90ct20.gb.1  
lammps-stable\_290ct2020/bench/POTENTIALS/log.90ct20.gb.4  
lammps-stable\_290ct2020/bench/POTENTIALS/log.90ct20.granular.1  
lammps-stable\_290ct2020/bench/POTENTIALS/log.90ct20.granular.4  
lammps-stable\_290ct2020/bench/POTENTIALS/log.90ct20.lj.1  
lammps-stable\_290ct2020/bench/POTENTIALS/log.90ct20.lj.4  
lammps-stable\_290ct2020/bench/POTENTIALS/log.90ct20.meamc.1  
lammps-stable\_290ct2020/bench/POTENTIALS/log.90ct20.meamc.4  
lammps-stable\_290ct2020/bench/POTENTIALS/log.90ct20.peri.1  
lammps-stable\_290ct2020/bench/POTENTIALS/log.90ct20.peri.4  
lammps-stable\_290ct2020/bench/POTENTIALS/log.90ct20.protein.1  
lammps-stable\_290ct2020/bench/POTENTIALS/log.90ct20.protein.4  
lammps-stable\_290ct2020/bench/POTENTIALS/log.90ct20.reaxc.1  
lammps-stable\_290ct2020/bench/POTENTIALS/log.90ct20.reaxc.4  
lammps-stable\_290ct2020/bench/POTENTIALS/log.90ct20.rebo.1  
lammps-stable\_290ct2020/bench/POTENTIALS/log.90ct20.rebo.4  
lammps-stable\_290ct2020/bench/POTENTIALS/log.90ct20.spce.1  
lammps-stable\_290ct2020/bench/POTENTIALS/log.90ct20.spce.4  
lammps-stable\_290ct2020/bench/POTENTIALS/log.90ct20.sw.1  
lammps-stable\_290ct2020/bench/POTENTIALS/log.90ct20.sw.4

lammps-stable\_290ct2020/bench/POTENTIALS/log.90ct20.tersoff.1  
lammps-stable\_290ct2020/bench/POTENTIALS/log.90ct20.tersoff.4  
lammps-stable\_290ct2020/bench/README  
lammps-stable\_290ct2020/bench/data.chain  
lammps-stable\_290ct2020/bench/data.chute  
lammps-stable\_290ct2020/bench/data.rhodo  
lammps-stable\_290ct2020/bench/in.chain  
lammps-stable\_290ct2020/bench/in.chain.scaled  
lammps-stable\_290ct2020/bench/in.chute  
lammps-stable\_290ct2020/bench/in.chute.scaled  
lammps-stable\_290ct2020/bench/in.eam  
lammps-stable\_290ct2020/bench/in.lj  
lammps-stable\_290ct2020/bench/in.rhodo  
lammps-stable\_290ct2020/bench/in.rhodo.scaled  
lammps-stable\_290ct2020/bench/log.60ct16.chain.fixed.icc.1  
lammps-stable\_290ct2020/bench/log.60ct16.chain.fixed.icc.4  
lammps-stable\_290ct2020/bench/log.60ct16.chain.scaled.icc.4  
lammps-stable\_290ct2020/bench/log.60ct16.chute.fixed.icc.1  
lammps-stable\_290ct2020/bench/log.60ct16.chute.fixed.icc.4  
lammps-stable\_290ct2020/bench/log.60ct16.chute.scaled.icc.4  
lammps-stable\_290ct2020/bench/log.60ct16.eam.fixed.icc.1  
lammps-stable\_290ct2020/bench/log.60ct16.eam.fixed.icc.4  
lammps-stable\_290ct2020/bench/log.60ct16.eam.scaled.icc.4  
lammps-stable\_290ct2020/bench/log.60ct16.lj.fixed.icc.1  
lammps-stable\_290ct2020/bench/log.60ct16.lj.fixed.icc.4  
lammps-stable\_290ct2020/bench/log.60ct16.lj.scaled.icc.4  
lammps-stable\_290ct2020/bench/log.60ct16.rhodo.fixed.icc.1  
lammps-stable\_290ct2020/bench/log.60ct16.rhodo.fixed.icc.4  
lammps-stable\_290ct2020/bench/log.60ct16.rhodo.scaled.icc.4  
lammps-stable\_290ct2020/cmake/  
lammps-stable\_290ct2020/cmake/CMakeLists.txt  
lammps-stable\_290ct2020/cmake/LAMMPSConfig.cmake.in  
lammps-stable\_290ct2020/cmake/Modules/  
lammps-stable\_290ct2020/cmake/Modules/CheckGeneratorSupport.cmake  
lammps-stable\_290ct2020/cmake/Modules/CodeCoverage.cmake  
lammps-stable\_290ct2020/cmake/Modules/CodingStandard.cmake  
lammps-stable\_290ct2020/cmake/Modules/Documentation.cmake  
lammps-stable\_290ct2020/cmake/Modules/FindCUB.cmake  
lammps-stable\_290ct2020/cmake/Modules/FindClangFormat.cmake  
lammps-stable\_290ct2020/cmake/Modules/FindFFTW3.cmake  
lammps-stable\_290ct2020/cmake/Modules/FindFFTW3F.cmake  
lammps-stable\_290ct2020/cmake/Modules/FindMKL.cmake  
lammps-stable\_290ct2020/cmake/Modules/FindMSCG.cmake  
lammps-stable\_290ct2020/cmake/Modules/FindNetCDF.cmake  
lammps-stable\_290ct2020/cmake/Modules/FindPNetCDF.cmake  
lammps-stable\_290ct2020/cmake/Modules/FindQUIP.cmake  
lammps-stable\_290ct2020/cmake/Modules/FindTBB\_MALLOC.cmake  
lammps-stable\_290ct2020/cmake/Modules/FindVORO.cmake  
lammps-stable\_290ct2020/cmake/Modules/FindYAML.cmake  
lammps-stable\_290ct2020/cmake/Modules/FindZMQ.cmake  
lammps-stable\_290ct2020/cmake/Modules/GTest.cmake  
lammps-stable\_290ct2020/cmake/Modules/GenerateBinaryHeader.cmake  
lammps-stable\_290ct2020/cmake/Modules/LAMMPSUtils.cmake  
lammps-stable\_290ct2020/cmake/Modules/MPI4WIN.cmake  
lammps-stable\_290ct2020/cmake/Modules/OpenCLUtils.cmake  
lammps-stable\_290ct2020/cmake/Modules/Packages/  
lammps-stable\_290ct2020/cmake/Modules/Packages/COMPRESS.cmake  
lammps-stable\_290ct2020/cmake/Modules/Packages/CORESHELL.cmake  
lammps-stable\_290ct2020/cmake/Modules/Packages/GPU.cmake  
lammps-stable\_290ct2020/cmake/Modules/Packages/KIM.cmake

```
lammps-stable_290ct2020/cmake/Modules/Packages/KOKKOS.cmake
lammps-stable_290ct2020/cmake/Modules/Packages/KSPACE.cmake
lammps-stable_290ct2020/cmake/Modules/Packages/LATTE.cmake
lammps-stable_290ct2020/cmake/Modules/Packages/MESSAGE.cmake
lammps-stable_290ct2020/cmake/Modules/Packages/MSCG.cmake
lammps-stable_290ct2020/cmake/Modules/Packages/OPT.cmake
lammps-stable_290ct2020/cmake/Modules/Packages/PYTHON.cmake
lammps-stable_290ct2020/cmake/Modules/Packages/QEQ.cmake
lammps-stable_290ct2020/cmake/Modules/Packages/USER-COLVARS.cmake
lammps-stable_290ct2020/cmake/Modules/Packages/USER-H5MD.cmake
lammps-stable_290ct2020/cmake/Modules/Packages/USER-INTEL.cmake
lammps-stable_290ct2020/cmake/Modules/Packages/USER-MOLFILE.cmake
lammps-stable_290ct2020/cmake/Modules/Packages/USER-NETCDF.cmake
lammps-stable_290ct2020/cmake/Modules/Packages/USER-OMP.cmake
lammps-stable_290ct2020/cmake/Modules/Packages/USER-PLUMED.cmake
lammps-stable_290ct2020/cmake/Modules/Packages/USER-QMMM.cmake
lammps-stable_290ct2020/cmake/Modules/Packages/USER-QUIP.cmake
lammps-stable_290ct2020/cmake/Modules/Packages/USER-SCAFACOS.cmake
lammps-stable_290ct2020/cmake/Modules/Packages/USER-SDPD.cmake
lammps-stable_290ct2020/cmake/Modules/Packages/USER-SMD.cmake
lammps-stable_290ct2020/cmake/Modules/Packages/USER-VTK.cmake
lammps-stable_290ct2020/cmake/Modules/Packages/VORONOI.cmake
lammps-stable_290ct2020/cmake/Modules/PreventInSourceBuilds.cmake
lammps-stable_290ct2020/cmake/Modules/StyleHeaderUtils.cmake
lammps-stable_290ct2020/cmake/Modules/Testing.cmake
lammps-stable_290ct2020/cmake/Modules/Tools.cmake
lammps-stable_290ct2020/cmake/Modules/generate_lmpgitversion.cmake
lammps-stable_290ct2020/cmake/etc/
lammps-stable_290ct2020/cmake/etc/profile.d/
lammps-stable_290ct2020/cmake/etc/profile.d/lammps.csh.in
lammps-stable_290ct2020/cmake/etc/profile.d/lammps.sh.in
lammps-stable_290ct2020/cmake/gpu/
lammps-stable_290ct2020/cmake/gpu/lal_pppm_d.cu
lammps-stable_290ct2020/cmake/gpu/lal_pppm_f.cu
lammps-stable_290ct2020/cmake/iwyu/
lammps-stable_290ct2020/cmake/iwyu/iwyu-extra-map.imp
lammps-stable_290ct2020/cmake/pkgconfig/
lammps-stable_290ct2020/cmake/pkgconfig/liblammps.pc.in
lammps-stable_290ct2020/cmake/presets/
lammps-stable_290ct2020/cmake/presets/all_off.cmake
lammps-stable_290ct2020/cmake/presets/all_on.cmake
lammps-stable_290ct2020/cmake/presets/clang.cmake
lammps-stable_290ct2020/cmake/presets/download.cmake
lammps-stable_290ct2020/cmake/presets/gcc.cmake
lammps-stable_290ct2020/cmake/presets/hip.cmake
lammps-stable_290ct2020/cmake/presets/intel.cmake
lammps-stable_290ct2020/cmake/presets/kokkos-cuda.cmake
lammps-stable_290ct2020/cmake/presets/kokkos-openmp.cmake
lammps-stable_290ct2020/cmake/presets/kokkos-serial.cmake
lammps-stable_290ct2020/cmake/presets/mingw-cross.cmake
lammps-stable_290ct2020/cmake/presets/minimal.cmake
lammps-stable_290ct2020/cmake/presets/most.cmake
lammps-stable_290ct2020/cmake/presets/nolib.cmake
lammps-stable_290ct2020/doc/
lammps-stable_290ct2020/doc/Makefile
lammps-stable_290ct2020/doc/README
lammps-stable_290ct2020/doc/documentation_conventions.md
lammps-stable_290ct2020/doc/doxygen/
lammps-stable_290ct2020/doc/doxygen/Doxyfile.in
lammps-stable_290ct2020/doc/doxygen/lammps-logo.png
```

lammps-stable\_290ct2020/doc/github-development-workflow.md  
lammps-stable\_290ct2020/doc/graphviz/  
lammps-stable\_290ct2020/doc/graphviz/Makefile  
lammps-stable\_290ct2020/doc/graphviz/lammps-classes.dot  
lammps-stable\_290ct2020/doc/graphviz/lammps-invoke-python.dot  
lammps-stable\_290ct2020/doc/graphviz/pylammps-invoke-lammps.dot  
lammps-stable\_290ct2020/doc/graphviz/python-invoke-lammps.dot  
lammps-stable\_290ct2020/doc/include-file-conventions.md  
lammps-stable\_290ct2020/doc/lammps.1  
lammps-stable\_290ct2020/doc/msi2lmp.1  
lammps-stable\_290ct2020/doc/src/  
lammps-stable\_290ct2020/doc/src/2001/  
lammps-stable\_290ct2020/doc/src/2001/README.html  
lammps-stable\_290ct2020/doc/src/2001/basics.html  
lammps-stable\_290ct2020/doc/src/2001/data\_format.html  
lammps-stable\_290ct2020/doc/src/2001/deficiencies.html  
lammps-stable\_290ct2020/doc/src/2001/force\_fields.html  
lammps-stable\_290ct2020/doc/src/2001/history.html  
lammps-stable\_290ct2020/doc/src/2001/input\_commands.html  
lammps-stable\_290ct2020/doc/src/2001/units.html  
lammps-stable\_290ct2020/doc/src/99/  
lammps-stable\_290ct2020/doc/src/99/README.html  
lammps-stable\_290ct2020/doc/src/99/basics.html  
lammps-stable\_290ct2020/doc/src/99/crib.html  
lammps-stable\_290ct2020/doc/src/99/data\_format.html  
lammps-stable\_290ct2020/doc/src/99/force\_fields.html  
lammps-stable\_290ct2020/doc/src/99/history.html  
lammps-stable\_290ct2020/doc/src/99/input\_commands.html  
lammps-stable\_290ct2020/doc/src/99/units.html  
lammps-stable\_290ct2020/doc/src/Bibliography.rst  
lammps-stable\_290ct2020/doc/src/Build.rst  
lammps-stable\_290ct2020/doc/src/Build\_basics.rst  
lammps-stable\_290ct2020/doc/src/Build\_cmake.rst  
lammps-stable\_290ct2020/doc/src/Build\_development.rst  
lammps-stable\_290ct2020/doc/src/Build\_extras.rst  
lammps-stable\_290ct2020/doc/src/Build\_link.rst  
lammps-stable\_290ct2020/doc/src/Build\_make.rst  
lammps-stable\_290ct2020/doc/src/Build\_manual.rst  
lammps-stable\_290ct2020/doc/src/Build\_package.rst  
lammps-stable\_290ct2020/doc/src/Build\_settings.rst  
lammps-stable\_290ct2020/doc/src/Build\_windows.rst  
lammps-stable\_290ct2020/doc/src/Classes.rst  
lammps-stable\_290ct2020/doc/src/Classes\_atom.rst  
lammps-stable\_290ct2020/doc/src/Classes\_input.rst  
lammps-stable\_290ct2020/doc/src/Classes\_lammps.rst  
lammps-stable\_290ct2020/doc/src/Commands.rst  
lammps-stable\_290ct2020/doc/src/Commands\_all.rst  
lammps-stable\_290ct2020/doc/src/Commands\_bond.rst  
lammps-stable\_290ct2020/doc/src/Commands\_category.rst  
lammps-stable\_290ct2020/doc/src/Commands\_compute.rst  
lammps-stable\_290ct2020/doc/src/Commands\_fix.rst  
lammps-stable\_290ct2020/doc/src/Commands\_input.rst  
lammps-stable\_290ct2020/doc/src/Commands\_kspace.rst  
lammps-stable\_290ct2020/doc/src/Commands\_pair.rst  
lammps-stable\_290ct2020/doc/src/Commands\_parse.rst  
lammps-stable\_290ct2020/doc/src/Commands\_removed.rst  
lammps-stable\_290ct2020/doc/src/Commands\_structure.rst  
lammps-stable\_290ct2020/doc/src/Cplusplus.rst  
lammps-stable\_290ct2020/doc/src/Developer.rst  
lammps-stable\_290ct2020/doc/src/Developer\_flow.rst

lammps-stable\_290ct2020/doc/src/Developer\_org.rst  
lammps-stable\_290ct2020/doc/src/Developer\_utils.rst  
lammps-stable\_290ct2020/doc/src/Developer\_write.rst  
lammps-stable\_290ct2020/doc/src/Errors.rst  
lammps-stable\_290ct2020/doc/src/Errors\_bugs.rst  
lammps-stable\_290ct2020/doc/src/Errors\_common.rst  
lammps-stable\_290ct2020/doc/src/Errors\_debug.rst  
lammps-stable\_290ct2020/doc/src/Errors\_messages.rst  
lammps-stable\_290ct2020/doc/src/Errors\_warnings.rst  
lammps-stable\_290ct2020/doc/src/Examples.rst  
lammps-stable\_290ct2020/doc/src/Fortran.rst  
lammps-stable\_290ct2020/doc/src/Howto.rst  
lammps-stable\_290ct2020/doc/src/Howto\_2d.rst  
lammps-stable\_290ct2020/doc/src/Howto\_barostat.rst  
lammps-stable\_290ct2020/doc/src/Howto\_bioFF.rst  
lammps-stable\_290ct2020/doc/src/Howto\_body.rst  
lammps-stable\_290ct2020/doc/src/Howto\_chunk.rst  
lammps-stable\_290ct2020/doc/src/Howto\_client\_server.rst  
lammps-stable\_290ct2020/doc/src/Howto\_cmake.rst  
lammps-stable\_290ct2020/doc/src/Howto\_coresHELL.rst  
lammps-stable\_290ct2020/doc/src/Howto\_couple.rst  
lammps-stable\_290ct2020/doc/src/Howto\_diffusion.rst  
lammps-stable\_290ct2020/doc/src/Howto\_dispersion.rst  
lammps-stable\_290ct2020/doc/src/Howto\_drude.rst  
lammps-stable\_290ct2020/doc/src/Howto\_drude2.rst  
lammps-stable\_290ct2020/doc/src/Howto\_elastic.rst  
lammps-stable\_290ct2020/doc/src/Howto\_github.rst  
lammps-stable\_290ct2020/doc/src/Howto\_granular.rst  
lammps-stable\_290ct2020/doc/src/Howto\_kappa.rst  
lammps-stable\_290ct2020/doc/src/Howto\_library.rst  
lammps-stable\_290ct2020/doc/src/Howto\_manifold.rst  
lammps-stable\_290ct2020/doc/src/Howto\_multiple.rst  
lammps-stable\_290ct2020/doc/src/Howto\_nemd.rst  
lammps-stable\_290ct2020/doc/src/Howto\_output.rst  
lammps-stable\_290ct2020/doc/src/Howto\_polarizable.rst  
lammps-stable\_290ct2020/doc/src/Howto\_pylammps.rst  
lammps-stable\_290ct2020/doc/src/Howto\_replica.rst  
lammps-stable\_290ct2020/doc/src/Howto\_restart.rst  
lammps-stable\_290ct2020/doc/src/Howto\_spc.rst  
lammps-stable\_290ct2020/doc/src/Howto\_spherical.rst  
lammps-stable\_290ct2020/doc/src/Howto\_spins.rst  
lammps-stable\_290ct2020/doc/src/Howto\_temperature.rst  
lammps-stable\_290ct2020/doc/src/Howto\_thermostat.rst  
lammps-stable\_290ct2020/doc/src/Howto\_tip3p.rst  
lammps-stable\_290ct2020/doc/src/Howto\_tip4p.rst  
lammps-stable\_290ct2020/doc/src/Howto\_triclinic.rst  
lammps-stable\_290ct2020/doc/src/Howto\_viscosity.rst  
lammps-stable\_290ct2020/doc/src/Howto\_viz.rst  
lammps-stable\_290ct2020/doc/src/Howto\_walls.rst  
lammps-stable\_290ct2020/doc/src/Howto\_wsl.rst  
lammps-stable\_290ct2020/doc/src/Install.rst  
lammps-stable\_290ct2020/doc/src/Install\_conda.rst  
lammps-stable\_290ct2020/doc/src/Install\_git.rst  
lammps-stable\_290ct2020/doc/src/Install\_linux.rst  
lammps-stable\_290ct2020/doc/src/Install\_mac.rst  
lammps-stable\_290ct2020/doc/src/Install\_patch.rst  
lammps-stable\_290ct2020/doc/src/Install\_tarball.rst  
lammps-stable\_290ct2020/doc/src/Install\_windows.rst  
lammps-stable\_290ct2020/doc/src/Intro.rst  
lammps-stable\_290ct2020/doc/src/Intro\_authors.rst

lammps-stable\_290ct2020/doc/src/Intro\_citing.rst  
lammps-stable\_290ct2020/doc/src/Intro\_features.rst  
lammps-stable\_290ct2020/doc/src/Intro\_nonfeatures.rst  
lammps-stable\_290ct2020/doc/src/Intro\_opensource.rst  
lammps-stable\_290ct2020/doc/src/Intro\_overview.rst  
lammps-stable\_290ct2020/doc/src/Intro\_website.rst  
lammps-stable\_290ct2020/doc/src/JPG/  
lammps-stable\_290ct2020/doc/src/JPG/atc\_nanotube.jpg  
lammps-stable\_290ct2020/doc/src/JPG/bondswap.jpg  
lammps-stable\_290ct2020/doc/src/JPG/ccmake-config.png  
lammps-stable\_290ct2020/doc/src/JPG/ccmake-initial.png  
lammps-stable\_290ct2020/doc/src/JPG/ccmake-options.png  
lammps-stable\_290ct2020/doc/src/JPG/cmake-codeblocks.png  
lammps-stable\_290ct2020/doc/src/JPG/cmake-gui-initial.png  
lammps-stable\_290ct2020/doc/src/JPG/cmake-gui-options.png  
lammps-stable\_290ct2020/doc/src/JPG/cmake-gui-popup.png  
lammps-stable\_290ct2020/doc/src/JPG/coul\_soft.jpg  
lammps-stable\_290ct2020/doc/src/JPG/coverage-file-branches.png  
lammps-stable\_290ct2020/doc/src/JPG/coverage-file-top.png  
lammps-stable\_290ct2020/doc/src/JPG/coverage-overview-manybody.png  
lammps-stable\_290ct2020/doc/src/JPG/coverage-overview-top.png  
lammps-stable\_290ct2020/doc/src/JPG/dihedral\_sign.jpg  
lammps-stable\_290ct2020/doc/src/JPG/dihedral\_spherical\_angles.jpg  
lammps-stable\_290ct2020/doc/src/JPG/dreiding\_hbond.jpg  
lammps-stable\_290ct2020/doc/src/JPG/dynamical\_matrix\_phonons.jpg  
lammps-stable\_290ct2020/doc/src/JPG/examples\_edpd.jpg  
lammps-stable\_290ct2020/doc/src/JPG/examples\_mdpd.gif  
lammps-stable\_290ct2020/doc/src/JPG/examples\_mdpd\_first.jpg  
lammps-stable\_290ct2020/doc/src/JPG/examples\_mdpd\_last.jpg  
lammps-stable\_290ct2020/doc/src/JPG/examples\_tdpd.jpg  
lammps-stable\_290ct2020/doc/src/JPG/fix\_integration\_spin\_stdecomposition.jpg  
lammps-stable\_290ct2020/doc/src/JPG/fix\_wall\_ees\_image.jpg  
lammps-stable\_290ct2020/doc/src/JPG/improper\_distance.jpg  
lammps-stable\_290ct2020/doc/src/JPG/lammps-classes.png  
lammps-stable\_290ct2020/doc/src/JPG/lammps-invoke-python.png  
lammps-stable\_290ct2020/doc/src/JPG/lj\_soft.jpg  
lammps-stable\_290ct2020/doc/src/JPG/offload\_knc.png  
lammps-stable\_290ct2020/doc/src/JPG/pair\_atm\_dia.jpg  
lammps-stable\_290ct2020/doc/src/JPG/pair\_body\_rounded.jpg  
lammps-stable\_290ct2020/doc/src/JPG/pair\_cosine\_squared\_graphs.jpg  
lammps-stable\_290ct2020/doc/src/JPG/pimd.jpg  
lammps-stable\_290ct2020/doc/src/JPG/pylammps-invoke-lammps.png  
lammps-stable\_290ct2020/doc/src/JPG/pylammps\_dihedral.jpg  
lammps-stable\_290ct2020/doc/src/JPG/pylammps\_mc\_disordered.jpg  
lammps-stable\_290ct2020/doc/src/JPG/pylammps\_mc\_energies\_plot.jpg  
lammps-stable\_290ct2020/doc/src/JPG/pylammps\_mc\_minimum.jpg  
lammps-stable\_290ct2020/doc/src/JPG/python-invoke-lammps.png  
lammps-stable\_290ct2020/doc/src/JPG/qbmsst\_init.jpg  
lammps-stable\_290ct2020/doc/src/JPG/qbmsst\_shock.jpg  
lammps-stable\_290ct2020/doc/src/JPG/rhodo\_staggered.jpg  
lammps-stable\_290ct2020/doc/src/JPG/third\_order\_force\_constant.png  
lammps-stable\_290ct2020/doc/src/JPG/tutorial\_additional\_changes.png  
lammps-stable\_290ct2020/doc/src/JPG/tutorial\_automated\_checks.png  
lammps-stable\_290ct2020/doc/src/JPG/tutorial\_automated\_checks\_passed.png  
lammps-stable\_290ct2020/doc/src/JPG/tutorial\_branch.png  
lammps-stable\_290ct2020/doc/src/JPG/tutorial\_changes\_others.png  
lammps-stable\_290ct2020/doc/src/JPG/tutorial\_create\_new\_pull\_request1.png  
lammps-stable\_290ct2020/doc/src/JPG/tutorial\_create\_new\_pull\_request2.png  
lammps-stable\_290ct2020/doc/src/JPG/tutorial\_edits\_maintainers.png  
lammps-stable\_290ct2020/doc/src/JPG/tutorial\_fork.png



lammps-stable\_290ct2020/doc/src/JPG/tutorial\_https\_block.png  
lammps-stable\_290ct2020/doc/src/JPG/tutorial\_merged.png  
lammps-stable\_290ct2020/doc/src/JPG/tutorial\_new\_pull\_request.png  
lammps-stable\_290ct2020/doc/src/JPG/tutorial\_pull\_request2.png  
lammps-stable\_290ct2020/doc/src/JPG/tutorial\_pull\_request3.png  
lammps-stable\_290ct2020/doc/src/JPG/tutorial\_pull\_request4.png  
lammps-stable\_290ct2020/doc/src/JPG/tutorial\_pull\_request\_feature\_branch1.png  
lammps-stable\_290ct2020/doc/src/JPG/tutorial\_reverse\_pull\_request.png  
lammps-stable\_290ct2020/doc/src/JPG/tutorial\_reverse\_pull\_request2.png  
lammps-stable\_290ct2020/doc/src/JPG/tutorial\_reverse\_pull\_request3.png  
lammps-stable\_290ct2020/doc/src/JPG/tutorial\_reverse\_pull\_request4.png  
lammps-stable\_290ct2020/doc/src/JPG/tutorial\_reverse\_pull\_request5.png  
lammps-stable\_290ct2020/doc/src/JPG/tutorial\_reverse\_pull\_request6.png  
lammps-stable\_290ct2020/doc/src/JPG/tutorial\_reverse\_pull\_request7.png  
lammps-stable\_290ct2020/doc/src/JPG/tutorial\_steve\_assignee.png  
lammps-stable\_290ct2020/doc/src/JPG/uef\_frames.jpg  
lammps-stable\_290ct2020/doc/src/JPG/umbrella.jpg  
lammps-stable\_290ct2020/doc/src/JPG/user\_intel.png  
lammps-stable\_290ct2020/doc/src/JPG/zeeman\_langevin.jpg  
lammps-stable\_290ct2020/doc/src/Library.rst  
lammps-stable\_290ct2020/doc/src/Library\_add.rst  
lammps-stable\_290ct2020/doc/src/Library\_atoms.rst  
lammps-stable\_290ct2020/doc/src/Library\_config.rst  
lammps-stable\_290ct2020/doc/src/Library\_create.rst  
lammps-stable\_290ct2020/doc/src/Library\_execute.rst  
lammps-stable\_290ct2020/doc/src/Library\_neighbor.rst  
lammps-stable\_290ct2020/doc/src/Library\_objects.rst  
lammps-stable\_290ct2020/doc/src/Library\_properties.rst  
lammps-stable\_290ct2020/doc/src/Library\_scatter.rst  
lammps-stable\_290ct2020/doc/src/Library\_utility.rst  
lammps-stable\_290ct2020/doc/src/Manual.rst  
lammps-stable\_290ct2020/doc/src/Manual\_version.rst  
lammps-stable\_290ct2020/doc/src/Modify.rst  
lammps-stable\_290ct2020/doc/src/Modify\_atom.rst  
lammps-stable\_290ct2020/doc/src/Modify\_body.rst  
lammps-stable\_290ct2020/doc/src/Modify\_bond.rst  
lammps-stable\_290ct2020/doc/src/Modify\_command.rst  
lammps-stable\_290ct2020/doc/src/Modify\_compute.rst  
lammps-stable\_290ct2020/doc/src/Modify\_contribute.rst  
lammps-stable\_290ct2020/doc/src/Modify\_dump.rst  
lammps-stable\_290ct2020/doc/src/Modify\_fix.rst  
lammps-stable\_290ct2020/doc/src/Modify\_kspace.rst  
lammps-stable\_290ct2020/doc/src/Modify\_min.rst  
lammps-stable\_290ct2020/doc/src/Modify\_overview.rst  
lammps-stable\_290ct2020/doc/src/Modify\_pair.rst  
lammps-stable\_290ct2020/doc/src/Modify\_region.rst  
lammps-stable\_290ct2020/doc/src/Modify\_thermo.rst  
lammps-stable\_290ct2020/doc/src/Modify\_variable.rst  
lammps-stable\_290ct2020/doc/src/PDF/  
lammps-stable\_290ct2020/doc/src/PDF/PDLammps\_EPS.pdf  
lammps-stable\_290ct2020/doc/src/PDF/PDLammps\_VES.pdf  
lammps-stable\_290ct2020/doc/src/PDF/PDLammps\_overview.pdf  
lammps-stable\_290ct2020/doc/src/PDF/SMD\_LAMMPS\_userguide.pdf  
lammps-stable\_290ct2020/doc/src/PDF/SPH\_LAMMPS\_userguide.pdf  
lammps-stable\_290ct2020/doc/src/PDF/USER-CGDNA.pdf  
lammps-stable\_290ct2020/doc/src/PDF/colvars-refman-lammps.pdf  
lammps-stable\_290ct2020/doc/src/PDF/kspace.pdf  
lammps-stable\_290ct2020/doc/src/PDF/pair\_gayberne\_extra.pdf  
lammps-stable\_290ct2020/doc/src/PDF/pair\_gayberne\_extra.tex  
lammps-stable\_290ct2020/doc/src/PDF/pair\_resquared\_extra.pdf

lammps-stable\_290ct2020/doc/src/PDF/pair\_resquared\_extra.tex  
lammps-stable\_290ct2020/doc/src/Packages.rst  
lammps-stable\_290ct2020/doc/src/Packages\_details.rst  
lammps-stable\_290ct2020/doc/src/Packages\_standard.rst  
lammps-stable\_290ct2020/doc/src/Packages\_user.rst  
lammps-stable\_290ct2020/doc/src/Python\_atoms.rst  
lammps-stable\_290ct2020/doc/src/Python\_call.rst  
lammps-stable\_290ct2020/doc/src/Python\_config.rst  
lammps-stable\_290ct2020/doc/src/Python\_create.rst  
lammps-stable\_290ct2020/doc/src/Python\_error.rst  
lammps-stable\_290ct2020/doc/src/Python\_examples.rst  
lammps-stable\_290ct2020/doc/src/Python\_execute.rst  
lammps-stable\_290ct2020/doc/src/Python\_ext.rst  
lammps-stable\_290ct2020/doc/src/Python\_head.rst  
lammps-stable\_290ct2020/doc/src/Python\_install.rst  
lammps-stable\_290ct2020/doc/src/Python\_launch.rst  
lammps-stable\_290ct2020/doc/src/Python\_module.rst  
lammps-stable\_290ct2020/doc/src/Python\_neighbor.rst  
lammps-stable\_290ct2020/doc/src/Python\_objects.rst  
lammps-stable\_290ct2020/doc/src/Python\_overview.rst  
lammps-stable\_290ct2020/doc/src/Python\_properties.rst  
lammps-stable\_290ct2020/doc/src/Python\_run.rst  
lammps-stable\_290ct2020/doc/src/Python\_scatter.rst  
lammps-stable\_290ct2020/doc/src/Python\_trouble.rst  
lammps-stable\_290ct2020/doc/src/Run\_basics.rst  
lammps-stable\_290ct2020/doc/src/Run\_head.rst  
lammps-stable\_290ct2020/doc/src/Run\_options.rst  
lammps-stable\_290ct2020/doc/src/Run\_output.rst  
lammps-stable\_290ct2020/doc/src/Run\_windows.rst  
lammps-stable\_290ct2020/doc/src/Speed.rst  
lammps-stable\_290ct2020/doc/src/Speed\_bench.rst  
lammps-stable\_290ct2020/doc/src/Speed\_compare.rst  
lammps-stable\_290ct2020/doc/src/Speed\_gpu.rst  
lammps-stable\_290ct2020/doc/src/Speed\_intel.rst  
lammps-stable\_290ct2020/doc/src/Speed\_kokkos.rst  
lammps-stable\_290ct2020/doc/src/Speed\_measure.rst  
lammps-stable\_290ct2020/doc/src/Speed\_omp.rst  
lammps-stable\_290ct2020/doc/src/Speed\_opt.rst  
lammps-stable\_290ct2020/doc/src/Speed\_packages.rst  
lammps-stable\_290ct2020/doc/src/Speed\_tips.rst  
lammps-stable\_290ct2020/doc/src/Tools.rst  
lammps-stable\_290ct2020/doc/src/\_ext/  
lammps-stable\_290ct2020/doc/src/\_ext/tab\_or\_note.py  
lammps-stable\_290ct2020/doc/src/\_ext/table\_from\_list.py  
lammps-stable\_290ct2020/doc/src/accel\_styles.rst  
lammps-stable\_290ct2020/doc/src/angle\_charmm.rst  
lammps-stable\_290ct2020/doc/src/angle\_class2.rst  
lammps-stable\_290ct2020/doc/src/angle\_coeff.rst  
lammps-stable\_290ct2020/doc/src/angle\_cosine.rst  
lammps-stable\_290ct2020/doc/src/angle\_cosine\_buck6d.rst  
lammps-stable\_290ct2020/doc/src/angle\_cosine\_delta.rst  
lammps-stable\_290ct2020/doc/src/angle\_cosine\_periodic.rst  
lammps-stable\_290ct2020/doc/src/angle\_cosine\_shift.rst  
lammps-stable\_290ct2020/doc/src/angle\_cosine\_shift\_exp.rst  
lammps-stable\_290ct2020/doc/src/angle\_cosine\_squared.rst  
lammps-stable\_290ct2020/doc/src/angle\_cross.rst  
lammps-stable\_290ct2020/doc/src/angle\_dipole.rst  
lammps-stable\_290ct2020/doc/src/angle\_fourier.rst  
lammps-stable\_290ct2020/doc/src/angle\_fourier\_simple.rst  
lammps-stable\_290ct2020/doc/src/angle\_harmonic.rst

lammps-stable\_290ct2020/doc/src/angle\_hybrid.rst  
lammps-stable\_290ct2020/doc/src/angle\_mm3.rst  
lammps-stable\_290ct2020/doc/src/angle\_none.rst  
lammps-stable\_290ct2020/doc/src/angle\_quartic.rst  
lammps-stable\_290ct2020/doc/src/angle\_sdk.rst  
lammps-stable\_290ct2020/doc/src/angle\_style.rst  
lammps-stable\_290ct2020/doc/src/angle\_table.rst  
lammps-stable\_290ct2020/doc/src/angle\_zero.rst  
lammps-stable\_290ct2020/doc/src/angles.rst  
lammps-stable\_290ct2020/doc/src/atc\_add\_molecule.rst  
lammps-stable\_290ct2020/doc/src/atc\_add\_species.rst  
lammps-stable\_290ct2020/doc/src/atc\_atom\_element\_map.rst  
lammps-stable\_290ct2020/doc/src/atc\_atom\_weight.rst  
lammps-stable\_290ct2020/doc/src/atc\_atomic\_charge.rst  
lammps-stable\_290ct2020/doc/src/atc\_boundary\_dynamics.rst  
lammps-stable\_290ct2020/doc/src/atc\_boundary\_faceset.rst  
lammps-stable\_290ct2020/doc/src/atc\_boundary\_type.rst  
lammps-stable\_290ct2020/doc/src/atc\_consistent\_fe\_initialization.rst  
lammps-stable\_290ct2020/doc/src/atc\_control\_localized\_lambda.rst  
lammps-stable\_290ct2020/doc/src/atc\_control\_momentum.rst  
lammps-stable\_290ct2020/doc/src/atc\_control\_thermal.rst  
lammps-stable\_290ct2020/doc/src/atc\_decomposition.rst  
lammps-stable\_290ct2020/doc/src/atc\_electron\_integration.rst  
lammps-stable\_290ct2020/doc/src/atc\_equilibrium\_start.rst  
lammps-stable\_290ct2020/doc/src/atc\_extrinsic\_exchange.rst  
lammps-stable\_290ct2020/doc/src/atc\_fe\_md\_boundary.rst  
lammps-stable\_290ct2020/doc/src/atc\_filter\_scale.rst  
lammps-stable\_290ct2020/doc/src/atc\_filter\_type.rst  
lammps-stable\_290ct2020/doc/src/atc\_fix.rst  
lammps-stable\_290ct2020/doc/src/atc\_fix\_flux.rst  
lammps-stable\_290ct2020/doc/src/atc\_hardy\_computes.rst  
lammps-stable\_290ct2020/doc/src/atc\_hardy\_fields.rst  
lammps-stable\_290ct2020/doc/src/atc\_hardy\_gradients.rst  
lammps-stable\_290ct2020/doc/src/atc\_hardy\_kernel.rst  
lammps-stable\_290ct2020/doc/src/atc\_hardy\_on\_the\_fly.rst  
lammps-stable\_290ct2020/doc/src/atc\_hardy\_rates.rst  
lammps-stable\_290ct2020/doc/src/atc\_initial.rst  
lammps-stable\_290ct2020/doc/src/atc\_internal\_element\_set.rst  
lammps-stable\_290ct2020/doc/src/atc\_internal\_quadrature.rst  
lammps-stable\_290ct2020/doc/src/atc\_kernel\_bandwidth.rst  
lammps-stable\_290ct2020/doc/src/atc\_lumped\_lambda\_solve.rst  
lammps-stable\_290ct2020/doc/src/atc\_mask\_direction.rst  
lammps-stable\_290ct2020/doc/src/atc\_mass\_matrix.rst  
lammps-stable\_290ct2020/doc/src/atc\_material.rst  
lammps-stable\_290ct2020/doc/src/atc\_mesh\_add\_to\_nodeset.rst  
lammps-stable\_290ct2020/doc/src/atc\_mesh\_create.rst  
lammps-stable\_290ct2020/doc/src/atc\_mesh\_create\_elementset.rst  
lammps-stable\_290ct2020/doc/src/atc\_mesh\_create\_faceset\_box.rst  
lammps-stable\_290ct2020/doc/src/atc\_mesh\_create\_faceset\_plane.rst  
lammps-stable\_290ct2020/doc/src/atc\_mesh\_create\_nodeset.rst  
lammps-stable\_290ct2020/doc/src/atc\_mesh\_delete\_elements.rst  
lammps-stable\_290ct2020/doc/src/atc\_mesh\_nodeset\_to\_elementset.rst  
lammps-stable\_290ct2020/doc/src/atc\_mesh\_output.rst  
lammps-stable\_290ct2020/doc/src/atc\_mesh\_quadrature.rst  
lammps-stable\_290ct2020/doc/src/atc\_mesh\_read.rst  
lammps-stable\_290ct2020/doc/src/atc\_mesh\_write.rst  
lammps-stable\_290ct2020/doc/src/atc\_output.rst  
lammps-stable\_290ct2020/doc/src/atc\_output\_boundary\_integral.rst  
lammps-stable\_290ct2020/doc/src/atc\_output\_contour\_integral.rst  
lammps-stable\_290ct2020/doc/src/atc\_output\_nodeset.rst

lammps-stable\_290ct2020/doc/src/atc\_output\_volume\_integral.rst  
lammps-stable\_290ct2020/doc/src/atc\_pair\_interactions.rst  
lammps-stable\_290ct2020/doc/src/atc\_poisson\_solver.rst  
lammps-stable\_290ct2020/doc/src/atc\_read\_restart.rst  
lammps-stable\_290ct2020/doc/src/atc\_remove\_molecule.rst  
lammps-stable\_290ct2020/doc/src/atc\_remove\_source.rst  
lammps-stable\_290ct2020/doc/src/atc\_remove\_species.rst  
lammps-stable\_290ct2020/doc/src/atc\_reset\_atomic\_reference.rst  
lammps-stable\_290ct2020/doc/src/atc\_reset\_time.rst  
lammps-stable\_290ct2020/doc/src/atc\_sample\_frequency.rst  
lammps-stable\_290ct2020/doc/src/atc\_set\_reference\_pe.rst  
lammps-stable\_290ct2020/doc/src/atc\_source.rst  
lammps-stable\_290ct2020/doc/src/atc\_source\_integration.rst  
lammps-stable\_290ct2020/doc/src/atc\_temperature\_definition.rst  
lammps-stable\_290ct2020/doc/src/atc\_time\_filter.rst  
lammps-stable\_290ct2020/doc/src/atc\_time\_integration.rst  
lammps-stable\_290ct2020/doc/src/atc\_track\_displacement.rst  
lammps-stable\_290ct2020/doc/src/atc\_unfix.rst  
lammps-stable\_290ct2020/doc/src/atc\_unfix\_flux.rst  
lammps-stable\_290ct2020/doc/src/atc\_write\_atom\_weights.rst  
lammps-stable\_290ct2020/doc/src/atc\_write\_restart.rst  
lammps-stable\_290ct2020/doc/src/atom\_modify.rst  
lammps-stable\_290ct2020/doc/src/atom\_style.rst  
lammps-stable\_290ct2020/doc/src/balance.rst  
lammps-stable\_290ct2020/doc/src/bond\_class2.rst  
lammps-stable\_290ct2020/doc/src/bond\_coeff.rst  
lammps-stable\_290ct2020/doc/src/bond\_fene.rst  
lammps-stable\_290ct2020/doc/src/bond\_fene\_expand.rst  
lammps-stable\_290ct2020/doc/src/bond\_gromos.rst  
lammps-stable\_290ct2020/doc/src/bond\_harmonic.rst  
lammps-stable\_290ct2020/doc/src/bond\_harmonic\_shift.rst  
lammps-stable\_290ct2020/doc/src/bond\_harmonic\_shift\_cut.rst  
lammps-stable\_290ct2020/doc/src/bond\_hybrid.rst  
lammps-stable\_290ct2020/doc/src/bond\_mm3.rst  
lammps-stable\_290ct2020/doc/src/bond\_morse.rst  
lammps-stable\_290ct2020/doc/src/bond\_none.rst  
lammps-stable\_290ct2020/doc/src/bond\_nonlinear.rst  
lammps-stable\_290ct2020/doc/src/bond\_oxdna.rst  
lammps-stable\_290ct2020/doc/src/bond\_quartic.rst  
lammps-stable\_290ct2020/doc/src/bond\_special.rst  
lammps-stable\_290ct2020/doc/src/bond\_style.rst  
lammps-stable\_290ct2020/doc/src/bond\_table.rst  
lammps-stable\_290ct2020/doc/src/bond\_write.rst  
lammps-stable\_290ct2020/doc/src/bond\_zero.rst  
lammps-stable\_290ct2020/doc/src/bonds.rst  
lammps-stable\_290ct2020/doc/src/boundary.rst  
lammps-stable\_290ct2020/doc/src/box.rst  
lammps-stable\_290ct2020/doc/src/change\_box.rst  
lammps-stable\_290ct2020/doc/src/clear.rst  
lammps-stable\_290ct2020/doc/src/comm\_modify.rst  
lammps-stable\_290ct2020/doc/src/comm\_style.rst  
lammps-stable\_290ct2020/doc/src/commands\_list.rst  
lammps-stable\_290ct2020/doc/src/compute.rst  
lammps-stable\_290ct2020/doc/src/compute\_ackland\_atom.rst  
lammps-stable\_290ct2020/doc/src/compute\_adf.rst  
lammps-stable\_290ct2020/doc/src/compute\_angle.rst  
lammps-stable\_290ct2020/doc/src/compute\_angle\_local.rst  
lammps-stable\_290ct2020/doc/src/compute\_angmom\_chunk.rst  
lammps-stable\_290ct2020/doc/src/compute\_basal\_atom.rst  
lammps-stable\_290ct2020/doc/src/compute\_body\_local.rst

lammps-stable\_290ct2020/doc/src/compute\_bond.rst  
lammps-stable\_290ct2020/doc/src/compute\_bond\_local.rst  
lammps-stable\_290ct2020/doc/src/compute\_centro\_atom.rst  
lammps-stable\_290ct2020/doc/src/compute\_chunk\_atom.rst  
lammps-stable\_290ct2020/doc/src/compute\_chunk\_spread\_atom.rst  
lammps-stable\_290ct2020/doc/src/compute\_cluster\_atom.rst  
lammps-stable\_290ct2020/doc/src/compute\_cna\_atom.rst  
lammps-stable\_290ct2020/doc/src/compute\_cnp\_atom.rst  
lammps-stable\_290ct2020/doc/src/compute\_com.rst  
lammps-stable\_290ct2020/doc/src/compute\_com\_chunk.rst  
lammps-stable\_290ct2020/doc/src/compute\_contact\_atom.rst  
lammps-stable\_290ct2020/doc/src/compute\_coord\_atom.rst  
lammps-stable\_290ct2020/doc/src/compute\_damage\_atom.rst  
lammps-stable\_290ct2020/doc/src/compute\_dihedral.rst  
lammps-stable\_290ct2020/doc/src/compute\_dihedral\_local.rst  
lammps-stable\_290ct2020/doc/src/compute\_dilatation\_atom.rst  
lammps-stable\_290ct2020/doc/src/compute\_dipole\_chunk.rst  
lammps-stable\_290ct2020/doc/src/compute\_displace\_atom.rst  
lammps-stable\_290ct2020/doc/src/compute\_dpd.rst  
lammps-stable\_290ct2020/doc/src/compute\_dpd\_atom.rst  
lammps-stable\_290ct2020/doc/src/compute\_edpd\_temp\_atom.rst  
lammps-stable\_290ct2020/doc/src/compute\_entropy\_atom.rst  
lammps-stable\_290ct2020/doc/src/compute\_erotate\_asphere.rst  
lammps-stable\_290ct2020/doc/src/compute\_erotate\_rigid.rst  
lammps-stable\_290ct2020/doc/src/compute\_erotate\_sphere.rst  
lammps-stable\_290ct2020/doc/src/compute\_erotate\_sphere\_atom.rst  
lammps-stable\_290ct2020/doc/src/compute\_event\_displace.rst  
lammps-stable\_290ct2020/doc/src/compute\_fep.rst  
lammps-stable\_290ct2020/doc/src/compute\_global\_atom.rst  
lammps-stable\_290ct2020/doc/src/compute\_group\_group.rst  
lammps-stable\_290ct2020/doc/src/compute\_gyration.rst  
lammps-stable\_290ct2020/doc/src/compute\_gyration\_chunk.rst  
lammps-stable\_290ct2020/doc/src/compute\_gyration\_shape.rst  
lammps-stable\_290ct2020/doc/src/compute\_gyration\_shape\_chunk.rst  
lammps-stable\_290ct2020/doc/src/compute\_heat\_flux.rst  
lammps-stable\_290ct2020/doc/src/compute\_hexorder\_atom.rst  
lammps-stable\_290ct2020/doc/src/compute\_hma.rst  
lammps-stable\_290ct2020/doc/src/compute\_improper.rst  
lammps-stable\_290ct2020/doc/src/compute\_improper\_local.rst  
lammps-stable\_290ct2020/doc/src/compute\_inertia\_chunk.rst  
lammps-stable\_290ct2020/doc/src/compute\_ke.rst  
lammps-stable\_290ct2020/doc/src/compute\_ke\_atom.rst  
lammps-stable\_290ct2020/doc/src/compute\_ke\_atom\_eff.rst  
lammps-stable\_290ct2020/doc/src/compute\_ke\_eff.rst  
lammps-stable\_290ct2020/doc/src/compute\_ke\_rigid.rst  
lammps-stable\_290ct2020/doc/src/compute\_mesont.rst  
lammps-stable\_290ct2020/doc/src/compute\_mliap.rst  
lammps-stable\_290ct2020/doc/src/compute\_modify.rst  
lammps-stable\_290ct2020/doc/src/compute\_momentum.rst  
lammps-stable\_290ct2020/doc/src/compute\_msd.rst  
lammps-stable\_290ct2020/doc/src/compute\_msd\_chunk.rst  
lammps-stable\_290ct2020/doc/src/compute\_msd\_nongauss.rst  
lammps-stable\_290ct2020/doc/src/compute\_omega\_chunk.rst  
lammps-stable\_290ct2020/doc/src/compute\_orientorder\_atom.rst  
lammps-stable\_290ct2020/doc/src/compute\_pair.rst  
lammps-stable\_290ct2020/doc/src/compute\_pair\_local.rst  
lammps-stable\_290ct2020/doc/src/compute\_pe.rst  
lammps-stable\_290ct2020/doc/src/compute\_pe\_atom.rst  
lammps-stable\_290ct2020/doc/src/compute\_plasticity\_atom.rst  
lammps-stable\_290ct2020/doc/src/compute\_pressure.rst

lammps-stable\_290ct2020/doc/src/compute\_pressure\_cylinder.rst  
lammps-stable\_290ct2020/doc/src/compute\_pressure\_uf.rst  
lammps-stable\_290ct2020/doc/src/compute\_property\_atom.rst  
lammps-stable\_290ct2020/doc/src/compute\_property\_chunk.rst  
lammps-stable\_290ct2020/doc/src/compute\_property\_local.rst  
lammps-stable\_290ct2020/doc/src/compute\_ptm\_atom.rst  
lammps-stable\_290ct2020/doc/src/compute\_rdf.rst  
lammps-stable\_290ct2020/doc/src/compute\_reduce.rst  
lammps-stable\_290ct2020/doc/src/compute\_reduce\_chunk.rst  
lammps-stable\_290ct2020/doc/src/compute\_rigid\_local.rst  
lammps-stable\_290ct2020/doc/src/compute\_saed.rst  
lammps-stable\_290ct2020/doc/src/compute\_slice.rst  
lammps-stable\_290ct2020/doc/src/compute\_smd\_contact\_radius.rst  
lammps-stable\_290ct2020/doc/src/compute\_smd\_damage.rst  
lammps-stable\_290ct2020/doc/src/compute\_smd\_hourglass\_error.rst  
lammps-stable\_290ct2020/doc/src/compute\_smd\_internal\_energy.rst  
lammps-stable\_290ct2020/doc/src/compute\_smd\_plastic\_strain.rst  
lammps-stable\_290ct2020/doc/src/compute\_smd\_plastic\_strain\_rate.rst  
lammps-stable\_290ct2020/doc/src/compute\_smd\_rho.rst  
lammps-stable\_290ct2020/doc/src/compute\_smd\_tlsph\_defgrad.rst  
lammps-stable\_290ct2020/doc/src/compute\_smd\_tlsph\_dt.rst  
lammps-stable\_290ct2020/doc/src/compute\_smd\_tlsph\_num\_neighs.rst  
lammps-stable\_290ct2020/doc/src/compute\_smd\_tlsph\_shape.rst  
lammps-stable\_290ct2020/doc/src/compute\_smd\_tlsph\_strain.rst  
lammps-stable\_290ct2020/doc/src/compute\_smd\_tlsph\_strain\_rate.rst  
lammps-stable\_290ct2020/doc/src/compute\_smd\_tlsph\_stress.rst  
lammps-stable\_290ct2020/doc/src/compute\_smd\_triangle\_vertices.rst  
lammps-stable\_290ct2020/doc/src/compute\_smd\_ulsph\_effm.rst  
lammps-stable\_290ct2020/doc/src/compute\_smd\_ulsph\_num\_neighs.rst  
lammps-stable\_290ct2020/doc/src/compute\_smd\_ulsph\_strain.rst  
lammps-stable\_290ct2020/doc/src/compute\_smd\_ulsph\_strain\_rate.rst  
lammps-stable\_290ct2020/doc/src/compute\_smd\_ulsph\_stress.rst  
lammps-stable\_290ct2020/doc/src/compute\_smd\_vol.rst  
lammps-stable\_290ct2020/doc/src/compute\_sna\_atom.rst  
lammps-stable\_290ct2020/doc/src/compute\_sph\_e\_atom.rst  
lammps-stable\_290ct2020/doc/src/compute\_sph\_rho\_atom.rst  
lammps-stable\_290ct2020/doc/src/compute\_sph\_t\_atom.rst  
lammps-stable\_290ct2020/doc/src/compute\_spin.rst  
lammps-stable\_290ct2020/doc/src/compute\_stress\_atom.rst  
lammps-stable\_290ct2020/doc/src/compute\_stress\_mop.rst  
lammps-stable\_290ct2020/doc/src/compute\_tally.rst  
lammps-stable\_290ct2020/doc/src/compute\_tdpd\_cc\_atom.rst  
lammps-stable\_290ct2020/doc/src/compute\_temp.rst  
lammps-stable\_290ct2020/doc/src/compute\_temp\_asphere.rst  
lammps-stable\_290ct2020/doc/src/compute\_temp\_body.rst  
lammps-stable\_290ct2020/doc/src/compute\_temp\_chunk.rst  
lammps-stable\_290ct2020/doc/src/compute\_temp\_com.rst  
lammps-stable\_290ct2020/doc/src/compute\_temp\_cs.rst  
lammps-stable\_290ct2020/doc/src/compute\_temp\_deform.rst  
lammps-stable\_290ct2020/doc/src/compute\_temp\_deform\_eff.rst  
lammps-stable\_290ct2020/doc/src/compute\_temp\_drude.rst  
lammps-stable\_290ct2020/doc/src/compute\_temp\_eff.rst  
lammps-stable\_290ct2020/doc/src/compute\_temp\_partial.rst  
lammps-stable\_290ct2020/doc/src/compute\_temp\_profile.rst  
lammps-stable\_290ct2020/doc/src/compute\_temp\_ramp.rst  
lammps-stable\_290ct2020/doc/src/compute\_temp\_region.rst  
lammps-stable\_290ct2020/doc/src/compute\_temp\_region\_eff.rst  
lammps-stable\_290ct2020/doc/src/compute\_temp\_rotate.rst  
lammps-stable\_290ct2020/doc/src/compute\_temp\_sphere.rst  
lammps-stable\_290ct2020/doc/src/compute\_temp\_uf.rst

lammps-stable\_290ct2020/doc/src/compute\_ti.rst  
lammps-stable\_290ct2020/doc/src/compute\_torque\_chunk.rst  
lammps-stable\_290ct2020/doc/src/compute\_vacf.rst  
lammps-stable\_290ct2020/doc/src/compute\_vcm\_chunk.rst  
lammps-stable\_290ct2020/doc/src/compute\_viscosity\_cos.rst  
lammps-stable\_290ct2020/doc/src/compute\_voronoi\_atom.rst  
lammps-stable\_290ct2020/doc/src/compute\_xrd.rst  
lammps-stable\_290ct2020/doc/src/computes.rst  
lammps-stable\_290ct2020/doc/src/create\_atoms.rst  
lammps-stable\_290ct2020/doc/src/create\_bonds.rst  
lammps-stable\_290ct2020/doc/src/create\_box.rst  
lammps-stable\_290ct2020/doc/src/delete\_atoms.rst  
lammps-stable\_290ct2020/doc/src/delete\_bonds.rst  
lammps-stable\_290ct2020/doc/src/dielectric.rst  
lammps-stable\_290ct2020/doc/src/dihedral\_charmm.rst  
lammps-stable\_290ct2020/doc/src/dihedral\_class2.rst  
lammps-stable\_290ct2020/doc/src/dihedral\_coeff.rst  
lammps-stable\_290ct2020/doc/src/dihedral\_cosine\_shift\_exp.rst  
lammps-stable\_290ct2020/doc/src/dihedral\_fourier.rst  
lammps-stable\_290ct2020/doc/src/dihedral\_harmonic.rst  
lammps-stable\_290ct2020/doc/src/dihedral\_helix.rst  
lammps-stable\_290ct2020/doc/src/dihedral\_hybrid.rst  
lammps-stable\_290ct2020/doc/src/dihedral\_multi\_harmonic.rst  
lammps-stable\_290ct2020/doc/src/dihedral\_nharmonic.rst  
lammps-stable\_290ct2020/doc/src/dihedral\_none.rst  
lammps-stable\_290ct2020/doc/src/dihedral\_opls.rst  
lammps-stable\_290ct2020/doc/src/dihedral\_quadratic.rst  
lammps-stable\_290ct2020/doc/src/dihedral\_spherical.rst  
lammps-stable\_290ct2020/doc/src/dihedral\_style.rst  
lammps-stable\_290ct2020/doc/src/dihedral\_table.rst  
lammps-stable\_290ct2020/doc/src/dihedral\_table\_cut.rst  
lammps-stable\_290ct2020/doc/src/dihedral\_zero.rst  
lammps-stable\_290ct2020/doc/src/dihedrals.rst  
lammps-stable\_290ct2020/doc/src/dimension.rst  
lammps-stable\_290ct2020/doc/src/displace\_atoms.rst  
lammps-stable\_290ct2020/doc/src/dump.rst  
lammps-stable\_290ct2020/doc/src/dump\_adios.rst  
lammps-stable\_290ct2020/doc/src/dump\_cfg\_ufef.rst  
lammps-stable\_290ct2020/doc/src/dump\_h5md.rst  
lammps-stable\_290ct2020/doc/src/dump\_image.rst  
lammps-stable\_290ct2020/doc/src/dump\_modify.rst  
lammps-stable\_290ct2020/doc/src/dump\_molfile.rst  
lammps-stable\_290ct2020/doc/src/dump\_netcdf.rst  
lammps-stable\_290ct2020/doc/src/dump\_vtk.rst  
lammps-stable\_290ct2020/doc/src/dynamical\_matrix.rst  
lammps-stable\_290ct2020/doc/src/echo.rst  
lammps-stable\_290ct2020/doc/src/fix.rst  
lammps-stable\_290ct2020/doc/src/fix\_accelerate\_cos.rst  
lammps-stable\_290ct2020/doc/src/fix\_adapt.rst  
lammps-stable\_290ct2020/doc/src/fix\_adapt\_fep.rst  
lammps-stable\_290ct2020/doc/src/fix\_addforce.rst  
lammps-stable\_290ct2020/doc/src/fix\_addtorque.rst  
lammps-stable\_290ct2020/doc/src/fix\_append\_atoms.rst  
lammps-stable\_290ct2020/doc/src/fix\_atc.rst  
lammps-stable\_290ct2020/doc/src/fix\_atom\_swap.rst  
lammps-stable\_290ct2020/doc/src/fix\_ave\_atom.rst  
lammps-stable\_290ct2020/doc/src/fix\_ave\_chunk.rst  
lammps-stable\_290ct2020/doc/src/fix\_ave\_correlate.rst  
lammps-stable\_290ct2020/doc/src/fix\_ave\_correlate\_long.rst  
lammps-stable\_290ct2020/doc/src/fix\_ave\_histo.rst

lammps-stable\_290ct2020/doc/src/fix\_ave\_time.rst  
lammps-stable\_290ct2020/doc/src/fix\_aveforce.rst  
lammps-stable\_290ct2020/doc/src/fix\_balance.rst  
lammps-stable\_290ct2020/doc/src/fix\_bocs.rst  
lammps-stable\_290ct2020/doc/src/fix\_bond\_break.rst  
lammps-stable\_290ct2020/doc/src/fix\_bond\_create.rst  
lammps-stable\_290ct2020/doc/src/fix\_bond\_react.rst  
lammps-stable\_290ct2020/doc/src/fix\_bond\_swap.rst  
lammps-stable\_290ct2020/doc/src/fix\_box\_relax.rst  
lammps-stable\_290ct2020/doc/src/fix\_client\_md.rst  
lammps-stable\_290ct2020/doc/src/fix\_cmap.rst  
lammps-stable\_290ct2020/doc/src/fix\_colvars.rst  
lammps-stable\_290ct2020/doc/src/fix\_controller.rst  
lammps-stable\_290ct2020/doc/src/fix\_deform.rst  
lammps-stable\_290ct2020/doc/src/fix\_deposit.rst  
lammps-stable\_290ct2020/doc/src/fix\_dpd\_energy.rst  
lammps-stable\_290ct2020/doc/src/fix\_dpd\_source.rst  
lammps-stable\_290ct2020/doc/src/fix\_drag.rst  
lammps-stable\_290ct2020/doc/src/fix\_drude.rst  
lammps-stable\_290ct2020/doc/src/fix\_drude\_transform.rst  
lammps-stable\_290ct2020/doc/src/fix\_dt\_reset.rst  
lammps-stable\_290ct2020/doc/src/fix\_efield.rst  
lammps-stable\_290ct2020/doc/src/fix\_ehex.rst  
lammps-stable\_290ct2020/doc/src/fix\_electron\_stopping.rst  
lammps-stable\_290ct2020/doc/src/fix\_enforce2d.rst  
lammps-stable\_290ct2020/doc/src/fix\_eos\_cv.rst  
lammps-stable\_290ct2020/doc/src/fix\_eos\_table.rst  
lammps-stable\_290ct2020/doc/src/fix\_eos\_table\_rx.rst  
lammps-stable\_290ct2020/doc/src/fix\_evaporate.rst  
lammps-stable\_290ct2020/doc/src/fix\_external.rst  
lammps-stable\_290ct2020/doc/src/fix\_ffl.rst  
lammps-stable\_290ct2020/doc/src/fix\_filter\_corotate.rst  
lammps-stable\_290ct2020/doc/src/fix\_flow\_gauss.rst  
lammps-stable\_290ct2020/doc/src/fix\_freeze.rst  
lammps-stable\_290ct2020/doc/src/fix\_gcmc.rst  
lammps-stable\_290ct2020/doc/src/fix\_gld.rst  
lammps-stable\_290ct2020/doc/src/fix\_gle.rst  
lammps-stable\_290ct2020/doc/src/fix\_gravity.rst  
lammps-stable\_290ct2020/doc/src/fix\_grem.rst  
lammps-stable\_290ct2020/doc/src/fix\_halt.rst  
lammps-stable\_290ct2020/doc/src/fix\_heat.rst  
lammps-stable\_290ct2020/doc/src/fix\_hyper\_global.rst  
lammps-stable\_290ct2020/doc/src/fix\_hyper\_local.rst  
lammps-stable\_290ct2020/doc/src/fix\_imd.rst  
lammps-stable\_290ct2020/doc/src/fix\_indent.rst  
lammps-stable\_290ct2020/doc/src/fix\_ipi.rst  
lammps-stable\_290ct2020/doc/src/fix\_langevin.rst  
lammps-stable\_290ct2020/doc/src/fix\_langevin\_drude.rst  
lammps-stable\_290ct2020/doc/src/fix\_langevin\_eff.rst  
lammps-stable\_290ct2020/doc/src/fix\_langevin\_spin.rst  
lammps-stable\_290ct2020/doc/src/fix\_latte.rst  
lammps-stable\_290ct2020/doc/src/fix\_lb\_fluid.rst  
lammps-stable\_290ct2020/doc/src/fix\_lb\_momentum.rst  
lammps-stable\_290ct2020/doc/src/fix\_lb\_pc.rst  
lammps-stable\_290ct2020/doc/src/fix\_lb\_rigid\_pc\_sphere.rst  
lammps-stable\_290ct2020/doc/src/fix\_lb\_viscous.rst  
lammps-stable\_290ct2020/doc/src/fix\_lineforce.rst  
lammps-stable\_290ct2020/doc/src/fix\_manifoldforce.rst  
lammps-stable\_290ct2020/doc/src/fix\_meso\_move.rst  
lammps-stable\_290ct2020/doc/src/fix\_modify.rst



lammps-stable\_290ct2020/doc/src/fix\_modify\_atc\_commands.rst  
lammps-stable\_290ct2020/doc/src/fix\_momentum.rst  
lammps-stable\_290ct2020/doc/src/fix\_move.rst  
lammps-stable\_290ct2020/doc/src/fix\_mscg.rst  
lammps-stable\_290ct2020/doc/src/fix\_msst.rst  
lammps-stable\_290ct2020/doc/src/fix\_mvv\_dpd.rst  
lammps-stable\_290ct2020/doc/src/fix\_neb.rst  
lammps-stable\_290ct2020/doc/src/fix\_neb\_spin.rst  
lammps-stable\_290ct2020/doc/src/fix\_nh.rst  
lammps-stable\_290ct2020/doc/src/fix\_nh\_eff.rst  
lammps-stable\_290ct2020/doc/src/fix\_nh\_ufef.rst  
lammps-stable\_290ct2020/doc/src/fix\_nph\_asphere.rst  
lammps-stable\_290ct2020/doc/src/fix\_nph\_body.rst  
lammps-stable\_290ct2020/doc/src/fix\_nph\_sphere.rst  
lammps-stable\_290ct2020/doc/src/fix\_nphug.rst  
lammps-stable\_290ct2020/doc/src/fix\_npt\_asphere.rst  
lammps-stable\_290ct2020/doc/src/fix\_npt\_body.rst  
lammps-stable\_290ct2020/doc/src/fix\_npt\_cauchy.rst  
lammps-stable\_290ct2020/doc/src/fix\_npt\_sphere.rst  
lammps-stable\_290ct2020/doc/src/fix\_numdiff.rst  
lammps-stable\_290ct2020/doc/src/fix\_nve.rst  
lammps-stable\_290ct2020/doc/src/fix\_nve\_asphere.rst  
lammps-stable\_290ct2020/doc/src/fix\_nve\_asphere\_noforce.rst  
lammps-stable\_290ct2020/doc/src/fix\_nve\_awpmd.rst  
lammps-stable\_290ct2020/doc/src/fix\_nve\_body.rst  
lammps-stable\_290ct2020/doc/src/fix\_nve\_dot.rst  
lammps-stable\_290ct2020/doc/src/fix\_nve\_dotc\_langevin.rst  
lammps-stable\_290ct2020/doc/src/fix\_nve\_eff.rst  
lammps-stable\_290ct2020/doc/src/fix\_nve\_limit.rst  
lammps-stable\_290ct2020/doc/src/fix\_nve\_line.rst  
lammps-stable\_290ct2020/doc/src/fix\_nve\_manifold\_rattle.rst  
lammps-stable\_290ct2020/doc/src/fix\_nve\_noforce.rst  
lammps-stable\_290ct2020/doc/src/fix\_nve\_sphere.rst  
lammps-stable\_290ct2020/doc/src/fix\_nve\_spin.rst  
lammps-stable\_290ct2020/doc/src/fix\_nve\_tri.rst  
lammps-stable\_290ct2020/doc/src/fix\_nvkl.rst  
lammps-stable\_290ct2020/doc/src/fix\_nvt\_asphere.rst  
lammps-stable\_290ct2020/doc/src/fix\_nvt\_body.rst  
lammps-stable\_290ct2020/doc/src/fix\_nvt\_manifold\_rattle.rst  
lammps-stable\_290ct2020/doc/src/fix\_nvt\_sllod.rst  
lammps-stable\_290ct2020/doc/src/fix\_nvt\_sllod\_eff.rst  
lammps-stable\_290ct2020/doc/src/fix\_nvt\_sphere.rst  
lammps-stable\_290ct2020/doc/src/fix\_oneway.rst  
lammps-stable\_290ct2020/doc/src/fix\_orient.rst  
lammps-stable\_290ct2020/doc/src/fix\_orient\_eco.rst  
lammps-stable\_290ct2020/doc/src/fix\_pafi.rst  
lammps-stable\_290ct2020/doc/src/fix\_phonon.rst  
lammps-stable\_290ct2020/doc/src/fix\_pimd.rst  
lammps-stable\_290ct2020/doc/src/fix\_plane\_force.rst  
lammps-stable\_290ct2020/doc/src/fix\_plumed.rst  
lammps-stable\_290ct2020/doc/src/fix\_poems.rst  
lammps-stable\_290ct2020/doc/src/fix\_pour.rst  
lammps-stable\_290ct2020/doc/src/fix\_precession\_spin.rst  
lammps-stable\_290ct2020/doc/src/fix\_press\_berendsen.rst  
lammps-stable\_290ct2020/doc/src/fix\_print.rst  
lammps-stable\_290ct2020/doc/src/fix\_propel\_self.rst  
lammps-stable\_290ct2020/doc/src/fix\_property\_atom.rst  
lammps-stable\_290ct2020/doc/src/fix\_python\_invoke.rst  
lammps-stable\_290ct2020/doc/src/fix\_python\_move.rst  
lammps-stable\_290ct2020/doc/src/fix\_qbmsst.rst

lammps-stable\_290ct2020/doc/src/fix\_geq.rst  
lammps-stable\_290ct2020/doc/src/fix\_geq\_comb.rst  
lammps-stable\_290ct2020/doc/src/fix\_geq\_reax.rst  
lammps-stable\_290ct2020/doc/src/fix\_qmmm.rst  
lammps-stable\_290ct2020/doc/src/fix\_qtb.rst  
lammps-stable\_290ct2020/doc/src/fix\_reaxc\_bonds.rst  
lammps-stable\_290ct2020/doc/src/fix\_reaxc\_species.rst  
lammps-stable\_290ct2020/doc/src/fix\_recenter.rst  
lammps-stable\_290ct2020/doc/src/fix\_restrain.rst  
lammps-stable\_290ct2020/doc/src/fix\_rhok.rst  
lammps-stable\_290ct2020/doc/src/fix\_rigid.rst  
lammps-stable\_290ct2020/doc/src/fix\_rigid\_meso.rst  
lammps-stable\_290ct2020/doc/src/fix\_rx.rst  
lammps-stable\_290ct2020/doc/src/fix\_saed\_vtk.rst  
lammps-stable\_290ct2020/doc/src/fix\_setforce.rst  
lammps-stable\_290ct2020/doc/src/fix\_shake.rst  
lammps-stable\_290ct2020/doc/src/fix\_shardlow.rst  
lammps-stable\_290ct2020/doc/src/fix\_smd.rst  
lammps-stable\_290ct2020/doc/src/fix\_smd\_adjust\_dt.rst  
lammps-stable\_290ct2020/doc/src/fix\_smd\_integrate\_tlsph.rst  
lammps-stable\_290ct2020/doc/src/fix\_smd\_integrate\_ulsph.rst  
lammps-stable\_290ct2020/doc/src/fix\_smd\_move\_triangulated\_surface.rst  
lammps-stable\_290ct2020/doc/src/fix\_smd\_setvel.rst  
lammps-stable\_290ct2020/doc/src/fix\_smd\_wall\_surface.rst  
lammps-stable\_290ct2020/doc/src/fix\_sph.rst  
lammps-stable\_290ct2020/doc/src/fix\_sph\_stationary.rst  
lammps-stable\_290ct2020/doc/src/fix\_spring.rst  
lammps-stable\_290ct2020/doc/src/fix\_spring\_chunk.rst  
lammps-stable\_290ct2020/doc/src/fix\_spring\_rg.rst  
lammps-stable\_290ct2020/doc/src/fix\_spring\_self.rst  
lammps-stable\_290ct2020/doc/src/fix\_srd.rst  
lammps-stable\_290ct2020/doc/src/fix\_store\_force.rst  
lammps-stable\_290ct2020/doc/src/fix\_store\_state.rst  
lammps-stable\_290ct2020/doc/src/fix\_temp\_berendsen.rst  
lammps-stable\_290ct2020/doc/src/fix\_temp\_csvr.rst  
lammps-stable\_290ct2020/doc/src/fix\_temp\_rescale.rst  
lammps-stable\_290ct2020/doc/src/fix\_temp\_rescale\_eff.rst  
lammps-stable\_290ct2020/doc/src/fix\_tfmc.rst  
lammps-stable\_290ct2020/doc/src/fix\_thermal\_conductivity.rst  
lammps-stable\_290ct2020/doc/src/fix\_ti\_spring.rst  
lammps-stable\_290ct2020/doc/src/fix\_tmd.rst  
lammps-stable\_290ct2020/doc/src/fix\_ttm.rst  
lammps-stable\_290ct2020/doc/src/fix\_tune\_kspace.rst  
lammps-stable\_290ct2020/doc/src/fix\_vector.rst  
lammps-stable\_290ct2020/doc/src/fix\_viscosity.rst  
lammps-stable\_290ct2020/doc/src/fix\_viscous.rst  
lammps-stable\_290ct2020/doc/src/fix\_wall.rst  
lammps-stable\_290ct2020/doc/src/fix\_wall\_body\_polygon.rst  
lammps-stable\_290ct2020/doc/src/fix\_wall\_body\_polyhedron.rst  
lammps-stable\_290ct2020/doc/src/fix\_wall\_ees.rst  
lammps-stable\_290ct2020/doc/src/fix\_wall\_gran.rst  
lammps-stable\_290ct2020/doc/src/fix\_wall\_gran\_region.rst  
lammps-stable\_290ct2020/doc/src/fix\_wall\_piston.rst  
lammps-stable\_290ct2020/doc/src/fix\_wall\_reflect.rst  
lammps-stable\_290ct2020/doc/src/fix\_wall\_reflect\_stochastic.rst  
lammps-stable\_290ct2020/doc/src/fix\_wall\_region.rst  
lammps-stable\_290ct2020/doc/src/fix\_wall\_srd.rst  
lammps-stable\_290ct2020/doc/src/fix\_widom.rst  
lammps-stable\_290ct2020/doc/src/fixes.rst  
lammps-stable\_290ct2020/doc/src/group.rst

lammps-stable\_290ct2020/doc/src/group2ndx.rst  
lammps-stable\_290ct2020/doc/src/hyper.rst  
lammps-stable\_290ct2020/doc/src/if.rst  
lammps-stable\_290ct2020/doc/src/img/  
lammps-stable\_290ct2020/doc/src/img/balance\_nonuniform.jpg  
lammps-stable\_290ct2020/doc/src/img/balance\_rcb.jpg  
lammps-stable\_290ct2020/doc/src/img/balance\_uniform.jpg  
lammps-stable\_290ct2020/doc/src/img/dump1.jpg  
lammps-stable\_290ct2020/doc/src/img/dump2.jpg  
lammps-stable\_290ct2020/doc/src/img/gran\_funnel.png  
lammps-stable\_290ct2020/doc/src/img/gran\_mixer.png  
lammps-stable\_290ct2020/doc/src/img/hop1.jpg  
lammps-stable\_290ct2020/doc/src/img/hop2.jpg  
lammps-stable\_290ct2020/doc/src/img/saed\_ewald\_intersect.jpg  
lammps-stable\_290ct2020/doc/src/img/saed\_mesh.jpg  
lammps-stable\_290ct2020/doc/src/img/screenshot\_atomeye.jpg  
lammps-stable\_290ct2020/doc/src/img/screenshot\_gl.jpg  
lammps-stable\_290ct2020/doc/src/img/screenshot\_pymol.jpg  
lammps-stable\_290ct2020/doc/src/img/screenshot\_vmd.jpg  
lammps-stable\_290ct2020/doc/src/img/sinusoid.jpg  
lammps-stable\_290ct2020/doc/src/img/wsl\_tutorial/  
lammps-stable\_290ct2020/doc/src/img/wsl\_tutorial/compilation\_result.png  
lammps-stable\_290ct2020/doc/src/img/wsl\_tutorial/first\_login.png  
lammps-stable\_290ct2020/doc/src/img/wsl\_tutorial/osinfo.png  
lammps-stable\_290ct2020/doc/src/img/wsl\_tutorial/powershell.png  
lammps-stable\_290ct2020/doc/src/img/wsl\_tutorial/ubuntu\_in\_store.png  
lammps-stable\_290ct2020/doc/src/img/wsl\_tutorial/updates.png  
lammps-stable\_290ct2020/doc/src/img/wsl\_tutorial/windows\_firewall.png  
lammps-stable\_290ct2020/doc/src/img/wsl\_tutorial/windows\_update.png  
lammps-stable\_290ct2020/doc/src/img/wsl\_tutorial/wsl\_install1.png  
lammps-stable\_290ct2020/doc/src/img/wsl\_tutorial/wsl\_install2.png  
lammps-stable\_290ct2020/doc/src/img/wsl\_tutorial/wsl\_install3.png  
lammps-stable\_290ct2020/doc/src/img/wsl\_tutorial/wsl\_integration.png  
lammps-stable\_290ct2020/doc/src/img/xrd\_mesh.jpg  
lammps-stable\_290ct2020/doc/src/improper\_class2.rst  
lammps-stable\_290ct2020/doc/src/improper\_coeff.rst  
lammps-stable\_290ct2020/doc/src/improper\_cossq.rst  
lammps-stable\_290ct2020/doc/src/improper\_cvff.rst  
lammps-stable\_290ct2020/doc/src/improper\_distance.rst  
lammps-stable\_290ct2020/doc/src/improper\_distharm.rst  
lammps-stable\_290ct2020/doc/src/improper\_fourier.rst  
lammps-stable\_290ct2020/doc/src/improper\_harmonic.rst  
lammps-stable\_290ct2020/doc/src/improper\_hybrid.rst  
lammps-stable\_290ct2020/doc/src/improper\_inversion\_harmonic.rst  
lammps-stable\_290ct2020/doc/src/improper\_none.rst  
lammps-stable\_290ct2020/doc/src/improper\_ring.rst  
lammps-stable\_290ct2020/doc/src/improper\_sqdistharm.rst  
lammps-stable\_290ct2020/doc/src/improper\_style.rst  
lammps-stable\_290ct2020/doc/src/improper\_umbrella.rst  
lammps-stable\_290ct2020/doc/src/improper\_zero.rst  
lammps-stable\_290ct2020/doc/src/impropers.rst  
lammps-stable\_290ct2020/doc/src/include.rst  
lammps-stable\_290ct2020/doc/src/info.rst  
lammps-stable\_290ct2020/doc/src/jump.rst  
lammps-stable\_290ct2020/doc/src/kim\_commands.rst  
lammps-stable\_290ct2020/doc/src/kspace\_modify.rst  
lammps-stable\_290ct2020/doc/src/kspace\_style.rst  
lammps-stable\_290ct2020/doc/src/label.rst  
lammps-stable\_290ct2020/doc/src/lattice.rst  
lammps-stable\_290ct2020/doc/src/log.rst

lammps-stable\_290ct2020/doc/src/mass.rst  
lammps-stable\_290ct2020/doc/src/message.rst  
lammps-stable\_290ct2020/doc/src/min\_modify.rst  
lammps-stable\_290ct2020/doc/src/min\_spin.rst  
lammps-stable\_290ct2020/doc/src/min\_style.rst  
lammps-stable\_290ct2020/doc/src/minimize.rst  
lammps-stable\_290ct2020/doc/src/molecule.rst  
lammps-stable\_290ct2020/doc/src/neb.rst  
lammps-stable\_290ct2020/doc/src/neb\_spin.rst  
lammps-stable\_290ct2020/doc/src/neigh\_modify.rst  
lammps-stable\_290ct2020/doc/src/neighbor.rst  
lammps-stable\_290ct2020/doc/src/newton.rst  
lammps-stable\_290ct2020/doc/src/next.rst  
lammps-stable\_290ct2020/doc/src/package.rst  
lammps-stable\_290ct2020/doc/src/pair\_adp.rst  
lammps-stable\_290ct2020/doc/src/pair\_agni.rst  
lammps-stable\_290ct2020/doc/src/pair\_airebo.rst  
lammps-stable\_290ct2020/doc/src/pair\_atm.rst  
lammps-stable\_290ct2020/doc/src/pair\_awpmd.rst  
lammps-stable\_290ct2020/doc/src/pair\_beck.rst  
lammps-stable\_290ct2020/doc/src/pair\_body\_nparticle.rst  
lammps-stable\_290ct2020/doc/src/pair\_body\_rounded\_polygon.rst  
lammps-stable\_290ct2020/doc/src/pair\_body\_rounded\_polyhedron.rst  
lammps-stable\_290ct2020/doc/src/pair\_bop.rst  
lammps-stable\_290ct2020/doc/src/pair\_born.rst  
lammps-stable\_290ct2020/doc/src/pair\_brownian.rst  
lammps-stable\_290ct2020/doc/src/pair\_buck.rst  
lammps-stable\_290ct2020/doc/src/pair\_buck6d\_coul\_gauss.rst  
lammps-stable\_290ct2020/doc/src/pair\_buck\_long.rst  
lammps-stable\_290ct2020/doc/src/pair\_charmm.rst  
lammps-stable\_290ct2020/doc/src/pair\_class2.rst  
lammps-stable\_290ct2020/doc/src/pair\_coeff.rst  
lammps-stable\_290ct2020/doc/src/pair\_colloid.rst  
lammps-stable\_290ct2020/doc/src/pair\_comb.rst  
lammps-stable\_290ct2020/doc/src/pair\_cosine\_squared.rst  
lammps-stable\_290ct2020/doc/src/pair\_coul.rst  
lammps-stable\_290ct2020/doc/src/pair\_coul\_diel.rst  
lammps-stable\_290ct2020/doc/src/pair\_coul\_shield.rst  
lammps-stable\_290ct2020/doc/src/pair\_coul\_slater.rst  
lammps-stable\_290ct2020/doc/src/pair\_coul\_tt.rst  
lammps-stable\_290ct2020/doc/src/pair\_cs.rst  
lammps-stable\_290ct2020/doc/src/pair\_dipole.rst  
lammps-stable\_290ct2020/doc/src/pair\_dpd.rst  
lammps-stable\_290ct2020/doc/src/pair\_dpd\_fdt.rst  
lammps-stable\_290ct2020/doc/src/pair\_drip.rst  
lammps-stable\_290ct2020/doc/src/pair\_dsmc.rst  
lammps-stable\_290ct2020/doc/src/pair\_e3b.rst  
lammps-stable\_290ct2020/doc/src/pair\_eam.rst  
lammps-stable\_290ct2020/doc/src/pair\_edip.rst  
lammps-stable\_290ct2020/doc/src/pair\_eff.rst  
lammps-stable\_290ct2020/doc/src/pair\_eim.rst  
lammps-stable\_290ct2020/doc/src/pair\_exp6\_rx.rst  
lammps-stable\_290ct2020/doc/src/pair\_extep.rst  
lammps-stable\_290ct2020/doc/src/pair\_fep\_soft.rst  
lammps-stable\_290ct2020/doc/src/pair\_gauss.rst  
lammps-stable\_290ct2020/doc/src/pair\_gayberne.rst  
lammps-stable\_290ct2020/doc/src/pair\_gran.rst  
lammps-stable\_290ct2020/doc/src/pair\_granular.rst  
lammps-stable\_290ct2020/doc/src/pair\_gromacs.rst  
lammps-stable\_290ct2020/doc/src/pair\_gw.rst

lammps-stable\_290ct2020/doc/src/pair\_hbond\_dreiding.rst  
lammps-stable\_290ct2020/doc/src/pair\_hybrid.rst  
lammps-stable\_290ct2020/doc/src/pair\_ilp\_graphene\_hbn.rst  
lammps-stable\_290ct2020/doc/src/pair\_kim.rst  
lammps-stable\_290ct2020/doc/src/pair\_kolmogorov\_crespi\_full.rst  
lammps-stable\_290ct2020/doc/src/pair\_kolmogorov\_crespi\_z.rst  
lammps-stable\_290ct2020/doc/src/pair\_lcbop.rst  
lammps-stable\_290ct2020/doc/src/pair\_lebedeva\_z.rst  
lammps-stable\_290ct2020/doc/src/pair\_line\_lj.rst  
lammps-stable\_290ct2020/doc/src/pair\_list.rst  
lammps-stable\_290ct2020/doc/src/pair\_lj.rst  
lammps-stable\_290ct2020/doc/src/pair\_lj96.rst  
lammps-stable\_290ct2020/doc/src/pair\_lj\_cubic.rst  
lammps-stable\_290ct2020/doc/src/pair\_lj\_cut\_coul.rst  
lammps-stable\_290ct2020/doc/src/pair\_lj\_cut\_tip4p.rst  
lammps-stable\_290ct2020/doc/src/pair\_lj\_expand.rst  
lammps-stable\_290ct2020/doc/src/pair\_lj\_long.rst  
lammps-stable\_290ct2020/doc/src/pair\_lj\_smooth.rst  
lammps-stable\_290ct2020/doc/src/pair\_lj\_smooth\_linear.rst  
lammps-stable\_290ct2020/doc/src/pair\_lj\_switch3\_coulgauss\_long.rst  
lammps-stable\_290ct2020/doc/src/pair\_local\_density.rst  
lammps-stable\_290ct2020/doc/src/pair\_lubricate.rst  
lammps-stable\_290ct2020/doc/src/pair\_lubricateU.rst  
lammps-stable\_290ct2020/doc/src/pair\_mdf.rst  
lammps-stable\_290ct2020/doc/src/pair\_meam\_spline.rst  
lammps-stable\_290ct2020/doc/src/pair\_meam\_sw\_spline.rst  
lammps-stable\_290ct2020/doc/src/pair\_meamc.rst  
lammps-stable\_290ct2020/doc/src/pair\_mesocnt.rst  
lammps-stable\_290ct2020/doc/src/pair\_mesodpd.rst  
lammps-stable\_290ct2020/doc/src/pair\_mesont\_tpm.rst  
lammps-stable\_290ct2020/doc/src/pair\_mgpt.rst  
lammps-stable\_290ct2020/doc/src/pair\_mie.rst  
lammps-stable\_290ct2020/doc/src/pair\_mliap.rst  
lammps-stable\_290ct2020/doc/src/pair\_mm3\_switch3\_coulgauss\_long.rst  
lammps-stable\_290ct2020/doc/src/pair\_modify.rst  
lammps-stable\_290ct2020/doc/src/pair\_momb.rst  
lammps-stable\_290ct2020/doc/src/pair\_morse.rst  
lammps-stable\_290ct2020/doc/src/pair\_multi\_lucy.rst  
lammps-stable\_290ct2020/doc/src/pair\_multi\_lucy\_rx.rst  
lammps-stable\_290ct2020/doc/src/pair\_nb3b\_harmonic.rst  
lammps-stable\_290ct2020/doc/src/pair\_nm.rst  
lammps-stable\_290ct2020/doc/src/pair\_none.rst  
lammps-stable\_290ct2020/doc/src/pair\_oxdna.rst  
lammps-stable\_290ct2020/doc/src/pair\_oxdna2.rst  
lammps-stable\_290ct2020/doc/src/pair\_oxrna2.rst  
lammps-stable\_290ct2020/doc/src/pair\_peri.rst  
lammps-stable\_290ct2020/doc/src/pair\_polymorphic.rst  
lammps-stable\_290ct2020/doc/src/pair\_python.rst  
lammps-stable\_290ct2020/doc/src/pair\_quip.rst  
lammps-stable\_290ct2020/doc/src/pair\_reaxc.rst  
lammps-stable\_290ct2020/doc/src/pair\_resquared.rst  
lammps-stable\_290ct2020/doc/src/pair\_sdk.rst  
lammps-stable\_290ct2020/doc/src/pair\_sdpd\_taitwater\_isothermal.rst  
lammps-stable\_290ct2020/doc/src/pair\_smd\_hertz.rst  
lammps-stable\_290ct2020/doc/src/pair\_smd\_tlsph.rst  
lammps-stable\_290ct2020/doc/src/pair\_smd\_triangulated\_surface.rst  
lammps-stable\_290ct2020/doc/src/pair\_smd\_ulsph.rst  
lammps-stable\_290ct2020/doc/src/pair\_smtbq.rst  
lammps-stable\_290ct2020/doc/src/pair\_snap.rst  
lammps-stable\_290ct2020/doc/src/pair\_soft.rst

lammps-stable\_290ct2020/doc/src/pair\_sph\_heatconduction.rst  
lammps-stable\_290ct2020/doc/src/pair\_sph\_idealgas.rst  
lammps-stable\_290ct2020/doc/src/pair\_sph\_lj.rst  
lammps-stable\_290ct2020/doc/src/pair\_sph\_rhosum.rst  
lammps-stable\_290ct2020/doc/src/pair\_sph\_taitwater.rst  
lammps-stable\_290ct2020/doc/src/pair\_sph\_taitwater\_morris.rst  
lammps-stable\_290ct2020/doc/src/pair\_spin\_dipole.rst  
lammps-stable\_290ct2020/doc/src/pair\_spin\_dmi.rst  
lammps-stable\_290ct2020/doc/src/pair\_spin\_exchange.rst  
lammps-stable\_290ct2020/doc/src/pair\_spin\_magelec.rst  
lammps-stable\_290ct2020/doc/src/pair\_spin\_neel.rst  
lammps-stable\_290ct2020/doc/src/pair\_srp.rst  
lammps-stable\_290ct2020/doc/src/pair\_style.rst  
lammps-stable\_290ct2020/doc/src/pair\_sw.rst  
lammps-stable\_290ct2020/doc/src/pair\_table.rst  
lammps-stable\_290ct2020/doc/src/pair\_table\_rx.rst  
lammps-stable\_290ct2020/doc/src/pair\_tersoff.rst  
lammps-stable\_290ct2020/doc/src/pair\_tersoff\_mod.rst  
lammps-stable\_290ct2020/doc/src/pair\_tersoff\_zbl.rst  
lammps-stable\_290ct2020/doc/src/pair\_thole.rst  
lammps-stable\_290ct2020/doc/src/pair\_tri\_lj.rst  
lammps-stable\_290ct2020/doc/src/pair\_uvm.rst  
lammps-stable\_290ct2020/doc/src/pair\_vashishta.rst  
lammps-stable\_290ct2020/doc/src/pair\_write.rst  
lammps-stable\_290ct2020/doc/src/pair\_yukawa.rst  
lammps-stable\_290ct2020/doc/src/pair\_yukawa\_colloid.rst  
lammps-stable\_290ct2020/doc/src/pair\_zbl.rst  
lammps-stable\_290ct2020/doc/src/pair\_zero.rst  
lammps-stable\_290ct2020/doc/src/pairs.rst  
lammps-stable\_290ct2020/doc/src/partition.rst  
lammps-stable\_290ct2020/doc/src/prd.rst  
lammps-stable\_290ct2020/doc/src/print.rst  
lammps-stable\_290ct2020/doc/src/processors.rst  
lammps-stable\_290ct2020/doc/src/python.rst  
lammps-stable\_290ct2020/doc/src/quit.rst  
lammps-stable\_290ct2020/doc/src/read\_data.rst  
lammps-stable\_290ct2020/doc/src/read\_dump.rst  
lammps-stable\_290ct2020/doc/src/read\_restart.rst  
lammps-stable\_290ct2020/doc/src/region.rst  
lammps-stable\_290ct2020/doc/src/replicate.rst  
lammps-stable\_290ct2020/doc/src/rerun.rst  
lammps-stable\_290ct2020/doc/src/reset\_atom\_ids.rst  
lammps-stable\_290ct2020/doc/src/reset\_mol\_ids.rst  
lammps-stable\_290ct2020/doc/src/reset\_timestep.rst  
lammps-stable\_290ct2020/doc/src/restart.rst  
lammps-stable\_290ct2020/doc/src/run.rst  
lammps-stable\_290ct2020/doc/src/run\_style.rst  
lammps-stable\_290ct2020/doc/src/server.rst  
lammps-stable\_290ct2020/doc/src/server\_mc.rst  
lammps-stable\_290ct2020/doc/src/server\_md.rst  
lammps-stable\_290ct2020/doc/src/set.rst  
lammps-stable\_290ct2020/doc/src/shell.rst  
lammps-stable\_290ct2020/doc/src/special\_bonds.rst  
lammps-stable\_290ct2020/doc/src/suffix.rst  
lammps-stable\_290ct2020/doc/src/tad.rst  
lammps-stable\_290ct2020/doc/src/temper.rst  
lammps-stable\_290ct2020/doc/src/temper\_grem.rst  
lammps-stable\_290ct2020/doc/src/temper\_npt.rst  
lammps-stable\_290ct2020/doc/src/thermo.rst  
lammps-stable\_290ct2020/doc/src/thermo\_modify.rst

```
lammps-stable_290ct2020/doc/src/thermo_style.rst
lammps-stable_290ct2020/doc/src/third_order.rst
lammps-stable_290ct2020/doc/src/timer.rst
lammps-stable_290ct2020/doc/src/timestep.rst
lammps-stable_290ct2020/doc/src/uncompute.rst
lammps-stable_290ct2020/doc/src/undump.rst
lammps-stable_290ct2020/doc/src/unfix.rst
lammps-stable_290ct2020/doc/src/units.rst
lammps-stable_290ct2020/doc/src/variable.rst
lammps-stable_290ct2020/doc/src/velocity.rst
lammps-stable_290ct2020/doc/src/write_coeff.rst
lammps-stable_290ct2020/doc/src/write_data.rst
lammps-stable_290ct2020/doc/src/write_dump.rst
lammps-stable_290ct2020/doc/src/write_restart.rst
lammps-stable_290ct2020/doc/utils/
lammps-stable_290ct2020/doc/utils/check-packages.py
lammps-stable_290ct2020/doc/utils/check-styles.py
lammps-stable_290ct2020/doc/utils/converters/
lammps-stable_290ct2020/doc/utils/converters/.travis.yml
lammps-stable_290ct2020/doc/utils/converters/LICENSE
lammps-stable_290ct2020/doc/utils/converters/README.md
lammps-stable_290ct2020/doc/utils/converters/lammpsdoc/
lammps-stable_290ct2020/doc/utils/converters/lammpsdoc/__init__.py
lammps-stable_290ct2020/doc/utils/converters/lammpsdoc/doc_anchor_check.py
lammps-stable_290ct2020/doc/utils/converters/lammpsdoc/lammps_filters.py
lammps-stable_290ct2020/doc/utils/converters/lammpsdoc/rst_anchor_check.py
lammps-stable_290ct2020/doc/utils/converters/lammpsdoc/txt2html.py
lammps-stable_290ct2020/doc/utils/converters/lammpsdoc/txt2rst.py
lammps-stable_290ct2020/doc/utils/converters/setup.py
lammps-stable_290ct2020/doc/utils/converters/tests/
lammps-stable_290ct2020/doc/utils/converters/tests/test_lammps_filters.py
lammps-stable_290ct2020/doc/utils/converters/tests/test_txt2html.py
lammps-stable_290ct2020/doc/utils/converters/tests/test_txt2rst.py
lammps-stable_290ct2020/doc/utils/fixup_headers.py
lammps-stable_290ct2020/doc/utils/requirements.txt
lammps-stable_290ct2020/doc/utils/sphinx-config/
lammps-stable_290ct2020/doc/utils/sphinx-config/LAMMPSLexer.py
lammps-stable_290ct2020/doc/utils/sphinx-config/_static/
lammps-stable_290ct2020/doc/utils/sphinx-config/_static/css/
lammps-stable_290ct2020/doc/utils/sphinx-config/_static/css/lammps.css
lammps-stable_290ct2020/doc/utils/sphinx-config/_static/lammps-logo.png
lammps-stable_290ct2020/doc/utils/sphinx-config/_static/lammps.ico
lammps-stable_290ct2020/doc/utils/sphinx-config/_themes/
lammps-stable_290ct2020/doc/utils/sphinx-config/_themes/lammps_theme/
lammps-stable_290ct2020/doc/utils/sphinx-config/_themes/lammps_theme/apache-
license-2.0.txt
lammps-stable_290ct2020/doc/utils/sphinx-config/_themes/lammps_theme/LICENSE
lammps-stable_290ct2020/doc/utils/sphinx-config/_themes/lammps_theme/OFL-Lice
nse.txt
lammps-stable_290ct2020/doc/utils/sphinx-config/_themes/lammps_theme/README
lammps-stable_290ct2020/doc/utils/sphinx-config/_themes/lammps_theme/__init_
_.py
lammps-stable_290ct2020/doc/utils/sphinx-config/_themes/lammps_theme/breadcru
mbs.html
lammps-stable_290ct2020/doc/utils/sphinx-config/_themes/lammps_theme/footer.h
tml
lammps-stable_290ct2020/doc/utils/sphinx-config/_themes/lammps_theme/layout.h
tml
lammps-stable_290ct2020/doc/utils/sphinx-config/_themes/lammps_theme/locale/
lammps-stable_290ct2020/doc/utils/sphinx-config/_themes/lammps_theme/locale/d
```

```
e/
lammps-stable_290ct2020/doc/utis/sphinx-config/_themes/lammps_theme/locale/d
e/LC_MESSAGES/
lammps-stable_290ct2020/doc/utis/sphinx-config/_themes/lammps_theme/locale/d
e/LC_MESSAGES/sphinx.mo
lammps-stable_290ct2020/doc/utis/sphinx-config/_themes/lammps_theme/locale/d
e/LC_MESSAGES/sphinx.po
lammps-stable_290ct2020/doc/utis/sphinx-config/_themes/lammps_theme/locale/e
n/
lammps-stable_290ct2020/doc/utis/sphinx-config/_themes/lammps_theme/locale/e
n/LC_MESSAGES/
lammps-stable_290ct2020/doc/utis/sphinx-config/_themes/lammps_theme/locale/e
n/LC_MESSAGES/sphinx.mo
lammps-stable_290ct2020/doc/utis/sphinx-config/_themes/lammps_theme/locale/e
n/LC_MESSAGES/sphinx.po
lammps-stable_290ct2020/doc/utis/sphinx-config/_themes/lammps_theme/locale/e
s/
lammps-stable_290ct2020/doc/utis/sphinx-config/_themes/lammps_theme/locale/e
s/LC_MESSAGES/
lammps-stable_290ct2020/doc/utis/sphinx-config/_themes/lammps_theme/locale/e
s/LC_MESSAGES/sphinx.mo
lammps-stable_290ct2020/doc/utis/sphinx-config/_themes/lammps_theme/locale/e
s/LC_MESSAGES/sphinx.po
lammps-stable_290ct2020/doc/utis/sphinx-config/_themes/lammps_theme/locale/e
t/
lammps-stable_290ct2020/doc/utis/sphinx-config/_themes/lammps_theme/locale/e
t/LC_MESSAGES/
lammps-stable_290ct2020/doc/utis/sphinx-config/_themes/lammps_theme/locale/e
t/LC_MESSAGES/sphinx.mo
lammps-stable_290ct2020/doc/utis/sphinx-config/_themes/lammps_theme/locale/e
t/LC_MESSAGES/sphinx.po
lammps-stable_290ct2020/doc/utis/sphinx-config/_themes/lammps_theme/locale/f
r/
lammps-stable_290ct2020/doc/utis/sphinx-config/_themes/lammps_theme/locale/f
r/LC_MESSAGES/
lammps-stable_290ct2020/doc/utis/sphinx-config/_themes/lammps_theme/locale/f
r/LC_MESSAGES/sphinx.mo
lammps-stable_290ct2020/doc/utis/sphinx-config/_themes/lammps_theme/locale/f
r/LC_MESSAGES/sphinx.po
lammps-stable_290ct2020/doc/utis/sphinx-config/_themes/lammps_theme/locale/n
l/
lammps-stable_290ct2020/doc/utis/sphinx-config/_themes/lammps_theme/locale/n
l/LC_MESSAGES/
lammps-stable_290ct2020/doc/utis/sphinx-config/_themes/lammps_theme/locale/n
l/LC_MESSAGES/sphinx.mo
lammps-stable_290ct2020/doc/utis/sphinx-config/_themes/lammps_theme/locale/n
l/LC_MESSAGES/sphinx.po
lammps-stable_290ct2020/doc/utis/sphinx-config/_themes/lammps_theme/locale/p
t_BR/
lammps-stable_290ct2020/doc/utis/sphinx-config/_themes/lammps_theme/locale/p
t_BR/LC_MESSAGES/
lammps-stable_290ct2020/doc/utis/sphinx-config/_themes/lammps_theme/locale/p
t_BR/LC_MESSAGES/sphinx.mo
lammps-stable_290ct2020/doc/utis/sphinx-config/_themes/lammps_theme/locale/p
t_BR/LC_MESSAGES/sphinx.po
lammps-stable_290ct2020/doc/utis/sphinx-config/_themes/lammps_theme/locale/r
u/
lammps-stable_290ct2020/doc/utis/sphinx-config/_themes/lammps_theme/locale/r
u/LC_MESSAGES/
lammps-stable_290ct2020/doc/utis/sphinx-config/_themes/lammps_theme/locale/r
```



u/LC\_MESSAGES/sphinx.mo  
lammps-stable\_290ct2020/doc/utils/sphinx-config/\_themes/lampps\_theme/locale/r  
u/LC\_MESSAGES/sphinx.po  
lammps-stable\_290ct2020/doc/utils/sphinx-config/\_themes/lampps\_theme/locale/s  
phinx.pot  
lammps-stable\_290ct2020/doc/utils/sphinx-config/\_themes/lampps\_theme/locale/s  
v/  
lammps-stable\_290ct2020/doc/utils/sphinx-config/\_themes/lampps\_theme/locale/s  
v/LC\_MESSAGES/  
lammps-stable\_290ct2020/doc/utils/sphinx-config/\_themes/lampps\_theme/locale/s  
v/LC\_MESSAGES/sphinx.mo  
lammps-stable\_290ct2020/doc/utils/sphinx-config/\_themes/lampps\_theme/locale/s  
v/LC\_MESSAGES/sphinx.po  
lammps-stable\_290ct2020/doc/utils/sphinx-config/\_themes/lampps\_theme/locale/t  
r/  
lammps-stable\_290ct2020/doc/utils/sphinx-config/\_themes/lampps\_theme/locale/t  
r/LC\_MESSAGES/  
lammps-stable\_290ct2020/doc/utils/sphinx-config/\_themes/lampps\_theme/locale/t  
r/LC\_MESSAGES/sphinx.mo  
lammps-stable\_290ct2020/doc/utils/sphinx-config/\_themes/lampps\_theme/locale/t  
r/LC\_MESSAGES/sphinx.po  
lammps-stable\_290ct2020/doc/utils/sphinx-config/\_themes/lampps\_theme/locale/z  
h\_CN/  
lammps-stable\_290ct2020/doc/utils/sphinx-config/\_themes/lampps\_theme/locale/z  
h\_CN/LC\_MESSAGES/  
lammps-stable\_290ct2020/doc/utils/sphinx-config/\_themes/lampps\_theme/locale/z  
h\_CN/LC\_MESSAGES/sphinx.mo  
lammps-stable\_290ct2020/doc/utils/sphinx-config/\_themes/lampps\_theme/locale/z  
h\_CN/LC\_MESSAGES/sphinx.po  
lammps-stable\_290ct2020/doc/utils/sphinx-config/\_themes/lampps\_theme/search.h  
tml  
lammps-stable\_290ct2020/doc/utils/sphinx-config/\_themes/lampps\_theme/searchbo  
x.html  
lammps-stable\_290ct2020/doc/utils/sphinx-config/\_themes/lampps\_theme/static/  
lammps-stable\_290ct2020/doc/utils/sphinx-config/\_themes/lampps\_theme/static/c  
ss/  
lammps-stable\_290ct2020/doc/utils/sphinx-config/\_themes/lampps\_theme/static/c  
ss/badge\_only.css  
lammps-stable\_290ct2020/doc/utils/sphinx-config/\_themes/lampps\_theme/static/c  
ss/fonts/  
lammps-stable\_290ct2020/doc/utils/sphinx-config/\_themes/lampps\_theme/static/c  
ss/fonts/Roboto-Slab-Bold.woff  
lammps-stable\_290ct2020/doc/utils/sphinx-config/\_themes/lampps\_theme/static/c  
ss/fonts/Roboto-Slab-Bold.woff2  
lammps-stable\_290ct2020/doc/utils/sphinx-config/\_themes/lampps\_theme/static/c  
ss/fonts/Roboto-Slab-Regular.woff  
lammps-stable\_290ct2020/doc/utils/sphinx-config/\_themes/lampps\_theme/static/c  
ss/fonts/Roboto-Slab-Regular.woff2  
lammps-stable\_290ct2020/doc/utils/sphinx-config/\_themes/lampps\_theme/static/c  
ss/fonts/fontawesome-webfont.eot  
lammps-stable\_290ct2020/doc/utils/sphinx-config/\_themes/lampps\_theme/static/c  
ss/fonts/fontawesome-webfont.svg  
lammps-stable\_290ct2020/doc/utils/sphinx-config/\_themes/lampps\_theme/static/c  
ss/fonts/fontawesome-webfont.ttf  
lammps-stable\_290ct2020/doc/utils/sphinx-config/\_themes/lampps\_theme/static/c  
ss/fonts/fontawesome-webfont.woff  
lammps-stable\_290ct2020/doc/utils/sphinx-config/\_themes/lampps\_theme/static/c  
ss/fonts/fontawesome-webfont.woff2  
lammps-stable\_290ct2020/doc/utils/sphinx-config/\_themes/lampps\_theme/static/c  
ss/fonts/lato-bold-italic.woff

lammps-stable\_290ct2020/doc/utils/sphinx-config/\_themes/lammps\_theme/static/css/fonts/lato-bold-italic.woff2  
lammps-stable\_290ct2020/doc/utils/sphinx-config/\_themes/lammps\_theme/static/css/fonts/lato-bold.woff  
lammps-stable\_290ct2020/doc/utils/sphinx-config/\_themes/lammps\_theme/static/css/fonts/lato-bold.woff2  
lammps-stable\_290ct2020/doc/utils/sphinx-config/\_themes/lammps\_theme/static/css/fonts/lato-normal-italic.woff  
lammps-stable\_290ct2020/doc/utils/sphinx-config/\_themes/lammps\_theme/static/css/fonts/lato-normal-italic.woff2  
lammps-stable\_290ct2020/doc/utils/sphinx-config/\_themes/lammps\_theme/static/css/fonts/lato-normal.woff  
lammps-stable\_290ct2020/doc/utils/sphinx-config/\_themes/lammps\_theme/static/css/fonts/lato-normal.woff2  
lammps-stable\_290ct2020/doc/utils/sphinx-config/\_themes/lammps\_theme/static/css/theme.css  
lammps-stable\_290ct2020/doc/utils/sphinx-config/\_themes/lammps\_theme/static/fonts/  
lammps-stable\_290ct2020/doc/utils/sphinx-config/\_themes/lammps\_theme/static/fonts/FontAwesome.otf  
lammps-stable\_290ct2020/doc/utils/sphinx-config/\_themes/lammps\_theme/static/fonts/Inconsolata-Bold.ttf  
lammps-stable\_290ct2020/doc/utils/sphinx-config/\_themes/lammps\_theme/static/fonts/Inconsolata.ttf  
lammps-stable\_290ct2020/doc/utils/sphinx-config/\_themes/lammps\_theme/static/fonts/Lato-Bold.ttf  
lammps-stable\_290ct2020/doc/utils/sphinx-config/\_themes/lammps\_theme/static/fonts/Lato-Regular.ttf  
lammps-stable\_290ct2020/doc/utils/sphinx-config/\_themes/lammps\_theme/static/fonts/RobotoSlab-Bold.ttf  
lammps-stable\_290ct2020/doc/utils/sphinx-config/\_themes/lammps\_theme/static/fonts/RobotoSlab-Regular.ttf  
lammps-stable\_290ct2020/doc/utils/sphinx-config/\_themes/lammps\_theme/static/fonts/fontawesome-webfont.eot  
lammps-stable\_290ct2020/doc/utils/sphinx-config/\_themes/lammps\_theme/static/fonts/fontawesome-webfont.svg  
lammps-stable\_290ct2020/doc/utils/sphinx-config/\_themes/lammps\_theme/static/fonts/fontawesome-webfont.ttf  
lammps-stable\_290ct2020/doc/utils/sphinx-config/\_themes/lammps\_theme/static/fonts/fontawesome-webfont.woff  
lammps-stable\_290ct2020/doc/utils/sphinx-config/\_themes/lammps\_theme/static/js/  
lammps-stable\_290ct2020/doc/utils/sphinx-config/\_themes/lammps\_theme/static/js/badge\_only.js  
lammps-stable\_290ct2020/doc/utils/sphinx-config/\_themes/lammps\_theme/static/js/modernizr.min.js  
lammps-stable\_290ct2020/doc/utils/sphinx-config/\_themes/lammps\_theme/static/js/theme.js  
lammps-stable\_290ct2020/doc/utils/sphinx-config/\_themes/lammps\_theme/theme.conf  
lammps-stable\_290ct2020/doc/utils/sphinx-config/\_themes/lammps\_theme/version.s.html  
lammps-stable\_290ct2020/doc/utils/sphinx-config/conf.py.in  
lammps-stable\_290ct2020/doc/utils/sphinx-config/false\_positives.txt  
lammps-stable\_290ct2020/examples/  
lammps-stable\_290ct2020/examples/ASPHERE/  
lammps-stable\_290ct2020/examples/ASPHERE/README  
lammps-stable\_290ct2020/examples/ASPHERE/box/  
lammps-stable\_290ct2020/examples/ASPHERE/box/box.py  
lammps-stable\_290ct2020/examples/ASPHERE/box/data.box

```
lammps-stable_290ct2020/examples/ASPHERE/box/in.box
lammps-stable_290ct2020/examples/ASPHERE/box/in.box.mp
lammps-stable_290ct2020/examples/ASPHERE/box/log.1Feb14.box.g++.8
lammps-stable_290ct2020/examples/ASPHERE/box/log.1Feb14.box.mp.g++.8
lammps-stable_290ct2020/examples/ASPHERE/dimer/
lammps-stable_290ct2020/examples/ASPHERE/dimer/data.dimer
lammps-stable_290ct2020/examples/ASPHERE/dimer/dimer.py
lammps-stable_290ct2020/examples/ASPHERE/dimer/in.dimer
lammps-stable_290ct2020/examples/ASPHERE/dimer/in.dimer.mp
lammps-stable_290ct2020/examples/ASPHERE/dimer/log.1Feb14.dimer.g++.8
lammps-stable_290ct2020/examples/ASPHERE/dimer/log.1Feb14.dimer.mp.g++.8
lammps-stable_290ct2020/examples/ASPHERE/ellipsoid/
lammps-stable_290ct2020/examples/ASPHERE/ellipsoid/in.ellipsoid
lammps-stable_290ct2020/examples/ASPHERE/ellipsoid/in.ellipsoid.mp
lammps-stable_290ct2020/examples/ASPHERE/ellipsoid/log.1Feb14.ellipsoid.g++.8
lammps-stable_290ct2020/examples/ASPHERE/ellipsoid/log.1Feb14.ellipsoid.mp.
g++.8
lammps-stable_290ct2020/examples/ASPHERE/line/
lammps-stable_290ct2020/examples/ASPHERE/line/data.line
lammps-stable_290ct2020/examples/ASPHERE/line/data.line.srd
lammps-stable_290ct2020/examples/ASPHERE/line/in.line
lammps-stable_290ct2020/examples/ASPHERE/line/in.line.srd
lammps-stable_290ct2020/examples/ASPHERE/line/line.py
lammps-stable_290ct2020/examples/ASPHERE/line/line.srd.py
lammps-stable_290ct2020/examples/ASPHERE/line/line.srd.viz.py
lammps-stable_290ct2020/examples/ASPHERE/line/line.viz.py
lammps-stable_290ct2020/examples/ASPHERE/line/log.1Feb14.line.g++.8
lammps-stable_290ct2020/examples/ASPHERE/line/log.1Feb14.line.srd.g++.8
lammps-stable_290ct2020/examples/ASPHERE/poly/
lammps-stable_290ct2020/examples/ASPHERE/poly/in.poly
lammps-stable_290ct2020/examples/ASPHERE/poly/in.poly.mp
lammps-stable_290ct2020/examples/ASPHERE/poly/log.1Feb14.poly.g++.8
lammps-stable_290ct2020/examples/ASPHERE/poly/log.1Feb14.poly.mp.g++.8
lammps-stable_290ct2020/examples/ASPHERE/star/
lammps-stable_290ct2020/examples/ASPHERE/star/data.star
lammps-stable_290ct2020/examples/ASPHERE/star/in.star
lammps-stable_290ct2020/examples/ASPHERE/star/in.star.mp
lammps-stable_290ct2020/examples/ASPHERE/star/log.1Feb14.star.g++.8
lammps-stable_290ct2020/examples/ASPHERE/star/log.1Feb14.star.mp.g++.8
lammps-stable_290ct2020/examples/ASPHERE/star/star.py
lammps-stable_290ct2020/examples/ASPHERE/tri/
lammps-stable_290ct2020/examples/ASPHERE/tri/data.tri.srd
lammps-stable_290ct2020/examples/ASPHERE/tri/in.tri.srd
lammps-stable_290ct2020/examples/ASPHERE/tri/log.1Feb14.tri.srd.g++.8
lammps-stable_290ct2020/examples/ASPHERE/tri/tri.srd.py
lammps-stable_290ct2020/examples/ASPHERE/tri/tri.srd.viz.py
lammps-stable_290ct2020/examples/COUPLE/
lammps-stable_290ct2020/examples/COUPLE/README
lammps-stable_290ct2020/examples/COUPLE/fortran/
lammps-stable_290ct2020/examples/COUPLE/fortran/README
lammps-stable_290ct2020/examples/COUPLE/fortran/libfwrapper.c
lammps-stable_290ct2020/examples/COUPLE/fortran2/
lammps-stable_290ct2020/examples/COUPLE/fortran2/LAMMPS-wrapper.cpp
lammps-stable_290ct2020/examples/COUPLE/fortran2/LAMMPS-wrapper.h
lammps-stable_290ct2020/examples/COUPLE/fortran2/LAMMPS.F90
lammps-stable_290ct2020/examples/COUPLE/fortran2/Makefile
lammps-stable_290ct2020/examples/COUPLE/fortran2/README
lammps-stable_290ct2020/examples/COUPLE/fortran2/in.simple
lammps-stable_290ct2020/examples/COUPLE/fortran2/simple.f90
lammps-stable_290ct2020/examples/COUPLE/fortran_dftb/
```

```
lammps-stable_290ct2020/examples/COUPLE/fortran_dftb/LAMMPS-wrapper.cpp
lammps-stable_290ct2020/examples/COUPLE/fortran_dftb/LAMMPS-wrapper.h
lammps-stable_290ct2020/examples/COUPLE/fortran_dftb/LAMMPS-wrapper2.cpp
lammps-stable_290ct2020/examples/COUPLE/fortran_dftb/LAMMPS-wrapper2.h
lammps-stable_290ct2020/examples/COUPLE/fortran_dftb/LAMMPS.F90
lammps-stable_290ct2020/examples/COUPLE/fortran_dftb/README
lammps-stable_290ct2020/examples/COUPLE/fortran_dftb/data.diamond
lammps-stable_290ct2020/examples/COUPLE/fortran_dftb/dftb_in.hsd
lammps-stable_290ct2020/examples/COUPLE/fortran_dftb/dftb_pin.hsd
lammps-stable_290ct2020/examples/COUPLE/fortran_dftb/in.simple
lammps-stable_290ct2020/examples/COUPLE/fortran_dftb/log.simple
lammps-stable_290ct2020/examples/COUPLE/fortran_dftb/makefile
lammps-stable_290ct2020/examples/COUPLE/fortran_dftb/simple.f90
lammps-stable_290ct2020/examples/COUPLE/lammps_mc/
lammps-stable_290ct2020/examples/COUPLE/lammps_mc/Makefile
lammps-stable_290ct2020/examples/COUPLE/lammps_mc/README
lammps-stable_290ct2020/examples/COUPLE/lammps_mc/in.mc
lammps-stable_290ct2020/examples/COUPLE/lammps_mc/in.mc.server
lammps-stable_290ct2020/examples/COUPLE/lammps_mc/log.28Aug18.file.g++.1
lammps-stable_290ct2020/examples/COUPLE/lammps_mc/log.28Aug18.file.g++.4
lammps-stable_290ct2020/examples/COUPLE/lammps_mc/log.28Aug18.zmq.g++.1
lammps-stable_290ct2020/examples/COUPLE/lammps_mc/log.28Aug18.zmq.g++.4
lammps-stable_290ct2020/examples/COUPLE/lammps_mc/mc.cpp
lammps-stable_290ct2020/examples/COUPLE/lammps_mc/mc.h
lammps-stable_290ct2020/examples/COUPLE/lammps_mc/random_park.cpp
lammps-stable_290ct2020/examples/COUPLE/lammps_mc/random_park.h
lammps-stable_290ct2020/examples/COUPLE/lammps_nwchem/
lammps-stable_290ct2020/examples/COUPLE/lammps_nwchem/README
lammps-stable_290ct2020/examples/COUPLE/lammps_nwchem/ao_basis/
lammps-stable_290ct2020/examples/COUPLE/lammps_nwchem/ao_basis/data.h2o
lammps-stable_290ct2020/examples/COUPLE/lammps_nwchem/ao_basis/h2o.nw
lammps-stable_290ct2020/examples/COUPLE/lammps_nwchem/ao_basis/in.client.h2o
lammps-stable_290ct2020/examples/COUPLE/lammps_nwchem/ao_basis/in.client.h2o.
min
lammps-stable_290ct2020/examples/COUPLE/lammps_nwchem/ao_basis/log.client.out
put
lammps-stable_290ct2020/examples/COUPLE/lammps_nwchem/ao_basis/log.lammps.h2
o.31Jan20
lammps-stable_290ct2020/examples/COUPLE/lammps_nwchem/ao_basis/log.lammps.h2
o.min.31Jan20
lammps-stable_290ct2020/examples/COUPLE/lammps_nwchem/ao_basis/nwchem_lammps.
out
lammps-stable_290ct2020/examples/COUPLE/lammps_nwchem/ao_basis/nwchem_lammps.
out.h2o.31Jan20
lammps-stable_290ct2020/examples/COUPLE/lammps_nwchem/ao_basis/nwchem_lammps.
out.h2o.min.31Jan20
lammps-stable_290ct2020/examples/COUPLE/lammps_nwchem/nwchem_wrap.py
lammps-stable_290ct2020/examples/COUPLE/lammps_nwchem/planewave/
lammps-stable_290ct2020/examples/COUPLE/lammps_nwchem/planewave/data.W
lammps-stable_290ct2020/examples/COUPLE/lammps_nwchem/planewave/in.client.W
lammps-stable_290ct2020/examples/COUPLE/lammps_nwchem/planewave/in.client.W.m
in
lammps-stable_290ct2020/examples/COUPLE/lammps_nwchem/planewave/log.client.ou
tput
lammps-stable_290ct2020/examples/COUPLE/lammps_nwchem/planewave/log.lammps.W.
30ct19
lammps-stable_290ct2020/examples/COUPLE/lammps_nwchem/planewave/log.lammps.W.
min.30ct19
lammps-stable_290ct2020/examples/COUPLE/lammps_nwchem/planewave/nwchem_lamp
s.out
```

lammps-stable\_290ct2020/examples/COUPLE/lammps\_nwchem/planewave/nwchem\_lammps.out.W.30ct19  
lammps-stable\_290ct2020/examples/COUPLE/lammps\_nwchem/planewave/nwchem\_lammps.out.W.min.30ct19  
lammps-stable\_290ct2020/examples/COUPLE/lammps\_nwchem/planewave/w.nw  
lammps-stable\_290ct2020/examples/COUPLE/lammps\_quest/  
lammps-stable\_290ct2020/examples/COUPLE/lammps\_quest/Makefile.g++  
lammps-stable\_290ct2020/examples/COUPLE/lammps\_quest/README  
lammps-stable\_290ct2020/examples/COUPLE/lammps\_quest/in.lammps  
lammps-stable\_290ct2020/examples/COUPLE/lammps\_quest/lmpopath.h  
lammps-stable\_290ct2020/examples/COUPLE/lammps\_quest/lmpqst.cpp  
lammps-stable\_290ct2020/examples/COUPLE/lammps\_quest/log.lammps.1  
lammps-stable\_290ct2020/examples/COUPLE/lammps\_quest/log.lammps.4  
lammps-stable\_290ct2020/examples/COUPLE/lammps\_quest/qstexe.h  
lammps-stable\_290ct2020/examples/COUPLE/lammps\_quest/si\_111.in  
lammps-stable\_290ct2020/examples/COUPLE/lammps\_spparks/  
lammps-stable\_290ct2020/examples/COUPLE/lammps\_spparks/Makefile.g++  
lammps-stable\_290ct2020/examples/COUPLE/lammps\_spparks/README  
lammps-stable\_290ct2020/examples/COUPLE/lammps\_spparks/in.lammps  
lammps-stable\_290ct2020/examples/COUPLE/lammps\_spparks/in.spparks  
lammps-stable\_290ct2020/examples/COUPLE/lammps\_spparks/lmpopath.h  
lammps-stable\_290ct2020/examples/COUPLE/lammps\_spparks/lmpspk.cpp  
lammps-stable\_290ct2020/examples/COUPLE/lammps\_spparks/log.lammps.1  
lammps-stable\_290ct2020/examples/COUPLE/lammps\_spparks/log.lammps.4  
lammps-stable\_290ct2020/examples/COUPLE/lammps\_spparks/log.spparks.1  
lammps-stable\_290ct2020/examples/COUPLE/lammps\_spparks/log.spparks.4  
lammps-stable\_290ct2020/examples/COUPLE/lammps\_spparks/spkpath.h  
lammps-stable\_290ct2020/examples/COUPLE/lammps\_vasp/  
lammps-stable\_290ct2020/examples/COUPLE/lammps\_vasp/INCAR  
lammps-stable\_290ct2020/examples/COUPLE/lammps\_vasp/KPOINTS  
lammps-stable\_290ct2020/examples/COUPLE/lammps\_vasp/POSCAR\_W  
lammps-stable\_290ct2020/examples/COUPLE/lammps\_vasp/README  
lammps-stable\_290ct2020/examples/COUPLE/lammps\_vasp/data.W  
lammps-stable\_290ct2020/examples/COUPLE/lammps\_vasp/in.client.W  
lammps-stable\_290ct2020/examples/COUPLE/lammps\_vasp/log.client.output  
lammps-stable\_290ct2020/examples/COUPLE/lammps\_vasp/vasp\_wrap.py  
lammps-stable\_290ct2020/examples/COUPLE/lammps\_vasp/vasprun.xml  
lammps-stable\_290ct2020/examples/COUPLE/library/  
lammps-stable\_290ct2020/examples/COUPLE/library/Makefile.g++  
lammps-stable\_290ct2020/examples/COUPLE/library/README  
lammps-stable\_290ct2020/examples/COUPLE/library/error.cpp  
lammps-stable\_290ct2020/examples/COUPLE/library/error.h  
lammps-stable\_290ct2020/examples/COUPLE/library/files.cpp  
lammps-stable\_290ct2020/examples/COUPLE/library/files.h  
lammps-stable\_290ct2020/examples/COUPLE/library/irregular.cpp  
lammps-stable\_290ct2020/examples/COUPLE/library/irregular.h  
lammps-stable\_290ct2020/examples/COUPLE/library/lammps\_data\_write.cpp  
lammps-stable\_290ct2020/examples/COUPLE/library/lammps\_data\_write.h  
lammps-stable\_290ct2020/examples/COUPLE/library/many2many.cpp  
lammps-stable\_290ct2020/examples/COUPLE/library/many2many.h  
lammps-stable\_290ct2020/examples/COUPLE/library/many2one.cpp  
lammps-stable\_290ct2020/examples/COUPLE/library/many2one.h  
lammps-stable\_290ct2020/examples/COUPLE/library/memory.cpp  
lammps-stable\_290ct2020/examples/COUPLE/library/memory.h  
lammps-stable\_290ct2020/examples/COUPLE/library/one2many.cpp  
lammps-stable\_290ct2020/examples/COUPLE/library/one2many.h  
lammps-stable\_290ct2020/examples/COUPLE/library/send2one.cpp  
lammps-stable\_290ct2020/examples/COUPLE/library/send2one.h  
lammps-stable\_290ct2020/examples/COUPLE/multiple/  
lammps-stable\_290ct2020/examples/COUPLE/multiple/README

```
lammps-stable_290ct2020/examples/COUPLE/multiple/data.chain
lammps-stable_290ct2020/examples/COUPLE/multiple/in.chain
lammps-stable_290ct2020/examples/COUPLE/multiple/multiple.cpp
lammps-stable_290ct2020/examples/COUPLE/plugin/
lammps-stable_290ct2020/examples/COUPLE/plugin/README
lammps-stable_290ct2020/examples/COUPLE/plugin/in.lj
lammps-stable_290ct2020/examples/COUPLE/plugin/liblammpsplugin.c
lammps-stable_290ct2020/examples/COUPLE/plugin/liblammpsplugin.h
lammps-stable_290ct2020/examples/COUPLE/plugin/log.simple.plugin.1
lammps-stable_290ct2020/examples/COUPLE/plugin/log.simple.plugin.4
lammps-stable_290ct2020/examples/COUPLE/plugin/simple.c
lammps-stable_290ct2020/examples/COUPLE/python/
lammps-stable_290ct2020/examples/COUPLE/python/example.py
lammps-stable_290ct2020/examples/COUPLE/python/in.fix_external
lammps-stable_290ct2020/examples/COUPLE/simple/
lammps-stable_290ct2020/examples/COUPLE/simple/CMakeLists.txt
lammps-stable_290ct2020/examples/COUPLE/simple/README
lammps-stable_290ct2020/examples/COUPLE/simple/in.lj
lammps-stable_290ct2020/examples/COUPLE/simple/log.simple.c++.1
lammps-stable_290ct2020/examples/COUPLE/simple/log.simple.c++.4
lammps-stable_290ct2020/examples/COUPLE/simple/simple.c
lammps-stable_290ct2020/examples/COUPLE/simple/simple.cpp
lammps-stable_290ct2020/examples/COUPLE/simple/simple.f90
lammps-stable_290ct2020/examples/COUPLE/simple/simple_f77.f90
lammps-stable_290ct2020/examples/DIFFUSE/
lammps-stable_290ct2020/examples/DIFFUSE/README
lammps-stable_290ct2020/examples/DIFFUSE/in.msd.2d
lammps-stable_290ct2020/examples/DIFFUSE/in.vacf.2d
lammps-stable_290ct2020/examples/DIFFUSE/log.3Aug18.msd.2d.g++.8
lammps-stable_290ct2020/examples/DIFFUSE/log.3Aug18.vacf.2d.g++.8
lammps-stable_290ct2020/examples/ELASTIC/
lammps-stable_290ct2020/examples/ELASTIC/Si.sw
lammps-stable_290ct2020/examples/ELASTIC/compliance.py
lammps-stable_290ct2020/examples/ELASTIC/displace.mod
lammps-stable_290ct2020/examples/ELASTIC/in.elastic
lammps-stable_290ct2020/examples/ELASTIC/init.mod
lammps-stable_290ct2020/examples/ELASTIC/potential.mod
lammps-stable_290ct2020/examples/ELASTIC_T/
lammps-stable_290ct2020/examples/ELASTIC_T/Si.sw
lammps-stable_290ct2020/examples/ELASTIC_T/displace.mod
lammps-stable_290ct2020/examples/ELASTIC_T/in.elastic
lammps-stable_290ct2020/examples/ELASTIC_T/init.mod
lammps-stable_290ct2020/examples/ELASTIC_T/potential.mod
lammps-stable_290ct2020/examples/HEAT/
lammps-stable_290ct2020/examples/HEAT/README
lammps-stable_290ct2020/examples/HEAT/data.lj
lammps-stable_290ct2020/examples/HEAT/data.spce
lammps-stable_290ct2020/examples/HEAT/in.lj.ehex
lammps-stable_290ct2020/examples/HEAT/in.lj.hex
lammps-stable_290ct2020/examples/HEAT/in.spce.ehex
lammps-stable_290ct2020/examples/HEAT/in.spce.hex
lammps-stable_290ct2020/examples/HEAT/log.10May16.lj.ehex.g++.32
lammps-stable_290ct2020/examples/HEAT/log.10May16.lj.hex.g++.32
lammps-stable_290ct2020/examples/HEAT/log.10May16.spce.ehex.g++.32
lammps-stable_290ct2020/examples/HEAT/log.10May16.spce.hex.g++.32
lammps-stable_290ct2020/examples/HEAT/out.10May16.Elj.ehex.g++.32
lammps-stable_290ct2020/examples/HEAT/out.10May16.Elj.hex.g++.32
lammps-stable_290ct2020/examples/HEAT/out.10May16.Espce.ehex.g++.32
lammps-stable_290ct2020/examples/HEAT/out.10May16.Espce.hex.g++.32
lammps-stable_290ct2020/examples/HEAT/out.10May16.Tlj.ehex.g++.32
```

lammps-stable\_290ct2020/examples/HEAT/out.10May16.Tlj.hex.g++.32  
lammps-stable\_290ct2020/examples/HEAT/out.10May16.Tspce.ehex.g++.32  
lammps-stable\_290ct2020/examples/HEAT/out.10May16.Tspce.hex.g++.32  
lammps-stable\_290ct2020/examples/KAPPA/  
lammps-stable\_290ct2020/examples/KAPPA/README  
lammps-stable\_290ct2020/examples/KAPPA/in.ehex  
lammps-stable\_290ct2020/examples/KAPPA/in.heat  
lammps-stable\_290ct2020/examples/KAPPA/in.heatflux  
lammps-stable\_290ct2020/examples/KAPPA/in.langevin  
lammps-stable\_290ct2020/examples/KAPPA/in.mp  
lammps-stable\_290ct2020/examples/KAPPA/log.130ct16.ehex.g++.8  
lammps-stable\_290ct2020/examples/KAPPA/log.130ct16.heat.g++.8  
lammps-stable\_290ct2020/examples/KAPPA/log.130ct16.heatflux.g++.8  
lammps-stable\_290ct2020/examples/KAPPA/log.130ct16.langevin.g++.8  
lammps-stable\_290ct2020/examples/KAPPA/log.130ct16.mp.g++.8  
lammps-stable\_290ct2020/examples/KAPPA/profile.1Feb14.heatflux.g++.8  
lammps-stable\_290ct2020/examples/KAPPA/profile.1Feb14.langevin.g++.8  
lammps-stable\_290ct2020/examples/KAPPA/profile.1Feb14.mp.g++.8  
lammps-stable\_290ct2020/examples/KAPPA/profile.7Jun16.ehex.g++.8  
lammps-stable\_290ct2020/examples/KAPPA/profile.7Jun16.heat.g++.8  
lammps-stable\_290ct2020/examples/MC/  
lammps-stable\_290ct2020/examples/MC/README  
lammps-stable\_290ct2020/examples/MC/in.mc  
lammps-stable\_290ct2020/examples/MC/log.130ct16.mc.g++.1  
lammps-stable\_290ct2020/examples/README  
lammps-stable\_290ct2020/examples/SPIN/  
lammps-stable\_290ct2020/examples/SPIN/README  
lammps-stable\_290ct2020/examples/SPIN/bfo/  
lammps-stable\_290ct2020/examples/SPIN/bfo/in.spin.bfo  
lammps-stable\_290ct2020/examples/SPIN/bfo/log.14Apr20.spin.bfo.g++.1  
lammps-stable\_290ct2020/examples/SPIN/bfo/log.14Apr20.spin.bfo.g++.4  
lammps-stable\_290ct2020/examples/SPIN/cobalt\_fcc/  
lammps-stable\_290ct2020/examples/SPIN/cobalt\_fcc/Co\_PurjaPun\_2012.eam.alloy  
lammps-stable\_290ct2020/examples/SPIN/cobalt\_fcc/exchange\_fit\_fcc\_co/  
lammps-stable\_290ct2020/examples/SPIN/cobalt\_fcc/exchange\_fit\_fcc\_co/exchange  
\_fcc\_cobalt.dat  
lammps-stable\_290ct2020/examples/SPIN/cobalt\_fcc/exchange\_fit\_fcc\_co/exchange  
\_fit.py  
lammps-stable\_290ct2020/examples/SPIN/cobalt\_fcc/in.spin.cobalt\_fcc  
lammps-stable\_290ct2020/examples/SPIN/cobalt\_fcc/log.14Apr20.spin.cobalt\_fcc.  
g++.1  
lammps-stable\_290ct2020/examples/SPIN/cobalt\_fcc/log.14Apr20.spin.cobalt\_fcc.  
g++.4  
lammps-stable\_290ct2020/examples/SPIN/cobalt\_hcp/  
lammps-stable\_290ct2020/examples/SPIN/cobalt\_hcp/Co\_PurjaPun\_2012.eam.alloy  
lammps-stable\_290ct2020/examples/SPIN/cobalt\_hcp/exchange\_fit\_hcp\_co/  
lammps-stable\_290ct2020/examples/SPIN/cobalt\_hcp/exchange\_fit\_hcp\_co/exchange  
\_fit.py  
lammps-stable\_290ct2020/examples/SPIN/cobalt\_hcp/exchange\_fit\_hcp\_co/exchange  
\_hcp\_co.dat  
lammps-stable\_290ct2020/examples/SPIN/cobalt\_hcp/in.spin.cobalt\_hcp  
lammps-stable\_290ct2020/examples/SPIN/cobalt\_hcp/log.14Apr20.spin.cobalt\_hcp.  
g++.1  
lammps-stable\_290ct2020/examples/SPIN/cobalt\_hcp/log.14Apr20.spin.cobalt\_hcp.  
g++.4  
lammps-stable\_290ct2020/examples/SPIN/dipole\_spin/  
lammps-stable\_290ct2020/examples/SPIN/dipole\_spin/Fe\_Mishin2006.eam.alloy  
lammps-stable\_290ct2020/examples/SPIN/dipole\_spin/exchange\_fit\_bcc\_iron/  
lammps-stable\_290ct2020/examples/SPIN/dipole\_spin/exchange\_fit\_bcc\_iron/excha  
nge\_bcc\_iron.dat

```
lammps-stable_290ct2020/examples/SPIN/dipole_spin/exchange_fit_bcc_iron/exchange_fit.py
lammps-stable_290ct2020/examples/SPIN/dipole_spin/fe_dd.dat
lammps-stable_290ct2020/examples/SPIN/dipole_spin/in.spin.iron_dipole_cut
lammps-stable_290ct2020/examples/SPIN/dipole_spin/in.spin.iron_dipole_ewald
lammps-stable_290ct2020/examples/SPIN/dipole_spin/in.spin.iron_dipole_pppm
lammps-stable_290ct2020/examples/SPIN/dipole_spin/log.14Apr20.spin.iron_dipole_cut.g++.1
lammps-stable_290ct2020/examples/SPIN/dipole_spin/log.14Apr20.spin.iron_dipole_cut.g++.4
lammps-stable_290ct2020/examples/SPIN/dipole_spin/log.14Apr20.spin.iron_dipole_ewald.g++.1
lammps-stable_290ct2020/examples/SPIN/dipole_spin/log.14Apr20.spin.iron_dipole_ewald.g++.4
lammps-stable_290ct2020/examples/SPIN/dipole_spin/log.14Apr20.spin.iron_dipole_pppm.g++.1
lammps-stable_290ct2020/examples/SPIN/dipole_spin/log.14Apr20.spin.iron_dipole_pppm.g++.4
lammps-stable_290ct2020/examples/SPIN/gneb/
lammps-stable_290ct2020/examples/SPIN/gneb/README
lammps-stable_290ct2020/examples/SPIN/gneb/iron/
lammps-stable_290ct2020/examples/SPIN/gneb/iron/final.iron_spin
lammps-stable_290ct2020/examples/SPIN/gneb/iron/in.gneb.iron
lammps-stable_290ct2020/examples/SPIN/gneb/iron/initial.iron_spin
lammps-stable_290ct2020/examples/SPIN/gneb/skymion/
lammps-stable_290ct2020/examples/SPIN/gneb/skymion/final.skymion
lammps-stable_290ct2020/examples/SPIN/gneb/skymion/in.gneb.skymion
lammps-stable_290ct2020/examples/SPIN/gneb/skymion/initial.skymion
lammps-stable_290ct2020/examples/SPIN/iron/
lammps-stable_290ct2020/examples/SPIN/iron/Fe_Mishin2006.eam.alloy
lammps-stable_290ct2020/examples/SPIN/iron/exchange_fit_bcc_iron/
lammps-stable_290ct2020/examples/SPIN/iron/exchange_fit_bcc_iron/exchange_fit_bcc_iron.dat
lammps-stable_290ct2020/examples/SPIN/iron/exchange_fit_bcc_iron/exchange_fit.py
lammps-stable_290ct2020/examples/SPIN/iron/fe_dd.dat
lammps-stable_290ct2020/examples/SPIN/iron/in.spin.iron
lammps-stable_290ct2020/examples/SPIN/iron/in.spin.iron_cubic
lammps-stable_290ct2020/examples/SPIN/iron/log.14Apr20.spin.iron.g++.1
lammps-stable_290ct2020/examples/SPIN/iron/log.14Apr20.spin.iron.g++.4
lammps-stable_290ct2020/examples/SPIN/iron/log.14Apr20.spin.iron_cubic.g++.1
lammps-stable_290ct2020/examples/SPIN/iron/log.14Apr20.spin.iron_cubic.g++.4
lammps-stable_290ct2020/examples/SPIN/nickel/
lammps-stable_290ct2020/examples/SPIN/nickel/Ni99.eam.alloy
lammps-stable_290ct2020/examples/SPIN/nickel/exchange_fit_fcc_ni/
lammps-stable_290ct2020/examples/SPIN/nickel/exchange_fit_fcc_ni/exchange_fit_fcc_ni.dat
lammps-stable_290ct2020/examples/SPIN/nickel/exchange_fit_fcc_ni/exchange_fit_fcc_ni2.dat
lammps-stable_290ct2020/examples/SPIN/nickel/exchange_fit_fcc_ni/exchange_fit.py
lammps-stable_290ct2020/examples/SPIN/nickel/in.spin.nickel
lammps-stable_290ct2020/examples/SPIN/nickel/in.spin.nickel_cubic
lammps-stable_290ct2020/examples/SPIN/nickel/log.14Apr20.spin.nickel.g++.1
lammps-stable_290ct2020/examples/SPIN/nickel/log.14Apr20.spin.nickel.g++.4
lammps-stable_290ct2020/examples/SPIN/nickel/log.14Apr20.spin.nickel_cubic.g++.1
lammps-stable_290ct2020/examples/SPIN/nickel/log.14Apr20.spin.nickel_cubic.g++.4
lammps-stable_290ct2020/examples/SPIN/read_restart/
```



```
lammps-stable_290ct2020/examples/SPIN/read_restart/Co_PurjaPun_2012.eam.alloy
lammps-stable_290ct2020/examples/SPIN/read_restart/Norm_randXY_8x8x32.data
lammps-stable_290ct2020/examples/SPIN/read_restart/in.spin.read_data
lammps-stable_290ct2020/examples/SPIN/read_restart/in.spin.restart
lammps-stable_290ct2020/examples/SPIN/read_restart/in.spin.write_restart
lammps-stable_290ct2020/examples/SPIN/read_restart/log.14Apr20.spin.read_dat
a.g++.1
lammps-stable_290ct2020/examples/SPIN/read_restart/log.14Apr20.spin.read_dat
a.g++.4
lammps-stable_290ct2020/examples/SPIN/read_restart/log.14Apr20.spin.restart.
g++.1
lammps-stable_290ct2020/examples/SPIN/read_restart/log.14Apr20.spin.restart.
g++.4
lammps-stable_290ct2020/examples/SPIN/read_restart/log.14Apr20.spin.write_res
tart.g++.1
lammps-stable_290ct2020/examples/SPIN/read_restart/log.14Apr20.spin.write_res
tart.g++.4
lammps-stable_290ct2020/examples/SPIN/read_restart/restart_hcp_cobalt.equil
lammps-stable_290ct2020/examples/SPIN/run_spin_examples.sh
lammps-stable_290ct2020/examples/SPIN/run_spin_examples_serial.sh
lammps-stable_290ct2020/examples/SPIN/setforce_spin/
lammps-stable_290ct2020/examples/SPIN/setforce_spin/in.spin.setforce
lammps-stable_290ct2020/examples/SPIN/setforce_spin/log.14Apr20.spin.setforc
e.g++.1
lammps-stable_290ct2020/examples/SPIN/setforce_spin/log.14Apr20.spin.setforc
e.g++.4
lammps-stable_290ct2020/examples/SPIN/spinmin/
lammps-stable_290ct2020/examples/SPIN/spinmin/in.spin.bfo_min
lammps-stable_290ct2020/examples/SPIN/spinmin/in.spin.bfo_min_cg
lammps-stable_290ct2020/examples/SPIN/spinmin/in.spin.bfo_min_lbfgs
lammps-stable_290ct2020/examples/SPIN/spinmin/in.spin.iron_min
lammps-stable_290ct2020/examples/SPIN/spinmin/log.14Apr20.spin.bfo_min.g++.1
lammps-stable_290ct2020/examples/SPIN/spinmin/log.14Apr20.spin.bfo_min.g++.4
lammps-stable_290ct2020/examples/SPIN/spinmin/log.14Apr20.spin.bfo_min_cg.
g++.1
lammps-stable_290ct2020/examples/SPIN/spinmin/log.14Apr20.spin.bfo_min_cg.
g++.4
lammps-stable_290ct2020/examples/SPIN/spinmin/log.14Apr20.spin.bfo_min_lbfgs.
g++.1
lammps-stable_290ct2020/examples/SPIN/spinmin/log.14Apr20.spin.bfo_min_lbfgs.
g++.4
lammps-stable_290ct2020/examples/SPIN/spinmin/log.14Apr20.spin.iron_min.g++.1
lammps-stable_290ct2020/examples/SPIN/spinmin/log.14Apr20.spin.iron_min.g++.4
lammps-stable_290ct2020/examples/SPIN/test_problems/
lammps-stable_290ct2020/examples/SPIN/test_problems/README
lammps-stable_290ct2020/examples/SPIN/test_problems/validation_damped_exchang
e/
lammps-stable_290ct2020/examples/SPIN/test_problems/validation_damped_exchang
e/llg_exchange.py
lammps-stable_290ct2020/examples/SPIN/test_problems/validation_damped_exchang
e/plot_precession.py
lammps-stable_290ct2020/examples/SPIN/test_problems/validation_damped_exchang
e/run-test-exchange.sh
lammps-stable_290ct2020/examples/SPIN/test_problems/validation_damped_exchang
e/test-spin-precession.in
lammps-stable_290ct2020/examples/SPIN/test_problems/validation_damped_exchang
e/two_spins.data
lammps-stable_290ct2020/examples/SPIN/test_problems/validation_damped_precess
ion/
lammps-stable_290ct2020/examples/SPIN/test_problems/validation_damped_precess
```

```
ion/llg_precession.py
lammps-stable_290ct2020/examples/SPIN/test_problems/validation_damped_precession/plot_precession.py
lammps-stable_290ct2020/examples/SPIN/test_problems/validation_damped_precession/run-test-prec.sh
lammps-stable_290ct2020/examples/SPIN/test_problems/validation_damped_precession/test-spin-precession.in
lammps-stable_290ct2020/examples/SPIN/test_problems/validation_langevin_precession/
lammps-stable_290ct2020/examples/SPIN/test_problems/validation_langevin_precession/langevin.py
lammps-stable_290ct2020/examples/SPIN/test_problems/validation_langevin_precession/plot_precession.py
lammps-stable_290ct2020/examples/SPIN/test_problems/validation_langevin_precession/run-test-prec.sh
lammps-stable_290ct2020/examples/SPIN/test_problems/validation_langevin_precession/test-prec-spin.template
lammps-stable_290ct2020/examples/SPIN/test_problems/validation_nve/
lammps-stable_290ct2020/examples/SPIN/test_problems/validation_nve/Fe_Mishin2006.eam.alloy
lammps-stable_290ct2020/examples/SPIN/test_problems/validation_nve/in.spin.iron-nve
lammps-stable_290ct2020/examples/SPIN/test_problems/validation_nve/plot_nve.py
lammps-stable_290ct2020/examples/SPIN/test_problems/validation_nve/run-test-nve.sh
lammps-stable_290ct2020/examples/SPIN/test_problems/validation_nvt/
lammps-stable_290ct2020/examples/SPIN/test_problems/validation_nvt/Fe_Mishin2006.eam.alloy
lammps-stable_290ct2020/examples/SPIN/test_problems/validation_nvt/in.spin.nvt_lattice
lammps-stable_290ct2020/examples/SPIN/test_problems/validation_nvt/in.spin.nvt_spin
lammps-stable_290ct2020/examples/SPIN/test_problems/validation_nvt/plot_nvt.py
lammps-stable_290ct2020/examples/SPIN/test_problems/validation_nvt/run-test-nvt.sh
lammps-stable_290ct2020/examples/SPIN/vmd/
lammps-stable_290ct2020/examples/SPIN/vmd/prepare_vmd.sh
lammps-stable_290ct2020/examples/SPIN/vmd/vmd_nano.vmd
lammps-stable_290ct2020/examples/TIP4P/
lammps-stable_290ct2020/examples/TIP4P/gpu_dump/
lammps-stable_290ct2020/examples/TIP4P/gpu_dump/data.spce
lammps-stable_290ct2020/examples/TIP4P/gpu_dump/dump.force_cpu.19Dec19.tip4p.g++.1
lammps-stable_290ct2020/examples/TIP4P/gpu_dump/dump.force_gpu.19Dec19.tip4p.g++.1.gtx1070.dp
lammps-stable_290ct2020/examples/TIP4P/gpu_dump/in.tip4p
lammps-stable_290ct2020/examples/TIP4P/gpu_dump/log.19Dec19.tip4p.g++.1
lammps-stable_290ct2020/examples/TIP4P/gpu_dump/log.19Dec19.tip4p.g++.1.gtx1070.dp
lammps-stable_290ct2020/examples/UNITS/
lammps-stable_290ct2020/examples/UNITS/README
lammps-stable_290ct2020/examples/UNITS/in.ar.lj
lammps-stable_290ct2020/examples/UNITS/in.ar.metal
lammps-stable_290ct2020/examples/UNITS/in.ar.real
lammps-stable_290ct2020/examples/UNITS/log.ar.lj.80ct19.g++.1
lammps-stable_290ct2020/examples/UNITS/log.ar.lj.80ct19.g++.4
lammps-stable_290ct2020/examples/UNITS/log.ar.metal.80ct19.g++.1
lammps-stable_290ct2020/examples/UNITS/log.ar.metal.80ct19.g++.4
```

```
lammps-stable_290ct2020/examples/UNITS/log.ar.real.80ct19.g++.1
lammps-stable_290ct2020/examples/UNITS/log.ar.real.80ct19.g++.4
lammps-stable_290ct2020/examples/USER/
lammps-stable_290ct2020/examples/USER/adios/
lammps-stable_290ct2020/examples/USER/adios/balance/
lammps-stable_290ct2020/examples/USER/adios/balance/adios2_config.xml
lammps-stable_290ct2020/examples/USER/adios/balance/in.adios_balance
lammps-stable_290ct2020/examples/USER/adios/balance/in.adios_balance2
lammps-stable_290ct2020/examples/USER/adios/balance/log.balance
lammps-stable_290ct2020/examples/USER/adios/rerun/
lammps-stable_290ct2020/examples/USER/adios/rerun/README
lammps-stable_290ct2020/examples/USER/adios/rerun/adios2_config.xml
lammps-stable_290ct2020/examples/USER/adios/rerun/in.first
lammps-stable_290ct2020/examples/USER/adios/rerun/in.read_dump
lammps-stable_290ct2020/examples/USER/adios/rerun/in.rerun
lammps-stable_290ct2020/examples/USER/adios/rerun/log.20Jan20.first.g++.7.4
lammps-stable_290ct2020/examples/USER/adios/rerun/log.20Jan20.read_dump.g++.
7.4
lammps-stable_290ct2020/examples/USER/adios/rerun/log.20Jan20.rerun.g++.7.4
lammps-stable_290ct2020/examples/USER/atc/
lammps-stable_290ct2020/examples/USER/atc/README
lammps-stable_290ct2020/examples/USER/atc/cauchy_born/
lammps-stable_290ct2020/examples/USER/atc/cauchy_born/Ar_CauchyBorn.mat
lammps-stable_290ct2020/examples/USER/atc/cauchy_born/Ar_CauchyBorn_linear.ma
t
lammps-stable_290ct2020/examples/USER/atc/cauchy_born/Au_CauchyBorn.mat
lammps-stable_290ct2020/examples/USER/atc/cauchy_born/Au_CauchyBorn_linear.ma
t
lammps-stable_290ct2020/examples/USER/atc/cauchy_born/Au_eam.mat
lammps-stable_290ct2020/examples/USER/atc/cauchy_born/Au_eam_linear.mat
lammps-stable_290ct2020/examples/USER/atc/cauchy_born/Au_u3.eam
lammps-stable_290ct2020/examples/USER/atc/cauchy_born/Cu_CauchyBorn.mat
lammps-stable_290ct2020/examples/USER/atc/cauchy_born/cb_biaxial.screen
lammps-stable_290ct2020/examples/USER/atc/cauchy_born/cb_shear.screen
lammps-stable_290ct2020/examples/USER/atc/cauchy_born/cb_unistrain.screen
lammps-stable_290ct2020/examples/USER/atc/cauchy_born/cb_unistrain_eam.screen
lammps-stable_290ct2020/examples/USER/atc/cauchy_born/cb_unistrain_eam_linea
r.screen
lammps-stable_290ct2020/examples/USER/atc/cauchy_born/cb_unistrain_linear.scr
een
lammps-stable_290ct2020/examples/USER/atc/cauchy_born/cb_volumetric.screen
lammps-stable_290ct2020/examples/USER/atc/cauchy_born/flying_cube.screen
lammps-stable_290ct2020/examples/USER/atc/cauchy_born/ftcb_constV.screen
lammps-stable_290ct2020/examples/USER/atc/cauchy_born/ftcb_constV_setup.init
lammps-stable_290ct2020/examples/USER/atc/cauchy_born/in.cb_biaxial
lammps-stable_290ct2020/examples/USER/atc/cauchy_born/in.cb_shear
lammps-stable_290ct2020/examples/USER/atc/cauchy_born/in.cb_unistrain
lammps-stable_290ct2020/examples/USER/atc/cauchy_born/in.cb_unistrain_eam
lammps-stable_290ct2020/examples/USER/atc/cauchy_born/in.cb_unistrain_eam_lin
ear
lammps-stable_290ct2020/examples/USER/atc/cauchy_born/in.cb_unistrain_linear
lammps-stable_290ct2020/examples/USER/atc/cauchy_born/in.cb_volumetric
lammps-stable_290ct2020/examples/USER/atc/cauchy_born/in.flying_cube
lammps-stable_290ct2020/examples/USER/atc/cauchy_born/in.ftcb_constV
lammps-stable_290ct2020/examples/USER/atc/cauchy_born/in.read_xref
lammps-stable_290ct2020/examples/USER/atc/cauchy_born/read_xref.screen
lammps-stable_290ct2020/examples/USER/atc/cauchy_born/read_xref_0.data
lammps-stable_290ct2020/examples/USER/atc/cauchy_born/read_xref_1.init
lammps-stable_290ct2020/examples/USER/atc/drift_diffusion/
lammps-stable_290ct2020/examples/USER/atc/drift_diffusion/Ar_ddm.mat
```

lammps-stable\_290ct2020/examples/USER/atc/drift\_diffusion/CNT\_ddm.mat  
lammps-stable\_290ct2020/examples/USER/atc/drift\_diffusion/Cu\_cddm.mat  
lammps-stable\_290ct2020/examples/USER/atc/drift\_diffusion/SiGe\_ddm\_schrodinger.mat  
lammps-stable\_290ct2020/examples/USER/atc/drift\_diffusion/SiVacuum\_cddm\_schrodinger.mat  
lammps-stable\_290ct2020/examples/USER/atc/drift\_diffusion/SiVacuum\_ddm\_schrodinger.mat  
lammps-stable\_290ct2020/examples/USER/atc/drift\_diffusion/Si\_ddm.mat  
lammps-stable\_290ct2020/examples/USER/atc/drift\_diffusion/Si\_ddm\_eq.mat  
lammps-stable\_290ct2020/examples/USER/atc/drift\_diffusion/Si\_ddm\_schrodinger.mat  
lammps-stable\_290ct2020/examples/USER/atc/drift\_diffusion/Si\_ddm\_thermopower.mat  
lammps-stable\_290ct2020/examples/USER/atc/drift\_diffusion/convective\_pulse.screen  
lammps-stable\_290ct2020/examples/USER/atc/drift\_diffusion/ddm\_schrodinger.screen  
lammps-stable\_290ct2020/examples/USER/atc/drift\_diffusion/finite\_well.screen  
lammps-stable\_290ct2020/examples/USER/atc/drift\_diffusion/in.convective\_pulse  
lammps-stable\_290ct2020/examples/USER/atc/drift\_diffusion/in.ddm\_schrodinger  
lammps-stable\_290ct2020/examples/USER/atc/drift\_diffusion/in.finite\_well  
lammps-stable\_290ct2020/examples/USER/atc/drift\_diffusion/in.no\_atoms\_ddm  
lammps-stable\_290ct2020/examples/USER/atc/drift\_diffusion/in.null\_material\_ddm  
lammps-stable\_290ct2020/examples/USER/atc/drift\_diffusion/in.poisson1d\_noatoms  
lammps-stable\_290ct2020/examples/USER/atc/drift\_diffusion/in.poisson2d\_noatoms  
lammps-stable\_290ct2020/examples/USER/atc/drift\_diffusion/in.schrodinger-poisson2d\_Jconstraint  
lammps-stable\_290ct2020/examples/USER/atc/drift\_diffusion/in.schrodinger-poisson2d\_convective  
lammps-stable\_290ct2020/examples/USER/atc/drift\_diffusion/in.schrodinger-poisson2d\_noatoms  
lammps-stable\_290ct2020/examples/USER/atc/drift\_diffusion/no\_atoms\_ddm.screen  
lammps-stable\_290ct2020/examples/USER/atc/drift\_diffusion/null\_material\_ddm.screen  
lammps-stable\_290ct2020/examples/USER/atc/drift\_diffusion/poisson1d\_noatoms.screen  
lammps-stable\_290ct2020/examples/USER/atc/drift\_diffusion/poisson2d\_noatoms.screen  
lammps-stable\_290ct2020/examples/USER/atc/drift\_diffusion/schrodinger-poisson2d\_Jconstraint.screen  
lammps-stable\_290ct2020/examples/USER/atc/drift\_diffusion/schrodinger-poisson2d\_convective.screen  
lammps-stable\_290ct2020/examples/USER/atc/drift\_diffusion/schrodinger-poisson2d\_noatoms.screen  
lammps-stable\_290ct2020/examples/USER/atc/elastic/  
lammps-stable\_290ct2020/examples/USER/atc/elastic/Ar\_CauchyBorn.mat  
lammps-stable\_290ct2020/examples/USER/atc/elastic/Ar\_CauchyBornLinear.mat  
lammps-stable\_290ct2020/examples/USER/atc/elastic/Ar\_damped.mat  
lammps-stable\_290ct2020/examples/USER/atc/elastic/Ar\_elastic.mat  
lammps-stable\_290ct2020/examples/USER/atc/elastic/Ar\_thermo\_elastic.mat  
lammps-stable\_290ct2020/examples/USER/atc/elastic/Au\_elastic.mat  
lammps-stable\_290ct2020/examples/USER/atc/elastic/CNT.mat  
lammps-stable\_290ct2020/examples/USER/atc/elastic/CNT\_electrostatic.mat  
lammps-stable\_290ct2020/examples/USER/atc/elastic/CNT\_electrostatic2.mat  
lammps-stable\_290ct2020/examples/USER/atc/elastic/CNT\_id.mat  
lammps-stable\_290ct2020/examples/USER/atc/elastic/bar1d.screen

lammps-stable\_290ct2020/examples/USER/atc/elastic/bar1d\_damped.screen  
lammps-stable\_290ct2020/examples/USER/atc/elastic/bar1d\_flux.screen  
lammps-stable\_290ct2020/examples/USER/atc/elastic/bar1d\_frac\_step.screen  
lammps-stable\_290ct2020/examples/USER/atc/elastic/bar1d\_ghost\_flux.screen  
lammps-stable\_290ct2020/examples/USER/atc/elastic/bar1d\_thermo\_elastic.screen  
lammps-stable\_290ct2020/examples/USER/atc/elastic/cnt\_electrostatic.screen  
lammps-stable\_290ct2020/examples/USER/atc/elastic/cnt\_electrostatic2.screen  
lammps-stable\_290ct2020/examples/USER/atc/elastic/cnt\_fixed\_charge.screen  
lammps-stable\_290ct2020/examples/USER/atc/elastic/eam\_energy.screen  
lammps-stable\_290ct2020/examples/USER/atc/elastic/electron\_density.screen  
lammps-stable\_290ct2020/examples/USER/atc/elastic/electrostatic\_bending.scre  
n  
lammps-stable\_290ct2020/examples/USER/atc/elastic/electrostatic\_bending\_dos.s  
creen  
lammps-stable\_290ct2020/examples/USER/atc/elastic/in.bar1d  
lammps-stable\_290ct2020/examples/USER/atc/elastic/in.bar1d\_damped  
lammps-stable\_290ct2020/examples/USER/atc/elastic/in.bar1d\_flux  
lammps-stable\_290ct2020/examples/USER/atc/elastic/in.bar1d\_frac\_step  
lammps-stable\_290ct2020/examples/USER/atc/elastic/in.bar1d\_ghost\_flux  
lammps-stable\_290ct2020/examples/USER/atc/elastic/in.bar1d\_thermo\_elastic  
lammps-stable\_290ct2020/examples/USER/atc/elastic/in.eam\_energy  
lammps-stable\_290ct2020/examples/USER/atc/elastic/in.electron\_density  
lammps-stable\_290ct2020/examples/USER/atc/elastic/in.no\_atoms  
lammps-stable\_290ct2020/examples/USER/atc/elastic/in.no\_atoms\_cb  
lammps-stable\_290ct2020/examples/USER/atc/elastic/in.no\_atoms\_cb\_linear  
lammps-stable\_290ct2020/examples/USER/atc/elastic/no\_atoms.screen  
lammps-stable\_290ct2020/examples/USER/atc/elastic/no\_atoms\_cb.screen  
lammps-stable\_290ct2020/examples/USER/atc/elastic/no\_atoms\_cb\_linear.screen  
lammps-stable\_290ct2020/examples/USER/atc/elastic/temp.init  
lammps-stable\_290ct2020/examples/USER/atc/fluids/  
lammps-stable\_290ct2020/examples/USER/atc/fluids/Ar\_elastic.mat  
lammps-stable\_290ct2020/examples/USER/atc/fluids/Ar\_electrostatic.mat  
lammps-stable\_290ct2020/examples/USER/atc/fluids/Ar\_liquid.mat  
lammps-stable\_290ct2020/examples/USER/atc/fluids/Ar\_species.mat  
lammps-stable\_290ct2020/examples/USER/atc/fluids/Ar\_species\_dl.mat  
lammps-stable\_290ct2020/examples/USER/atc/fluids/Ar\_thermal.mat  
lammps-stable\_290ct2020/examples/USER/atc/fluids/Ar\_visc\_no\_atoms.mat  
lammps-stable\_290ct2020/examples/USER/atc/fluids/Ar\_viscosity.mat  
lammps-stable\_290ct2020/examples/USER/atc/fluids/bar1d\_fluids.screen  
lammps-stable\_290ct2020/examples/USER/atc/fluids/concentration.screen  
lammps-stable\_290ct2020/examples/USER/atc/fluids/concentration\_init.data  
lammps-stable\_290ct2020/examples/USER/atc/fluids/conducting\_interface.screen  
lammps-stable\_290ct2020/examples/USER/atc/fluids/dielectric.mat  
lammps-stable\_290ct2020/examples/USER/atc/fluids/dielectric\_interface.screen  
lammps-stable\_290ct2020/examples/USER/atc/fluids/double\_layer.screen  
lammps-stable\_290ct2020/examples/USER/atc/fluids/in.bar1d\_fluids  
lammps-stable\_290ct2020/examples/USER/atc/fluids/in.concentration  
lammps-stable\_290ct2020/examples/USER/atc/fluids/in.conducting\_interface  
lammps-stable\_290ct2020/examples/USER/atc/fluids/in.dielectric\_interface  
lammps-stable\_290ct2020/examples/USER/atc/fluids/in.double\_layer  
lammps-stable\_290ct2020/examples/USER/atc/fluids/in.liquid\_electrostatic  
lammps-stable\_290ct2020/examples/USER/atc/fluids/in.opp\_force  
lammps-stable\_290ct2020/examples/USER/atc/fluids/in.poisson  
lammps-stable\_290ct2020/examples/USER/atc/fluids/in.shear\_flow  
lammps-stable\_290ct2020/examples/USER/atc/fluids/in.shear\_no\_atoms  
lammps-stable\_290ct2020/examples/USER/atc/fluids/interface\_init.data  
lammps-stable\_290ct2020/examples/USER/atc/fluids/liquid\_electrostatic.screen  
lammps-stable\_290ct2020/examples/USER/atc/fluids/opp\_force.screen  
lammps-stable\_290ct2020/examples/USER/atc/fluids/poisson.screen  
lammps-stable\_290ct2020/examples/USER/atc/fluids/post\_eq.init

```
lammps-stable_290ct2020/examples/USER/atc/fluids/shear_flow.screen
lammps-stable_290ct2020/examples/USER/atc/fluids/shear_no_atoms.screen
lammps-stable_290ct2020/examples/USER/atc/fluids/temp.init
lammps-stable_290ct2020/examples/USER/atc/fluids/velocities.init
lammps-stable_290ct2020/examples/USER/atc/fluids/waternve.atm
lammps-stable_290ct2020/examples/USER/atc/hardy/
lammps-stable_290ct2020/examples/USER/atc/hardy/consistency.screen
lammps-stable_290ct2020/examples/USER/atc/hardy/eam_kernel_convergence.screen
lammps-stable_290ct2020/examples/USER/atc/hardy/eam_unistrain_cell.screen
lammps-stable_290ct2020/examples/USER/atc/hardy/eam_unistrain_mesh.screen
lammps-stable_290ct2020/examples/USER/atc/hardy/eam_unistrain_qcylinder.scre
n
lammps-stable_290ct2020/examples/USER/atc/hardy/eam_unistrain_qsphere.screen
lammps-stable_290ct2020/examples/USER/atc/hardy/eam_unistrain_step.screen
lammps-stable_290ct2020/examples/USER/atc/hardy/eam_volume_stretch.screen
lammps-stable_290ct2020/examples/USER/atc/hardy/eshelby_static.screen
lammps-stable_290ct2020/examples/USER/atc/hardy/in.consistency
lammps-stable_290ct2020/examples/USER/atc/hardy/in.eam_kernel_convergence
lammps-stable_290ct2020/examples/USER/atc/hardy/in.eam_unistrain_cell
lammps-stable_290ct2020/examples/USER/atc/hardy/in.eam_unistrain_mesh
lammps-stable_290ct2020/examples/USER/atc/hardy/in.eam_unistrain_qcylinder
lammps-stable_290ct2020/examples/USER/atc/hardy/in.eam_unistrain_qsphere
lammps-stable_290ct2020/examples/USER/atc/hardy/in.eam_unistrain_step
lammps-stable_290ct2020/examples/USER/atc/hardy/in.eam_volume_stretch
lammps-stable_290ct2020/examples/USER/atc/hardy/in.eshelby_static
lammps-stable_290ct2020/examples/USER/atc/hardy/in.nvt
lammps-stable_290ct2020/examples/USER/atc/hardy/nvt.data
lammps-stable_290ct2020/examples/USER/atc/hardy/nvt.init
lammps-stable_290ct2020/examples/USER/atc/hardy/nvt.screen
lammps-stable_290ct2020/examples/USER/atc/mesh/
lammps-stable_290ct2020/examples/USER/atc/mesh/Ar_ttm.mat
lammps-stable_290ct2020/examples/USER/atc/mesh/Si.mat
lammps-stable_290ct2020/examples/USER/atc/mesh/circle_temp.init
lammps-stable_290ct2020/examples/USER/atc/mesh/gaussianIC1d_hex.screen
lammps-stable_290ct2020/examples/USER/atc/mesh/gaussianIC2d_hex.screen
lammps-stable_290ct2020/examples/USER/atc/mesh/gaussianIC2d_hex20_uniform.scr
een
lammps-stable_290ct2020/examples/USER/atc/mesh/gaussianIC2d_hex27_uniform.scr
een
lammps-stable_290ct2020/examples/USER/atc/mesh/gaussianIC2d_hex_uniform.scre
n
lammps-stable_290ct2020/examples/USER/atc/mesh/gaussianIC2d_tet.screen
lammps-stable_290ct2020/examples/USER/atc/mesh/in.gaussianIC1d_hex
lammps-stable_290ct2020/examples/USER/atc/mesh/in.gaussianIC2d_hex
lammps-stable_290ct2020/examples/USER/atc/mesh/in.gaussianIC2d_hex20_uniform
lammps-stable_290ct2020/examples/USER/atc/mesh/in.gaussianIC2d_hex27_uniform
lammps-stable_290ct2020/examples/USER/atc/mesh/in.gaussianIC2d_tet
lammps-stable_290ct2020/examples/USER/atc/mesh/in.kernel2d_hex
lammps-stable_290ct2020/examples/USER/atc/mesh/in.kernel2d_tet
lammps-stable_290ct2020/examples/USER/atc/mesh/in.mesh2d_tet
lammps-stable_290ct2020/examples/USER/atc/mesh/in.semicircle
lammps-stable_290ct2020/examples/USER/atc/mesh/kernel2d_hex.screen
lammps-stable_290ct2020/examples/USER/atc/mesh/kernel2d_tet.screen
lammps-stable_290ct2020/examples/USER/atc/mesh/mesh2d_tet.screen
lammps-stable_290ct2020/examples/USER/atc/mesh/semicircle.init
lammps-stable_290ct2020/examples/USER/atc/mesh/semicircle.screen
lammps-stable_290ct2020/examples/USER/atc/mesh/si_semicircle.init
lammps-stable_290ct2020/examples/USER/atc/mesh/temp.init
lammps-stable_290ct2020/examples/USER/atc/molecule/
lammps-stable_290ct2020/examples/USER/atc/molecule/harmonic_bonds.init
```

```
lammps-stable_290ct2020/examples/USER/atc/molecule/harmonic_bonds.screen
lammps-stable_290ct2020/examples/USER/atc/molecule/in.harmonic_bonds
lammps-stable_290ct2020/examples/USER/atc/molecule/in.polarize
lammps-stable_290ct2020/examples/USER/atc/molecule/in.quartic_bonds
lammps-stable_290ct2020/examples/USER/atc/molecule/in.water
lammps-stable_290ct2020/examples/USER/atc/molecule/polarize.screen
lammps-stable_290ct2020/examples/USER/atc/molecule/quartic_bonds.data
lammps-stable_290ct2020/examples/USER/atc/molecule/quartic_bonds.screen
lammps-stable_290ct2020/examples/USER/atc/molecule/water.init
lammps-stable_290ct2020/examples/USER/atc/molecule/water.mat
lammps-stable_290ct2020/examples/USER/atc/molecule/water.screen
lammps-stable_290ct2020/examples/USER/atc/molecule/waterequil.init
lammps-stable_290ct2020/examples/USER/atc/thermal/
lammps-stable_290ct2020/examples/USER/atc/thermal/Ar_thermal.mat
lammps-stable_290ct2020/examples/USER/atc/thermal/all_atoms.init
lammps-stable_290ct2020/examples/USER/atc/thermal/bar1d.screen
lammps-stable_290ct2020/examples/USER/atc/thermal/bar1d_all_atoms.screen
lammps-stable_290ct2020/examples/USER/atc/thermal/bar1d_combined.screen
lammps-stable_290ct2020/examples/USER/atc/thermal/bar1d_flux.screen
lammps-stable_290ct2020/examples/USER/atc/thermal/bar1d_frac_step.screen
lammps-stable_290ct2020/examples/USER/atc/thermal/bar1d_hoover.screen
lammps-stable_290ct2020/examples/USER/atc/thermal/bar1d_interpolate.screen
lammps-stable_290ct2020/examples/USER/atc/thermal/bar1d_lumped.screen
lammps-stable_290ct2020/examples/USER/atc/thermal/in.bar1d
lammps-stable_290ct2020/examples/USER/atc/thermal/in.bar1d_all_atoms
lammps-stable_290ct2020/examples/USER/atc/thermal/in.bar1d_combined
lammps-stable_290ct2020/examples/USER/atc/thermal/in.bar1d_flux
lammps-stable_290ct2020/examples/USER/atc/thermal/in.bar1d_frac_step
lammps-stable_290ct2020/examples/USER/atc/thermal/in.bar1d_hoover
lammps-stable_290ct2020/examples/USER/atc/thermal/in.bar1d_interpolate
lammps-stable_290ct2020/examples/USER/atc/thermal/in.bar1d_lumped
lammps-stable_290ct2020/examples/USER/atc/thermal/in.no_atoms
lammps-stable_290ct2020/examples/USER/atc/thermal/no_atoms.screen
lammps-stable_290ct2020/examples/USER/atc/thermal/temp.init
lammps-stable_290ct2020/examples/USER/atc/two_temperature/
lammps-stable_290ct2020/examples/USER/atc/two_temperature/Ar_ttm.mat
lammps-stable_290ct2020/examples/USER/atc/two_temperature/Cu_ttm.mat
lammps-stable_290ct2020/examples/USER/atc/two_temperature/bar1d_ttm.screen
lammps-stable_290ct2020/examples/USER/atc/two_temperature/cutout.init
lammps-stable_290ct2020/examples/USER/atc/two_temperature/cutout.screen
lammps-stable_290ct2020/examples/USER/atc/two_temperature/gaussianIC_ttm.scre
en
lammps-stable_290ct2020/examples/USER/atc/two_temperature/in.bar1d_ttm
lammps-stable_290ct2020/examples/USER/atc/two_temperature/in.cutout
lammps-stable_290ct2020/examples/USER/atc/two_temperature/in.gaussianIC_ttm
lammps-stable_290ct2020/examples/USER/atc/two_temperature/in.no_atoms
lammps-stable_290ct2020/examples/USER/atc/two_temperature/in.restart
lammps-stable_290ct2020/examples/USER/atc/two_temperature/in.uniform_exchange
lammps-stable_290ct2020/examples/USER/atc/two_temperature/in.uniform_heating
lammps-stable_290ct2020/examples/USER/atc/two_temperature/no_atoms.screen
lammps-stable_290ct2020/examples/USER/atc/two_temperature/restart.screen
lammps-stable_290ct2020/examples/USER/atc/two_temperature/temp.init
lammps-stable_290ct2020/examples/USER/atc/two_temperature/uniform_exchange.in
it
lammps-stable_290ct2020/examples/USER/atc/two_temperature/uniform_exchange.sc
reen
lammps-stable_290ct2020/examples/USER/atc/two_temperature/uniform_heating.ini
t
lammps-stable_290ct2020/examples/USER/atc/two_temperature/uniform_heating.scr
een
```

```
lammps-stable_290ct2020/examples/USER/awpmd/  
lammps-stable_290ct2020/examples/USER/awpmd/README  
lammps-stable_290ct2020/examples/USER/awpmd/data.h_atom  
lammps-stable_290ct2020/examples/USER/awpmd/data.h_molecule  
lammps-stable_290ct2020/examples/USER/awpmd/in.h_atom  
lammps-stable_290ct2020/examples/USER/awpmd/in.h_molecule  
lammps-stable_290ct2020/examples/USER/awpmd/log.27Nov18.h_atom.g++.1  
lammps-stable_290ct2020/examples/USER/awpmd/log.27Nov18.h_atom.g++.4  
lammps-stable_290ct2020/examples/USER/awpmd/log.27Nov18.h_molecule.g++.1  
lammps-stable_290ct2020/examples/USER/awpmd/log.27Nov18.h_molecule.g++.4  
lammps-stable_290ct2020/examples/USER/bocs/  
lammps-stable_290ct2020/examples/USER/bocs/README  
lammps-stable_290ct2020/examples/USER/bocs/in.methanol  
lammps-stable_290ct2020/examples/USER/bocs/lammps_nb_MET-MET.table  
lammps-stable_290ct2020/examples/USER/bocs/log.27Nov18.methanol.g++.1  
lammps-stable_290ct2020/examples/USER/bocs/log.27Nov18.methanol.g++.4  
lammps-stable_290ct2020/examples/USER/bocs/methanol.data  
lammps-stable_290ct2020/examples/USER/cgdna/  
lammps-stable_290ct2020/examples/USER/cgdna/README  
lammps-stable_290ct2020/examples/USER/cgdna/examples/  
lammps-stable_290ct2020/examples/USER/cgdna/examples/oxDNA/  
lammps-stable_290ct2020/examples/USER/cgdna/examples/oxDNA/duplex1/  
lammps-stable_290ct2020/examples/USER/cgdna/examples/oxDNA/duplex1/data.duplex1  
lammps-stable_290ct2020/examples/USER/cgdna/examples/oxDNA/duplex1/in.duplex1  
lammps-stable_290ct2020/examples/USER/cgdna/examples/oxDNA/duplex1/log.30Jun20.duplex1.g++.1  
lammps-stable_290ct2020/examples/USER/cgdna/examples/oxDNA/duplex1/log.30Jun20.duplex1.g++.4  
lammps-stable_290ct2020/examples/USER/cgdna/examples/oxDNA/duplex2/  
lammps-stable_290ct2020/examples/USER/cgdna/examples/oxDNA/duplex2/data.duplex2  
lammps-stable_290ct2020/examples/USER/cgdna/examples/oxDNA/duplex2/in.duplex2  
lammps-stable_290ct2020/examples/USER/cgdna/examples/oxDNA/duplex2/log.30Jun20.duplex2.g++.1  
lammps-stable_290ct2020/examples/USER/cgdna/examples/oxDNA/duplex2/log.30Jun20.duplex2.g++.4  
lammps-stable_290ct2020/examples/USER/cgdna/examples/oxDNA2/  
lammps-stable_290ct2020/examples/USER/cgdna/examples/oxDNA2/duplex1/  
lammps-stable_290ct2020/examples/USER/cgdna/examples/oxDNA2/duplex1/data.duplex1  
lammps-stable_290ct2020/examples/USER/cgdna/examples/oxDNA2/duplex1/in.duplex1  
lammps-stable_290ct2020/examples/USER/cgdna/examples/oxDNA2/duplex1/log.30Jun20.duplex1.g++.1  
lammps-stable_290ct2020/examples/USER/cgdna/examples/oxDNA2/duplex1/log.30Jun20.duplex1.g++.4  
lammps-stable_290ct2020/examples/USER/cgdna/examples/oxDNA2/duplex2/  
lammps-stable_290ct2020/examples/USER/cgdna/examples/oxDNA2/duplex2/data.duplex2  
lammps-stable_290ct2020/examples/USER/cgdna/examples/oxDNA2/duplex2/in.duplex2  
lammps-stable_290ct2020/examples/USER/cgdna/examples/oxDNA2/duplex2/log.30Jun20.duplex2.g++.1  
lammps-stable_290ct2020/examples/USER/cgdna/examples/oxDNA2/duplex2/log.30Jun20.duplex2.g++.4  
lammps-stable_290ct2020/examples/USER/cgdna/examples/oxDNA2/duplex3/  
lammps-stable_290ct2020/examples/USER/cgdna/examples/oxDNA2/duplex3/data.duplex3  
lammps-stable_290ct2020/examples/USER/cgdna/examples/oxDNA2/duplex3/in.duplex3
```



```
3
lammps-stable_290ct2020/examples/USER/cgdna/examples/oxDNA2/duplex3/log.30Jun
20.duplex3.g++.1
lammps-stable_290ct2020/examples/USER/cgdna/examples/oxDNA2/duplex3/log.30Jun
20.duplex3.g++.4
lammps-stable_290ct2020/examples/USER/cgdna/examples/oxDNA2/unique_bp/
lammps-stable_290ct2020/examples/USER/cgdna/examples/oxDNA2/unique_bp/data.du
plex4.4type
lammps-stable_290ct2020/examples/USER/cgdna/examples/oxDNA2/unique_bp/data.du
plex4.8type
lammps-stable_290ct2020/examples/USER/cgdna/examples/oxDNA2/unique_bp/generat
e_unique.py
lammps-stable_290ct2020/examples/USER/cgdna/examples/oxDNA2/unique_bp/in.dupl
ex4.4type
lammps-stable_290ct2020/examples/USER/cgdna/examples/oxDNA2/unique_bp/in.dupl
ex4.8type
lammps-stable_290ct2020/examples/USER/cgdna/examples/oxDNA2/unique_bp/log.30J
un20.duplex4.4type.g++1
lammps-stable_290ct2020/examples/USER/cgdna/examples/oxDNA2/unique_bp/log.30J
un20.duplex4.4type.g++4
lammps-stable_290ct2020/examples/USER/cgdna/examples/oxDNA2/unique_bp/log.30J
un20.duplex4.8type.g++1
lammps-stable_290ct2020/examples/USER/cgdna/examples/oxDNA2/unique_bp/log.30J
un20.duplex4.8type.g++4
lammps-stable_290ct2020/examples/USER/cgdna/examples/oxRNA2/
lammps-stable_290ct2020/examples/USER/cgdna/examples/oxRNA2/duplex4/
lammps-stable_290ct2020/examples/USER/cgdna/examples/oxRNA2/duplex4/data.dupl
ex4
lammps-stable_290ct2020/examples/USER/cgdna/examples/oxRNA2/duplex4/in.duplex
4
lammps-stable_290ct2020/examples/USER/cgdna/examples/oxRNA2/duplex4/log.30Jun
20.duplex4.g++.1
lammps-stable_290ct2020/examples/USER/cgdna/examples/oxRNA2/duplex4/log.30Jun
20.duplex4.g++.4
lammps-stable_290ct2020/examples/USER/cgdna/util/
lammps-stable_290ct2020/examples/USER/cgdna/util/generate.py
lammps-stable_290ct2020/examples/USER/cgdna/util/generate_simple.py
lammps-stable_290ct2020/examples/USER/cgdna/util/input.ref
lammps-stable_290ct2020/examples/USER/cgdna/util/sequence.txt
lammps-stable_290ct2020/examples/USER/cgdna/util/sequence_simple.txt
lammps-stable_290ct2020/examples/USER/cgsdk/
lammps-stable_290ct2020/examples/USER/cgsdk/README
lammps-stable_290ct2020/examples/USER/cgsdk/peg-verlet/
lammps-stable_290ct2020/examples/USER/cgsdk/peg-verlet/data.pegc12e8.gz
lammps-stable_290ct2020/examples/USER/cgsdk/peg-verlet/in.pegc12e8
lammps-stable_290ct2020/examples/USER/cgsdk/peg-verlet/in.pegc12e8-angle
lammps-stable_290ct2020/examples/USER/cgsdk/peg-verlet/log.27Nov18.pegc12e8-a
ngle.g++.1
lammps-stable_290ct2020/examples/USER/cgsdk/peg-verlet/log.27Nov18.pegc12e8-a
ngle.g++.4
lammps-stable_290ct2020/examples/USER/cgsdk/peg-verlet/log.27Nov18.pegc12e8.
g++.1
lammps-stable_290ct2020/examples/USER/cgsdk/peg-verlet/log.27Nov18.pegc12e8.
g++.4
lammps-stable_290ct2020/examples/USER/cgsdk/sds-monolayer/
lammps-stable_290ct2020/examples/USER/cgsdk/sds-monolayer/data.sds.gz
lammps-stable_290ct2020/examples/USER/cgsdk/sds-monolayer/in.sds-hybrid
lammps-stable_290ct2020/examples/USER/cgsdk/sds-monolayer/in.sds-regular
lammps-stable_290ct2020/examples/USER/cgsdk/sds-monolayer/log.27Nov18.sds-hyb
rid.g++.1
```

```
lammps-stable_290ct2020/examples/USER/cgSDK/sds-monolayer/log.27Nov18.sds-hybrid.g++.4
lammps-stable_290ct2020/examples/USER/cgSDK/sds-monolayer/log.27Nov18.sds-regular.g++.1
lammps-stable_290ct2020/examples/USER/cgSDK/sds-monolayer/log.27Nov18.sds-regular.g++.4
lammps-stable_290ct2020/examples/USER/colvars/
lammps-stable_290ct2020/examples/USER/colvars/data.peptide
lammps-stable_290ct2020/examples/USER/colvars/in.peptide-colvars
lammps-stable_290ct2020/examples/USER/colvars/in.peptide-colvars2
lammps-stable_290ct2020/examples/USER/colvars/in.peptide-spring
lammps-stable_290ct2020/examples/USER/colvars/in.peptide-spring2
lammps-stable_290ct2020/examples/USER/colvars/log.27Nov18.peptide-colvars.g++.1
lammps-stable_290ct2020/examples/USER/colvars/log.27Nov18.peptide-colvars.g++.4
lammps-stable_290ct2020/examples/USER/colvars/log.27Nov18.peptide-colvars2.g++.1
lammps-stable_290ct2020/examples/USER/colvars/log.27Nov18.peptide-colvars2.g++.4
lammps-stable_290ct2020/examples/USER/colvars/log.27Nov18.peptide-spring.g++.1
lammps-stable_290ct2020/examples/USER/colvars/log.27Nov18.peptide-spring.g++.4
lammps-stable_290ct2020/examples/USER/colvars/log.27Nov18.peptide-spring2.g++.1
lammps-stable_290ct2020/examples/USER/colvars/log.27Nov18.peptide-spring2.g++.4
lammps-stable_290ct2020/examples/USER/colvars/out.colvars.state
lammps-stable_290ct2020/examples/USER/colvars/out.colvars.state.old
lammps-stable_290ct2020/examples/USER/colvars/out.colvars.traj
lammps-stable_290ct2020/examples/USER/colvars/out2.colvars.state
lammps-stable_290ct2020/examples/USER/colvars/out2.colvars.traj
lammps-stable_290ct2020/examples/USER/colvars/peptide.colvars
lammps-stable_290ct2020/examples/USER/colvars/peptide.colvars2
lammps-stable_290ct2020/examples/USER/colvars/peptide.psf
lammps-stable_290ct2020/examples/USER/colvars/peptide2.colvars.state
lammps-stable_290ct2020/examples/USER/colvars/peptide2.colvars.traj
lammps-stable_290ct2020/examples/USER/diffraction/
lammps-stable_290ct2020/examples/USER/diffraction/Output/
lammps-stable_290ct2020/examples/USER/diffraction/Output/bulkNi.hist.xrd.correct
lammps-stable_290ct2020/examples/USER/diffraction/Output/bulkNi.log.correct
lammps-stable_290ct2020/examples/USER/diffraction/Output/bulkNi_001.saed.0.vtk.correct
lammps-stable_290ct2020/examples/USER/diffraction/Output/bulkNi_001.saed.0_VisIt_Image.png
lammps-stable_290ct2020/examples/USER/diffraction/Output/log.cite
lammps-stable_290ct2020/examples/USER/diffraction/README
lammps-stable_290ct2020/examples/USER/diffraction/in.BulkNi
lammps-stable_290ct2020/examples/USER/diffraction/log.27Nov18.BulkNi.g++.1
lammps-stable_290ct2020/examples/USER/diffraction/log.27Nov18.BulkNi.g++.4
lammps-stable_290ct2020/examples/USER/dpd/
lammps-stable_290ct2020/examples/USER/dpd/README
lammps-stable_290ct2020/examples/USER/dpd/dpd-shardlow/
lammps-stable_290ct2020/examples/USER/dpd/dpd-shardlow/data.dpd
lammps-stable_290ct2020/examples/USER/dpd/dpd-shardlow/in.dpd-shardlow
lammps-stable_290ct2020/examples/USER/dpd/dpd-shardlow/log.dpd-shardlow.reference
lammps-stable_290ct2020/examples/USER/dpd/dpd-vv/
```

```
lammps-stable_290ct2020/examples/USER/dpd/dpd-vv/data.dpd
lammps-stable_290ct2020/examples/USER/dpd/dpd-vv/in.dpd-vv
lammps-stable_290ct2020/examples/USER/dpd/dpd-vv/log.dpd-vv.reference
lammps-stable_290ct2020/examples/USER/dpd/dpde-shardlow/
lammps-stable_290ct2020/examples/USER/dpd/dpde-shardlow/data.dpde
lammps-stable_290ct2020/examples/USER/dpd/dpde-shardlow/in.dpde-shardlow
lammps-stable_290ct2020/examples/USER/dpd/dpde-shardlow/log.dpde-shardlow.ref
erence
lammps-stable_290ct2020/examples/USER/dpd/dpde-vv/
lammps-stable_290ct2020/examples/USER/dpd/dpde-vv/data.dpd
lammps-stable_290ct2020/examples/USER/dpd/dpde-vv/in.dpde-vv
lammps-stable_290ct2020/examples/USER/dpd/dpde-vv/log.dpde-vv.reference
lammps-stable_290ct2020/examples/USER/dpd/dpdh-shardlow/
lammps-stable_290ct2020/examples/USER/dpd/dpdh-shardlow/data.dpdh
lammps-stable_290ct2020/examples/USER/dpd/dpdh-shardlow/in.dpdh-shardlow
lammps-stable_290ct2020/examples/USER/dpd/dpdh-shardlow/log.dpdh-shardlow.ref
erence
lammps-stable_290ct2020/examples/USER/dpd/dpdp-shardlow/
lammps-stable_290ct2020/examples/USER/dpd/dpdp-shardlow/data.dpd
lammps-stable_290ct2020/examples/USER/dpd/dpdp-shardlow/in.dpdp-shardlow
lammps-stable_290ct2020/examples/USER/dpd/dpdp-shardlow/log.dpdp-shardlow.ref
erence
lammps-stable_290ct2020/examples/USER/dpd/dpdrx-shardlow/
lammps-stable_290ct2020/examples/USER/dpd/dpdrx-shardlow/in.dpdrx-shardlow
lammps-stable_290ct2020/examples/USER/dpd/dpdrx-shardlow/kinetics.dpdrx
lammps-stable_290ct2020/examples/USER/dpd/dpdrx-shardlow/log.dpdrx-shardlow.r
eference
lammps-stable_290ct2020/examples/USER/dpd/dpdrx-shardlow/params.exp6
lammps-stable_290ct2020/examples/USER/dpd/dpdrx-shardlow/table.eos
lammps-stable_290ct2020/examples/USER/dpd/dpdrx-shardlow/thermo.dpdrx
lammps-stable_290ct2020/examples/USER/dpd/dpdrx-shardlow/thermo.dpdrx.new
lammps-stable_290ct2020/examples/USER/dpd/multi-lucy/
lammps-stable_290ct2020/examples/USER/dpd/multi-lucy/in.multi-lucy
lammps-stable_290ct2020/examples/USER/dpd/multi-lucy/log.multi-lucy.reference
lammps-stable_290ct2020/examples/USER/dpd/multi-lucy/table.multibody
lammps-stable_290ct2020/examples/USER/drude/
lammps-stable_290ct2020/examples/USER/drude/README
lammps-stable_290ct2020/examples/USER/drude/butane/
lammps-stable_290ct2020/examples/USER/drude/butane/data.butane
lammps-stable_290ct2020/examples/USER/drude/butane/in.butane.lang
lammps-stable_290ct2020/examples/USER/drude/butane/in.butane.nh
lammps-stable_290ct2020/examples/USER/drude/butane/log.27Nov18.butane.lang.
g++.1
lammps-stable_290ct2020/examples/USER/drude/butane/log.27Nov18.butane.lang.
g++.4
lammps-stable_290ct2020/examples/USER/drude/butane/log.27Nov18.butane.nh.g++.
1
lammps-stable_290ct2020/examples/USER/drude/butane/log.27Nov18.butane.nh.g++.
4
lammps-stable_290ct2020/examples/USER/drude/ethanol/
lammps-stable_290ct2020/examples/USER/drude/ethanol/data.ethanol
lammps-stable_290ct2020/examples/USER/drude/ethanol/in.ethanol.lang
lammps-stable_290ct2020/examples/USER/drude/ethanol/in.ethanol.nh
lammps-stable_290ct2020/examples/USER/drude/ethanol/log.27Nov18.ethanol.lang.
g++.1
lammps-stable_290ct2020/examples/USER/drude/ethanol/log.27Nov18.ethanol.lang.
g++.4
lammps-stable_290ct2020/examples/USER/drude/ethanol/log.27Nov18.ethanol.nh.
g++.1
lammps-stable_290ct2020/examples/USER/drude/ethanol/log.27Nov18.ethanol.nh.
```

```
g++.4
lammps-stable_290ct2020/examples/USER/drude/ethylene_glycol/
lammps-stable_290ct2020/examples/USER/drude/ethylene_glycol/data.ethylene_glycol
lammps-stable_290ct2020/examples/USER/drude/ethylene_glycol/in.ethylene_glycol
lammps-stable_290ct2020/examples/USER/drude/ethylene_glycol/log.18Sep20.ethylene_glycol.g++.1
lammps-stable_290ct2020/examples/USER/drude/ethylene_glycol/log.18Sep20.ethylene_glycol.g++.4
lammps-stable_290ct2020/examples/USER/drude/swm4-ndp/
lammps-stable_290ct2020/examples/USER/drude/swm4-ndp/data.swm4-ndp
lammps-stable_290ct2020/examples/USER/drude/swm4-ndp/in.swm4-ndp.lang
lammps-stable_290ct2020/examples/USER/drude/swm4-ndp/in.swm4-ndp.nh
lammps-stable_290ct2020/examples/USER/drude/swm4-ndp/log.27Nov18.swm4-ndp.lang.g++.1
lammps-stable_290ct2020/examples/USER/drude/swm4-ndp/log.27Nov18.swm4-ndp.lang.g++.4
lammps-stable_290ct2020/examples/USER/drude/swm4-ndp/log.27Nov18.swm4-ndp.nh.g++.1
lammps-stable_290ct2020/examples/USER/drude/swm4-ndp/log.27Nov18.swm4-ndp.nh.g++.4
lammps-stable_290ct2020/examples/USER/drude/toluene/
lammps-stable_290ct2020/examples/USER/drude/toluene/data.toluene
lammps-stable_290ct2020/examples/USER/drude/toluene/in.toluene.lang
lammps-stable_290ct2020/examples/USER/drude/toluene/in.toluene.nh
lammps-stable_290ct2020/examples/USER/drude/toluene/log.7Aug19.toluene.lang.g++.1
lammps-stable_290ct2020/examples/USER/drude/toluene/log.7Aug19.toluene.lang.g++.4
lammps-stable_290ct2020/examples/USER/drude/toluene/log.7Aug19.toluene.nh.g++.1
lammps-stable_290ct2020/examples/USER/drude/toluene/log.7Aug19.toluene.nh.g++.4
lammps-stable_290ct2020/examples/USER/eff/
lammps-stable_290ct2020/examples/USER/eff/Auger-Adamantane/
lammps-stable_290ct2020/examples/USER/eff/Auger-Adamantane/README
lammps-stable_290ct2020/examples/USER/eff/Auger-Adamantane/data.adamantane
lammps-stable_290ct2020/examples/USER/eff/Auger-Adamantane/data.adamantane_ionized
lammps-stable_290ct2020/examples/USER/eff/Auger-Adamantane/in.adamantane_ionized.nve
lammps-stable_290ct2020/examples/USER/eff/Be-solid/
lammps-stable_290ct2020/examples/USER/eff/Be-solid/README
lammps-stable_290ct2020/examples/USER/eff/Be-solid/data.Be-solid
lammps-stable_290ct2020/examples/USER/eff/Be-solid/in.Be-solid.spe
lammps-stable_290ct2020/examples/USER/eff/CH4/
lammps-stable_290ct2020/examples/USER/eff/CH4/README
lammps-stable_290ct2020/examples/USER/eff/CH4/data.ch4
lammps-stable_290ct2020/examples/USER/eff/CH4/data.ch4_ionized
lammps-stable_290ct2020/examples/USER/eff/CH4/in.ch4.dynamics
lammps-stable_290ct2020/examples/USER/eff/CH4/in.ch4.min
lammps-stable_290ct2020/examples/USER/eff/CH4/in.ch4_ionized.dynamics
lammps-stable_290ct2020/examples/USER/eff/ECP/
lammps-stable_290ct2020/examples/USER/eff/ECP/README
lammps-stable_290ct2020/examples/USER/eff/ECP/Si2H6/
lammps-stable_290ct2020/examples/USER/eff/ECP/Si2H6/data.Si2H6
lammps-stable_290ct2020/examples/USER/eff/ECP/Si2H6/data.Si2H6.ang
lammps-stable_290ct2020/examples/USER/eff/ECP/Si2H6/in.Si2H6
lammps-stable_290ct2020/examples/USER/eff/ECP/Si2H6/in.Si2H6.ang
```

```
lammps-stable_290ct2020/examples/USER/eff/ECP/SiC/
lammps-stable_290ct2020/examples/USER/eff/ECP/SiC/bulk/
lammps-stable_290ct2020/examples/USER/eff/ECP/SiC/bulk/data.SiC
lammps-stable_290ct2020/examples/USER/eff/ECP/SiC/bulk/in.SiC
lammps-stable_290ct2020/examples/USER/eff/ECP/SiH4/
lammps-stable_290ct2020/examples/USER/eff/ECP/SiH4/data.SiH4
lammps-stable_290ct2020/examples/USER/eff/ECP/SiH4/data.SiH4.ang
lammps-stable_290ct2020/examples/USER/eff/ECP/SiH4/in.SiH4
lammps-stable_290ct2020/examples/USER/eff/ECP/SiH4/in.SiH4.ang
lammps-stable_290ct2020/examples/USER/eff/H/
lammps-stable_290ct2020/examples/USER/eff/H/README
lammps-stable_290ct2020/examples/USER/eff/H/data.h_atom.ang
lammps-stable_290ct2020/examples/USER/eff/H/data.h_atom.bohr
lammps-stable_290ct2020/examples/USER/eff/H/in.h_atom.spe.ang
lammps-stable_290ct2020/examples/USER/eff/H/in.h_atom.spe.bohr
lammps-stable_290ct2020/examples/USER/eff/H2/
lammps-stable_290ct2020/examples/USER/eff/H2/README
lammps-stable_290ct2020/examples/USER/eff/H2/data.h2
lammps-stable_290ct2020/examples/USER/eff/H2/in.h2
lammps-stable_290ct2020/examples/USER/eff/H_plasma/
lammps-stable_290ct2020/examples/USER/eff/H_plasma/README
lammps-stable_290ct2020/examples/USER/eff/H_plasma/data.h2bulk
lammps-stable_290ct2020/examples/USER/eff/H_plasma/data.h2bulk.ang
lammps-stable_290ct2020/examples/USER/eff/H_plasma/in.h2bulk.npt
lammps-stable_290ct2020/examples/USER/eff/H_plasma/in.h2bulk.nve
lammps-stable_290ct2020/examples/USER/eff/H_plasma/in.h2bulk.nve.ang
lammps-stable_290ct2020/examples/USER/eff/Li-dendritic/
lammps-stable_290ct2020/examples/USER/eff/Li-dendritic/README
lammps-stable_290ct2020/examples/USER/eff/Li-dendritic/data.Li-dendritic
lammps-stable_290ct2020/examples/USER/eff/Li-dendritic/in.Li-dendritic.min
lammps-stable_290ct2020/examples/USER/eff/Li-dendritic/in.Li-dendritic.nvt
lammps-stable_290ct2020/examples/USER/eff/Li-solid/
lammps-stable_290ct2020/examples/USER/eff/Li-solid/README
lammps-stable_290ct2020/examples/USER/eff/Li-solid/data.Li.ang
lammps-stable_290ct2020/examples/USER/eff/Li-solid/data.Li.bohr
lammps-stable_290ct2020/examples/USER/eff/Li-solid/in.Li.ang
lammps-stable_290ct2020/examples/USER/eff/Li-solid/in.Li.bohr
lammps-stable_290ct2020/examples/USER/eff/README
lammps-stable_290ct2020/examples/USER/eff/fixed-core/
lammps-stable_290ct2020/examples/USER/eff/fixed-core/C2H6/
lammps-stable_290ct2020/examples/USER/eff/fixed-core/C2H6/data.C2H6fc.ang
lammps-stable_290ct2020/examples/USER/eff/fixed-core/C2H6/data.C2H6fc.bohr
lammps-stable_290ct2020/examples/USER/eff/fixed-core/C2H6/in.C2H6fc.ang
lammps-stable_290ct2020/examples/USER/eff/fixed-core/C2H6/in.C2H6fc.bohr
lammps-stable_290ct2020/examples/USER/eff/fixed-core/CH4/
lammps-stable_290ct2020/examples/USER/eff/fixed-core/CH4/data.CH4fc.ang
lammps-stable_290ct2020/examples/USER/eff/fixed-core/CH4/data.CH4fc.bohr
lammps-stable_290ct2020/examples/USER/eff/fixed-core/CH4/in.CH4fc.ang
lammps-stable_290ct2020/examples/USER/eff/fixed-core/CH4/in.CH4fc.bohr
lammps-stable_290ct2020/examples/USER/eff/fixed-core/CH4/in.CH4fc.spe.ang
lammps-stable_290ct2020/examples/USER/eff/fixed-core/CH4/in.CH4fc.spe.bohr
lammps-stable_290ct2020/examples/USER/eff/fixed-core/README
lammps-stable_290ct2020/examples/USER/fep/
lammps-stable_290ct2020/examples/USER/fep/C7inEthanol/
lammps-stable_290ct2020/examples/USER/fep/C7inEthanol/fep01/
lammps-stable_290ct2020/examples/USER/fep/C7inEthanol/fep01/data.init_conf_wi
th_heptane
lammps-stable_290ct2020/examples/USER/fep/C7inEthanol/fep01/in.insertion
lammps-stable_290ct2020/examples/USER/fep/C7inEthanol/fep01/log.lammps
lammps-stable_290ct2020/examples/USER/fep/C7inEthanol/fep10/
```

lammps-stable\_290ct2020/examples/USER/fep/C7inEthanol/fep10/data.init\_conf\_with\_heptane  
lammps-stable\_290ct2020/examples/USER/fep/C7inEthanol/fep10/in.deletion  
lammps-stable\_290ct2020/examples/USER/fep/C7inEthanol/fep10/log.lammps  
lammps-stable\_290ct2020/examples/USER/fep/CC-CO/  
lammps-stable\_290ct2020/examples/USER/fep/CC-CO/README  
lammps-stable\_290ct2020/examples/USER/fep/CC-CO/bar01/  
lammps-stable\_290ct2020/examples/USER/fep/CC-CO/bar01/bar01.lmp  
lammps-stable\_290ct2020/examples/USER/fep/CC-CO/bar01/in.bar01.lmp  
lammps-stable\_290ct2020/examples/USER/fep/CC-CO/bar01/log.lammps  
lammps-stable\_290ct2020/examples/USER/fep/CC-CO/bar10/  
lammps-stable\_290ct2020/examples/USER/fep/CC-CO/bar10/bar10.lmp  
lammps-stable\_290ct2020/examples/USER/fep/CC-CO/bar10/in.bar10.lmp  
lammps-stable\_290ct2020/examples/USER/fep/CC-CO/bar10/log.lammps  
lammps-stable\_290ct2020/examples/USER/fep/CC-CO/fdti01/  
lammps-stable\_290ct2020/examples/USER/fep/CC-CO/fdti01/fdti01.lmp  
lammps-stable\_290ct2020/examples/USER/fep/CC-CO/fdti01/in.fdti01.lmp  
lammps-stable\_290ct2020/examples/USER/fep/CC-CO/fdti01/log.lammps  
lammps-stable\_290ct2020/examples/USER/fep/CC-CO/fdti10/  
lammps-stable\_290ct2020/examples/USER/fep/CC-CO/fdti10/fdti10.lmp  
lammps-stable\_290ct2020/examples/USER/fep/CC-CO/fdti10/in.fdti10.lmp  
lammps-stable\_290ct2020/examples/USER/fep/CC-CO/fdti10/log.lammps  
lammps-stable\_290ct2020/examples/USER/fep/CC-CO/fep01/  
lammps-stable\_290ct2020/examples/USER/fep/CC-CO/fep01/data.0.lmp  
lammps-stable\_290ct2020/examples/USER/fep/CC-CO/fep01/fep01.lmp  
lammps-stable\_290ct2020/examples/USER/fep/CC-CO/fep01/in.fep01  
lammps-stable\_290ct2020/examples/USER/fep/CC-CO/fep01/in.fep01.lmp  
lammps-stable\_290ct2020/examples/USER/fep/CC-CO/fep01/log.lammps  
lammps-stable\_290ct2020/examples/USER/fep/CC-CO/fep01/log.reference  
lammps-stable\_290ct2020/examples/USER/fep/CC-CO/fep01/log.reference-omp  
lammps-stable\_290ct2020/examples/USER/fep/CC-CO/fep10/  
lammps-stable\_290ct2020/examples/USER/fep/CC-CO/fep10/fep10.lmp  
lammps-stable\_290ct2020/examples/USER/fep/CC-CO/fep10/in.fep10.lmp  
lammps-stable\_290ct2020/examples/USER/fep/CC-CO/fep10/log.lammps  
lammps-stable\_290ct2020/examples/USER/fep/CC-CO/mols/  
lammps-stable\_290ct2020/examples/USER/fep/CC-CO/mols/CC-CO.ff  
lammps-stable\_290ct2020/examples/USER/fep/CC-CO/mols/CC-CO.zmat  
lammps-stable\_290ct2020/examples/USER/fep/CC-CO/mols/CO-CC.zmat  
lammps-stable\_290ct2020/examples/USER/fep/CC-CO/mols/README  
lammps-stable\_290ct2020/examples/USER/fep/CC-CO/mols/data.0.lmp  
lammps-stable\_290ct2020/examples/USER/fep/CC-CO/mols/data.1.lmp  
lammps-stable\_290ct2020/examples/USER/fep/CC-CO/mols/spce.ff  
lammps-stable\_290ct2020/examples/USER/fep/CC-CO/mols/spce.zmat  
lammps-stable\_290ct2020/examples/USER/fep/CH4-CF4/  
lammps-stable\_290ct2020/examples/USER/fep/CH4-CF4/README  
lammps-stable\_290ct2020/examples/USER/fep/CH4-CF4/bar01/  
lammps-stable\_290ct2020/examples/USER/fep/CH4-CF4/bar01/bar01.lmp  
lammps-stable\_290ct2020/examples/USER/fep/CH4-CF4/bar01/in.bar01.lmp  
lammps-stable\_290ct2020/examples/USER/fep/CH4-CF4/bar01/log.lammps  
lammps-stable\_290ct2020/examples/USER/fep/CH4-CF4/bar10/  
lammps-stable\_290ct2020/examples/USER/fep/CH4-CF4/bar10/bar10.lmp  
lammps-stable\_290ct2020/examples/USER/fep/CH4-CF4/bar10/in.bar10.lmp  
lammps-stable\_290ct2020/examples/USER/fep/CH4-CF4/bar10/log.lammps  
lammps-stable\_290ct2020/examples/USER/fep/CH4-CF4/mols/  
lammps-stable\_290ct2020/examples/USER/fep/CH4-CF4/mols/CF4-CH4.zmat  
lammps-stable\_290ct2020/examples/USER/fep/CH4-CF4/mols/CH4-CF4.ff  
lammps-stable\_290ct2020/examples/USER/fep/CH4-CF4/mols/CH4-CF4.zmat  
lammps-stable\_290ct2020/examples/USER/fep/CH4-CF4/mols/data.0.lmp  
lammps-stable\_290ct2020/examples/USER/fep/CH4-CF4/mols/data.1.lmp  
lammps-stable\_290ct2020/examples/USER/fep/CH4-CF4/mols/spce.ff

```
lammps-stable_290ct2020/examples/USER/fep/CH4-CF4/mols/spce.zmat
lammps-stable_290ct2020/examples/USER/fep/CH4hyd/
lammps-stable_290ct2020/examples/USER/fep/CH4hyd/README
lammps-stable_290ct2020/examples/USER/fep/CH4hyd/fdti01/
lammps-stable_290ct2020/examples/USER/fep/CH4hyd/fdti01/fdti01.lmp
lammps-stable_290ct2020/examples/USER/fep/CH4hyd/fdti01/in.fdti01.lmp
lammps-stable_290ct2020/examples/USER/fep/CH4hyd/fdti01/log.lammps
lammps-stable_290ct2020/examples/USER/fep/CH4hyd/fdti10/
lammps-stable_290ct2020/examples/USER/fep/CH4hyd/fdti10/fdti10.lmp
lammps-stable_290ct2020/examples/USER/fep/CH4hyd/fdti10/in.fdti10.lmp
lammps-stable_290ct2020/examples/USER/fep/CH4hyd/fdti10/log.lammps
lammps-stable_290ct2020/examples/USER/fep/CH4hyd/fep01/
lammps-stable_290ct2020/examples/USER/fep/CH4hyd/fep01/fep01.lmp
lammps-stable_290ct2020/examples/USER/fep/CH4hyd/fep01/in.fep01.lmp
lammps-stable_290ct2020/examples/USER/fep/CH4hyd/fep01/log.lammps
lammps-stable_290ct2020/examples/USER/fep/CH4hyd/fep10/
lammps-stable_290ct2020/examples/USER/fep/CH4hyd/fep10/fep10.lmp
lammps-stable_290ct2020/examples/USER/fep/CH4hyd/fep10/in.fep10.lmp
lammps-stable_290ct2020/examples/USER/fep/CH4hyd/fep10/log.lammps
lammps-stable_290ct2020/examples/USER/fep/CH4hyd/mols/
lammps-stable_290ct2020/examples/USER/fep/CH4hyd/mols/data.lmp
lammps-stable_290ct2020/examples/USER/fep/CH4hyd/mols/methane.zmat
lammps-stable_290ct2020/examples/USER/fep/CH4hyd/mols/oplsaa.ff
lammps-stable_290ct2020/examples/USER/fep/CH4hyd/mols/tip4pew.ff
lammps-stable_290ct2020/examples/USER/fep/CH4hyd/mols/tip4pew.zmat
lammps-stable_290ct2020/examples/USER/fep/README
lammps-stable_290ct2020/examples/USER/lb/
lammps-stable_290ct2020/examples/USER/lb/confined_colloid/
lammps-stable_290ct2020/examples/USER/lb/confined_colloid/in.confined_colloid
s
lammps-stable_290ct2020/examples/USER/lb/confined_colloid/results64.out
lammps-stable_290ct2020/examples/USER/lb/dragforce/
lammps-stable_290ct2020/examples/USER/lb/dragforce/data.one_radius16d2
lammps-stable_290ct2020/examples/USER/lb/dragforce/defaultgamma_drag.out
lammps-stable_290ct2020/examples/USER/lb/dragforce/in.defaultgamma_drag
lammps-stable_290ct2020/examples/USER/lb/dragforce/in.setgamma_drag
lammps-stable_290ct2020/examples/USER/lb/dragforce/setgamma13d0_drag.out
lammps-stable_290ct2020/examples/USER/lb/fourspheres/
lammps-stable_290ct2020/examples/USER/lb/fourspheres/data.four
lammps-stable_290ct2020/examples/USER/lb/fourspheres/fourspheres_velocity0d00
01_defaultgamma.out
lammps-stable_290ct2020/examples/USER/lb/fourspheres/fourspheres_velocity0d00
01_setgamma.out
lammps-stable_290ct2020/examples/USER/lb/fourspheres/in.fourspheres_default_g
amma
lammps-stable_290ct2020/examples/USER/lb/fourspheres/in.fourspheres_set_gamma
lammps-stable_290ct2020/examples/USER/lb/microrheology/
lammps-stable_290ct2020/examples/USER/lb/microrheology/data.two
lammps-stable_290ct2020/examples/USER/lb/microrheology/in.microrheology_defau
lt_gamma
lammps-stable_290ct2020/examples/USER/lb/microrheology/in.microrheology_set_g
amma
lammps-stable_290ct2020/examples/USER/lb/microrheology/microrheology_defaultg
amma.out
lammps-stable_290ct2020/examples/USER/lb/microrheology/microrheology_setgamm
a.out
lammps-stable_290ct2020/examples/USER/lb/planewall/
lammps-stable_290ct2020/examples/USER/lb/planewall/data.one_radius16d2
lammps-stable_290ct2020/examples/USER/lb/planewall/in.planewall_default_gamma
lammps-stable_290ct2020/examples/USER/lb/planewall/in.planewall_set_gamma
```

```
lammps-stable_290ct2020/examples/USER/lb/planewall/wall_defaultgamma.out
lammps-stable_290ct2020/examples/USER/lb/planewall/wall_setgamma.out
lammps-stable_290ct2020/examples/USER/lb/polymer/
lammps-stable_290ct2020/examples/USER/lb/polymer/data.polymer
lammps-stable_290ct2020/examples/USER/lb/polymer/in.polymer_default_gamma
lammps-stable_290ct2020/examples/USER/lb/polymer/in.polymer_setgamma
lammps-stable_290ct2020/examples/USER/lb/polymer/out.polymer_default_gamma
lammps-stable_290ct2020/examples/USER/lb/polymer/out.polymer_setgamma
lammps-stable_290ct2020/examples/USER/manifold/
lammps-stable_290ct2020/examples/USER/manifold/diffusion/
lammps-stable_290ct2020/examples/USER/manifold/diffusion/README
lammps-stable_290ct2020/examples/USER/manifold/diffusion/msd.cyl.data
lammps-stable_290ct2020/examples/USER/manifold/diffusion/msd.cyl.in
lammps-stable_290ct2020/examples/USER/manifold/diffusion/msd.pdf
lammps-stable_290ct2020/examples/USER/manifold/diffusion/msd.plane.data
lammps-stable_290ct2020/examples/USER/manifold/diffusion/msd.plane.in
lammps-stable_290ct2020/examples/USER/manifold/diffusion/msd.sphere.data
lammps-stable_290ct2020/examples/USER/manifold/diffusion/msd.sphere.in
lammps-stable_290ct2020/examples/USER/manifold/diffusion/msd_plot2.pdf
lammps-stable_290ct2020/examples/USER/manifold/diffusion/plot_msd.gpl
lammps-stable_290ct2020/examples/USER/manifold/energy/
lammps-stable_290ct2020/examples/USER/manifold/energy/README
lammps-stable_290ct2020/examples/USER/manifold/energy/cylinder.data
lammps-stable_290ct2020/examples/USER/manifold/energy/cylinder.setup
lammps-stable_290ct2020/examples/USER/manifold/energy/energy.in
lammps-stable_290ct2020/examples/USER/manifold/energy/energy.plane.in
lammps-stable_290ct2020/examples/USER/manifold/energy/energy.sh
lammps-stable_290ct2020/examples/USER/manifold/energy/energy_conservation.pdf
lammps-stable_290ct2020/examples/USER/manifold/energy/energy_conservation.png
lammps-stable_290ct2020/examples/USER/manifold/energy/plane.anneal.data
lammps-stable_290ct2020/examples/USER/manifold/energy/plane.data
lammps-stable_290ct2020/examples/USER/manifold/energy/plot_energies.gpl
lammps-stable_290ct2020/examples/USER/manifold/energy/sphere.data
lammps-stable_290ct2020/examples/USER/manifold/energy/sphere.setup
lammps-stable_290ct2020/examples/USER/manifold/energy/torus.data
lammps-stable_290ct2020/examples/USER/manifold/energy/torus.setup
lammps-stable_290ct2020/examples/USER/manifold/thylakoid/
lammps-stable_290ct2020/examples/USER/manifold/thylakoid/README
lammps-stable_290ct2020/examples/USER/manifold/thylakoid/thylakoid.data
lammps-stable_290ct2020/examples/USER/manifold/thylakoid/thylakoid.in
lammps-stable_290ct2020/examples/USER/manifold/virus/
lammps-stable_290ct2020/examples/USER/manifold/virus/README
lammps-stable_290ct2020/examples/USER/manifold/virus/init.data
lammps-stable_290ct2020/examples/USER/manifold/virus/vir.in
lammps-stable_290ct2020/examples/USER/mesodpd/
lammps-stable_290ct2020/examples/USER/mesodpd/README
lammps-stable_290ct2020/examples/USER/mesodpd/edpd/
lammps-stable_290ct2020/examples/USER/mesodpd/edpd/in.edpd
lammps-stable_290ct2020/examples/USER/mesodpd/edpd/log.16Aug17.edpd.g++.1
lammps-stable_290ct2020/examples/USER/mesodpd/edpd/log.16Aug17.edpd.g++.4
lammps-stable_290ct2020/examples/USER/mesodpd/edpd/temp.profile.16Aug17.edpd.
g++.1
lammps-stable_290ct2020/examples/USER/mesodpd/edpd/temp.profile.16Aug17.edpd.
g++.4
lammps-stable_290ct2020/examples/USER/mesodpd/mdpd/
lammps-stable_290ct2020/examples/USER/mesodpd/mdpd/in.mdpd
lammps-stable_290ct2020/examples/USER/mesodpd/mdpd/log.16Aug17.mdpd.g++.1
lammps-stable_290ct2020/examples/USER/mesodpd/mdpd/log.16Aug17.mdpd.g++.4
lammps-stable_290ct2020/examples/USER/mesodpd/tdpd/
lammps-stable_290ct2020/examples/USER/mesodpd/tdpd/cc.profile.16Aug17.tdpd.
```



```
g++.1
lammps-stable_290ct2020/examples/USER/mesodpd/tdpd/cc.profile.16Aug17.tdpd.
g++.4
lammps-stable_290ct2020/examples/USER/mesodpd/tdpd/in.tdpd
lammps-stable_290ct2020/examples/USER/mesodpd/tdpd/log.16Aug17.tdpd.g++.1
lammps-stable_290ct2020/examples/USER/mesodpd/tdpd/log.16Aug17.tdpd.g++.4
lammps-stable_290ct2020/examples/USER/mesont/
lammps-stable_290ct2020/examples/USER/mesont/C_10_10.mesocnt
lammps-stable_290ct2020/examples/USER/mesont/README
lammps-stable_290ct2020/examples/USER/mesont/TABTP_10_10.mesont
lammps-stable_290ct2020/examples/USER/mesont/cnt.data
lammps-stable_290ct2020/examples/USER/mesont/data.bundle
lammps-stable_290ct2020/examples/USER/mesont/data.film
lammps-stable_290ct2020/examples/USER/mesont/in.bundle
lammps-stable_290ct2020/examples/USER/mesont/in.cnt
lammps-stable_290ct2020/examples/USER/mesont/in.film
lammps-stable_290ct2020/examples/USER/mesont/log.2Jun2020.bundle.g++.1
lammps-stable_290ct2020/examples/USER/mesont/log.2Jun2020.bundle.g++.4
lammps-stable_290ct2020/examples/USER/mesont/log.2Jun2020.film.g++.1
lammps-stable_290ct2020/examples/USER/mesont/log.2Jun2020.film.g++.4
lammps-stable_290ct2020/examples/USER/mesont/log.9Jan20.cnt.g++.1
lammps-stable_290ct2020/examples/USER/mesont/log.9Jan20.cnt.g++.4
lammps-stable_290ct2020/examples/USER/mgpt/
lammps-stable_290ct2020/examples/USER/mgpt/Ta6.8x.mgpt.README
lammps-stable_290ct2020/examples/USER/mgpt/Ta6.8x.mgpt.parmin
lammps-stable_290ct2020/examples/USER/mgpt/Ta6.8x.mgpt.potin
lammps-stable_290ct2020/examples/USER/mgpt/in.bcc0
lammps-stable_290ct2020/examples/USER/mgpt/in.vac0-bcc
lammps-stable_290ct2020/examples/USER/mgpt/in.vacmin-bcc
lammps-stable_290ct2020/examples/USER/mgpt/log.bcc0
lammps-stable_290ct2020/examples/USER/mgpt/log.vac0-bcc
lammps-stable_290ct2020/examples/USER/mgpt/log.vacmin-bcc
lammps-stable_290ct2020/examples/USER/misc/
lammps-stable_290ct2020/examples/USER/misc/addtorque/
lammps-stable_290ct2020/examples/USER/misc/addtorque/in.addtorque
lammps-stable_290ct2020/examples/USER/misc/addtorque/log.9Nov16.addtorque.
g++.1
lammps-stable_290ct2020/examples/USER/misc/addtorque/log.9Nov16.addtorque.
g++.4
lammps-stable_290ct2020/examples/USER/misc/agni/
lammps-stable_290ct2020/examples/USER/misc/agni/Al_jpc.agni
lammps-stable_290ct2020/examples/USER/misc/agni/adatom.data
lammps-stable_290ct2020/examples/USER/misc/agni/in.adatom
lammps-stable_290ct2020/examples/USER/misc/agni/in.vacancy
lammps-stable_290ct2020/examples/USER/misc/agni/log.21Feb17.adatom.g++.1
lammps-stable_290ct2020/examples/USER/misc/agni/log.21Feb17.adatom.g++.4
lammps-stable_290ct2020/examples/USER/misc/agni/log.21Feb17.vacancy.g++.1
lammps-stable_290ct2020/examples/USER/misc/agni/log.21Feb17.vacancy.g++.4
lammps-stable_290ct2020/examples/USER/misc/agni/vacancy.data
lammps-stable_290ct2020/examples/USER/misc/basal/
lammps-stable_290ct2020/examples/USER/misc/basal/almg.liu
lammps-stable_290ct2020/examples/USER/misc/basal/in.basal
lammps-stable_290ct2020/examples/USER/misc/cauchy/
lammps-stable_290ct2020/examples/USER/misc/cauchy/NiAlH_jea.eam.alloy
lammps-stable_290ct2020/examples/USER/misc/cauchy/README
lammps-stable_290ct2020/examples/USER/misc/cauchy/in.cauchystat
lammps-stable_290ct2020/examples/USER/misc/cauchy/log.2Jun2020.cauchystat.
g++.1
lammps-stable_290ct2020/examples/USER/misc/cnp/
lammps-stable_290ct2020/examples/USER/misc/cnp/Cu_Mishin1.eam
```

lammps-stable\_290ct2020/examples/USER/misc/cnp/in.cnp  
lammps-stable\_290ct2020/examples/USER/misc/cnp/log.31May17.cnp.g++.4  
lammps-stable\_290ct2020/examples/USER/misc/drip/  
lammps-stable\_290ct2020/examples/USER/misc/drip/C.drip  
lammps-stable\_290ct2020/examples/USER/misc/drip/CH.rebo  
lammps-stable\_290ct2020/examples/USER/misc/drip/README.txt  
lammps-stable\_290ct2020/examples/USER/misc/drip/data.C  
lammps-stable\_290ct2020/examples/USER/misc/drip/data.CH  
lammps-stable\_290ct2020/examples/USER/misc/drip/in.CH\_drip  
lammps-stable\_290ct2020/examples/USER/misc/drip/in.C\_drip  
lammps-stable\_290ct2020/examples/USER/misc/drip/log.30Apr19.CH\_drip.g++.1  
lammps-stable\_290ct2020/examples/USER/misc/drip/log.30Apr19.CH\_drip.g++.4  
lammps-stable\_290ct2020/examples/USER/misc/drip/log.30Apr19.C\_drip.g++.1  
lammps-stable\_290ct2020/examples/USER/misc/drip/log.30Apr19.C\_drip.g++.4  
lammps-stable\_290ct2020/examples/USER/misc/e3b/  
lammps-stable\_290ct2020/examples/USER/misc/e3b/README  
lammps-stable\_290ct2020/examples/USER/misc/e3b/e3b\_box.data  
lammps-stable\_290ct2020/examples/USER/misc/e3b/in.e3b-tip4p2005  
lammps-stable\_290ct2020/examples/USER/misc/e3b/log.29Mar2019.e3b-tip4p2005.  
g++.1  
lammps-stable\_290ct2020/examples/USER/misc/e3b/log.29Mar2019.e3b-tip4p2005.  
g++.4  
lammps-stable\_290ct2020/examples/USER/misc/edip/  
lammps-stable\_290ct2020/examples/USER/misc/edip/Si.edip  
lammps-stable\_290ct2020/examples/USER/misc/edip/SiC.edip  
lammps-stable\_290ct2020/examples/USER/misc/edip/data.SiC  
lammps-stable\_290ct2020/examples/USER/misc/edip/in.edip-Si  
lammps-stable\_290ct2020/examples/USER/misc/edip/in.edip-Si-multi  
lammps-stable\_290ct2020/examples/USER/misc/edip/in.edip-SiC  
lammps-stable\_290ct2020/examples/USER/misc/edip/log.4May2017.g++.edip-Si-mult  
i.1  
lammps-stable\_290ct2020/examples/USER/misc/edip/log.4May2017.g++.edip-Si-mult  
i.4  
lammps-stable\_290ct2020/examples/USER/misc/edip/log.4May2017.g++.edip-Si.1  
lammps-stable\_290ct2020/examples/USER/misc/edip/log.4May2017.g++.edip-Si.4  
lammps-stable\_290ct2020/examples/USER/misc/edip/log.4May2017.g++.edip-SiC.1  
lammps-stable\_290ct2020/examples/USER/misc/edip/log.4May2017.g++.edip-SiC.4  
lammps-stable\_290ct2020/examples/USER/misc/ees/  
lammps-stable\_290ct2020/examples/USER/misc/ees/Data\_region  
lammps-stable\_290ct2020/examples/USER/misc/ees/Data\_wall  
lammps-stable\_290ct2020/examples/USER/misc/ees/README  
lammps-stable\_290ct2020/examples/USER/misc/ees/in.fix\_wall  
lammps-stable\_290ct2020/examples/USER/misc/ees/in.fix\_wall\_region  
lammps-stable\_290ct2020/examples/USER/misc/ees/log.23Jun17.fix\_wall.g++.1  
lammps-stable\_290ct2020/examples/USER/misc/ees/log.23Jun17.fix\_wall.g++.4  
lammps-stable\_290ct2020/examples/USER/misc/ees/log.23Jun17.fix\_wall\_region.  
g++.1  
lammps-stable\_290ct2020/examples/USER/misc/ees/log.23Jun17.fix\_wall\_region.  
g++.4  
lammps-stable\_290ct2020/examples/USER/misc/electron\_stopping/  
lammps-stable\_290ct2020/examples/USER/misc/electron\_stopping/Si.Si.elstop  
lammps-stable\_290ct2020/examples/USER/misc/electron\_stopping/Si.sw  
lammps-stable\_290ct2020/examples/USER/misc/electron\_stopping/in.elstop  
lammps-stable\_290ct2020/examples/USER/misc/electron\_stopping/in.elstop.only  
lammps-stable\_290ct2020/examples/USER/misc/electron\_stopping/log.20Mar19.elst  
op.g++.1  
lammps-stable\_290ct2020/examples/USER/misc/electron\_stopping/log.20Mar19.elst  
op.g++.4  
lammps-stable\_290ct2020/examples/USER/misc/electron\_stopping/log.20Mar19.elst  
op.only.g++.1

lammps-stable\_290ct2020/examples/USER/misc/electron\_stopping/log.20Mar19.elst  
op.only.g++.4  
lammps-stable\_290ct2020/examples/USER/misc/entropy/  
lammps-stable\_290ct2020/examples/USER/misc/entropy/Na\_MendeleVM\_2014.eam.fs  
lammps-stable\_290ct2020/examples/USER/misc/entropy/data.interface  
lammps-stable\_290ct2020/examples/USER/misc/entropy/in.entropy  
lammps-stable\_290ct2020/examples/USER/misc/entropy/log.entropy  
lammps-stable\_290ct2020/examples/USER/misc/extep/  
lammps-stable\_290ct2020/examples/USER/misc/extep/BN.data  
lammps-stable\_290ct2020/examples/USER/misc/extep/in.extep-bn  
lammps-stable\_290ct2020/examples/USER/misc/extep/log.230ct17.extep-bn.g++.1  
lammps-stable\_290ct2020/examples/USER/misc/extep/log.230ct17.extep-bn.g++.4  
lammps-stable\_290ct2020/examples/USER/misc/filter\_corotate/  
lammps-stable\_290ct2020/examples/USER/misc/filter\_corotate/data.bpti  
lammps-stable\_290ct2020/examples/USER/misc/filter\_corotate/data.peptide  
lammps-stable\_290ct2020/examples/USER/misc/filter\_corotate/in.bpti  
lammps-stable\_290ct2020/examples/USER/misc/filter\_corotate/in.peptide  
lammps-stable\_290ct2020/examples/USER/misc/filter\_corotate/log.22Jun2017.bpt  
i.g++.1  
lammps-stable\_290ct2020/examples/USER/misc/filter\_corotate/log.22Jun2017.bpt  
i.g++.4  
lammps-stable\_290ct2020/examples/USER/misc/filter\_corotate/log.22Jun2017.pept  
ide.g++.1  
lammps-stable\_290ct2020/examples/USER/misc/filter\_corotate/log.22Jun2017.pept  
ide.g++.4  
lammps-stable\_290ct2020/examples/USER/misc/flow\_gauss/  
lammps-stable\_290ct2020/examples/USER/misc/flow\_gauss/README  
lammps-stable\_290ct2020/examples/USER/misc/flow\_gauss/in.GD  
lammps-stable\_290ct2020/examples/USER/misc/flow\_gauss/log.6Jul17.GD.g++.1  
lammps-stable\_290ct2020/examples/USER/misc/flow\_gauss/log.6Jul17.GD.g++.4  
lammps-stable\_290ct2020/examples/USER/misc/flow\_gauss/output-files/  
lammps-stable\_290ct2020/examples/USER/misc/flow\_gauss/output-files/GD.out  
lammps-stable\_290ct2020/examples/USER/misc/flow\_gauss/output-files/Vy\_profile  
lammps-stable\_290ct2020/examples/USER/misc/flow\_gauss/output-files/x\_profiles  
lammps-stable\_290ct2020/examples/USER/misc/gauss\_diel/  
lammps-stable\_290ct2020/examples/USER/misc/gauss\_diel/data.gauss-diel  
lammps-stable\_290ct2020/examples/USER/misc/gauss\_diel/in.gauss-diel  
lammps-stable\_290ct2020/examples/USER/misc/gauss\_diel/in.gauss-diel-cg  
lammps-stable\_290ct2020/examples/USER/misc/gauss\_diel/in.gauss-diel-split  
lammps-stable\_290ct2020/examples/USER/misc/gauss\_diel/log.gauss-diel  
lammps-stable\_290ct2020/examples/USER/misc/gauss\_diel/log.gauss-diel-cg  
lammps-stable\_290ct2020/examples/USER/misc/gauss\_diel/log.gauss-diel-split  
lammps-stable\_290ct2020/examples/USER/misc/gle/  
lammps-stable\_290ct2020/examples/USER/misc/gle/data.h2o-quantum  
lammps-stable\_290ct2020/examples/USER/misc/gle/data.h2o-smart  
lammps-stable\_290ct2020/examples/USER/misc/gle/in.h2o-quantum  
lammps-stable\_290ct2020/examples/USER/misc/gle/in.h2o-smart  
lammps-stable\_290ct2020/examples/USER/misc/gle/log.h2o-quantum  
lammps-stable\_290ct2020/examples/USER/misc/gle/log.h2o-smart  
lammps-stable\_290ct2020/examples/USER/misc/gle/qt-300k.A  
lammps-stable\_290ct2020/examples/USER/misc/gle/qt-300k.C  
lammps-stable\_290ct2020/examples/USER/misc/gle/smart.A  
lammps-stable\_290ct2020/examples/USER/misc/grem/  
lammps-stable\_290ct2020/examples/USER/misc/grem/README  
lammps-stable\_290ct2020/examples/USER/misc/grem/lj-6rep/  
lammps-stable\_290ct2020/examples/USER/misc/grem/lj-6rep/400/  
lammps-stable\_290ct2020/examples/USER/misc/grem/lj-6rep/400/restart.init  
lammps-stable\_290ct2020/examples/USER/misc/grem/lj-6rep/405/  
lammps-stable\_290ct2020/examples/USER/misc/grem/lj-6rep/405/restart.init  
lammps-stable\_290ct2020/examples/USER/misc/grem/lj-6rep/410/

```
lammps-stable_290ct2020/examples/USER/misc/grem/lj-6rep/410/restart.init
lammps-stable_290ct2020/examples/USER/misc/grem/lj-6rep/415/
lammps-stable_290ct2020/examples/USER/misc/grem/lj-6rep/415/restart.init
lammps-stable_290ct2020/examples/USER/misc/grem/lj-6rep/420/
lammps-stable_290ct2020/examples/USER/misc/grem/lj-6rep/420/restart.init
lammps-stable_290ct2020/examples/USER/misc/grem/lj-6rep/425/
lammps-stable_290ct2020/examples/USER/misc/grem/lj-6rep/425/restart.init
lammps-stable_290ct2020/examples/USER/misc/grem/lj-6rep/clean.sh
lammps-stable_290ct2020/examples/USER/misc/grem/lj-6rep/double-re-short.py
lammps-stable_290ct2020/examples/USER/misc/grem/lj-6rep/in.gREM
lammps-stable_290ct2020/examples/USER/misc/grem/lj-6rep/run.sh
lammps-stable_290ct2020/examples/USER/misc/grem/lj-6rep/walker.bkp
lammps-stable_290ct2020/examples/USER/misc/grem/lj-single/
lammps-stable_290ct2020/examples/USER/misc/grem/lj-single/in.gREM-npt
lammps-stable_290ct2020/examples/USER/misc/grem/lj-single/in.gREM-nvt
lammps-stable_290ct2020/examples/USER/misc/grem/lj-single/lj.data
lammps-stable_290ct2020/examples/USER/misc/grem/lj-single/log.gREM-npt.9Nov1
6.g++.1
lammps-stable_290ct2020/examples/USER/misc/grem/lj-single/log.gREM-npt.9Nov1
6.g++.4
lammps-stable_290ct2020/examples/USER/misc/grem/lj-single/log.gREM-nvt.9Nov1
6.g++.1
lammps-stable_290ct2020/examples/USER/misc/grem/lj-single/log.gREM-nvt.9Nov1
6.g++.4
lammps-stable_290ct2020/examples/USER/misc/grem/lj-temper/
lammps-stable_290ct2020/examples/USER/misc/grem/lj-temper/0/
lammps-stable_290ct2020/examples/USER/misc/grem/lj-temper/0/lj.data
lammps-stable_290ct2020/examples/USER/misc/grem/lj-temper/0/log.lammps.0
lammps-stable_290ct2020/examples/USER/misc/grem/lj-temper/1/
lammps-stable_290ct2020/examples/USER/misc/grem/lj-temper/1/lj.data
lammps-stable_290ct2020/examples/USER/misc/grem/lj-temper/1/log.lammps.1
lammps-stable_290ct2020/examples/USER/misc/grem/lj-temper/2/
lammps-stable_290ct2020/examples/USER/misc/grem/lj-temper/2/lj.data
lammps-stable_290ct2020/examples/USER/misc/grem/lj-temper/2/log.lammps.2
lammps-stable_290ct2020/examples/USER/misc/grem/lj-temper/3/
lammps-stable_290ct2020/examples/USER/misc/grem/lj-temper/3/lj.data
lammps-stable_290ct2020/examples/USER/misc/grem/lj-temper/3/log.lammps.3
lammps-stable_290ct2020/examples/USER/misc/grem/lj-temper/in.gREM-temper
lammps-stable_290ct2020/examples/USER/misc/hma/
lammps-stable_290ct2020/examples/USER/misc/hma/README
lammps-stable_290ct2020/examples/USER/misc/hma/hma.in
lammps-stable_290ct2020/examples/USER/misc/hma/log.6Nov18.hma.g++.1
lammps-stable_290ct2020/examples/USER/misc/hma/log.6Nov18.hma.g++.4
lammps-stable_290ct2020/examples/USER/misc/ilp_graphene_hbn/
lammps-stable_290ct2020/examples/USER/misc/ilp_graphene_hbn/BNC.tersoff
lammps-stable_290ct2020/examples/USER/misc/ilp_graphene_hbn/BNCH-old.ILP
lammps-stable_290ct2020/examples/USER/misc/ilp_graphene_hbn/Bi_gr_AB_stack_2L
_noH.data
lammps-stable_290ct2020/examples/USER/misc/ilp_graphene_hbn/gr_hBN_Cstack_2L
_noH.data
lammps-stable_290ct2020/examples/USER/misc/ilp_graphene_hbn/hBN_AA_prime_stac
k_2L_noH.data
lammps-stable_290ct2020/examples/USER/misc/ilp_graphene_hbn/hBN_AB_stack_2L_n
oH_equi_300K.data
lammps-stable_290ct2020/examples/USER/misc/ilp_graphene_hbn/in.bilayer-graphe
ne
lammps-stable_290ct2020/examples/USER/misc/ilp_graphene_hbn/in.bilayer-hBN
lammps-stable_290ct2020/examples/USER/misc/ilp_graphene_hbn/in.grhBN
lammps-stable_290ct2020/examples/USER/misc/ilp_graphene_hbn/in.ilp_graphene_h
bn
```

lammps-stable\_290ct2020/examples/USER/misc/ilp\_graphene\_hbn/log.31Jul19.bilayer-graphene.g++.1  
lammps-stable\_290ct2020/examples/USER/misc/ilp\_graphene\_hbn/log.31Jul19.bilayer-graphene.g++.4  
lammps-stable\_290ct2020/examples/USER/misc/ilp\_graphene\_hbn/log.31Jul19.bilayer-hBN.g++.1  
lammps-stable\_290ct2020/examples/USER/misc/ilp\_graphene\_hbn/log.31Jul19.bilayer-hBN.g++.4  
lammps-stable\_290ct2020/examples/USER/misc/ilp\_graphene\_hbn/log.31Jul19.grhBN.g++.1  
lammps-stable\_290ct2020/examples/USER/misc/ilp\_graphene\_hbn/log.31Jul19.grhBN.g++.4  
lammps-stable\_290ct2020/examples/USER/misc/ilp\_graphene\_hbn/log.31Jul19.ilp\_graphene\_hbn.g++.1  
lammps-stable\_290ct2020/examples/USER/misc/ilp\_graphene\_hbn/log.31Jul19.ilp\_graphene\_hbn.g++.4  
lammps-stable\_290ct2020/examples/USER/misc/imd/  
lammps-stable\_290ct2020/examples/USER/misc/imd/README  
lammps-stable\_290ct2020/examples/USER/misc/imd/bucky-plus-cnt-mol.psf  
lammps-stable\_290ct2020/examples/USER/misc/imd/bucky\_cnt\_imd.vmd  
lammps-stable\_290ct2020/examples/USER/misc/imd/data.bucky-plus-cnt  
lammps-stable\_290ct2020/examples/USER/misc/imd/data.deca-ala-solv  
lammps-stable\_290ct2020/examples/USER/misc/imd/deca-ala-solv.psf  
lammps-stable\_290ct2020/examples/USER/misc/imd/deca-ala-solv\_imd-demo.vmd  
lammps-stable\_290ct2020/examples/USER/misc/imd/deca-ala.psf  
lammps-stable\_290ct2020/examples/USER/misc/imd/deca-ala\_imd-demo.vmd  
lammps-stable\_290ct2020/examples/USER/misc/imd/falcon.tcl  
lammps-stable\_290ct2020/examples/USER/misc/imd/in.bucky-plus-cnt  
lammps-stable\_290ct2020/examples/USER/misc/imd/in.bucky-plus-cnt-gpu  
lammps-stable\_290ct2020/examples/USER/misc/imd/in.deca-ala-solv-filter\_imd  
lammps-stable\_290ct2020/examples/USER/misc/imd/in.deca-ala-solv\_imd  
lammps-stable\_290ct2020/examples/USER/misc/imd/in.deca-ala\_imd  
lammps-stable\_290ct2020/examples/USER/misc/imd/in.deca-ala\_imd-gpu  
lammps-stable\_290ct2020/examples/USER/misc/imd/in.melt\_imd  
lammps-stable\_290ct2020/examples/USER/misc/imd/in.melt\_imd-gpu  
lammps-stable\_290ct2020/examples/USER/misc/imd/melt.psf  
lammps-stable\_290ct2020/examples/USER/misc/imd/melt\_imd-demo.vmd  
lammps-stable\_290ct2020/examples/USER/misc/ipi/  
lammps-stable\_290ct2020/examples/USER/misc/ipi/C.opt.tersoff  
lammps-stable\_290ct2020/examples/USER/misc/ipi/README  
lammps-stable\_290ct2020/examples/USER/misc/ipi/data.graphene  
lammps-stable\_290ct2020/examples/USER/misc/ipi/i-pi\_input.xml  
lammps-stable\_290ct2020/examples/USER/misc/ipi/i-pi\_positions.xyz  
lammps-stable\_290ct2020/examples/USER/misc/ipi/in.graphene  
lammps-stable\_290ct2020/examples/USER/misc/kolmogorov\_crespi\_full/  
lammps-stable\_290ct2020/examples/USER/misc/kolmogorov\_crespi\_full/Bi\_gr\_AB\_stack\_2L\_noH.data  
lammps-stable\_290ct2020/examples/USER/misc/kolmogorov\_crespi\_full/Bi\_gr\_AB\_stack\_2L\_noH\_300K.data  
lammps-stable\_290ct2020/examples/USER/misc/kolmogorov\_crespi\_full/CC.KC-full  
lammps-stable\_290ct2020/examples/USER/misc/kolmogorov\_crespi\_full/CH.KC  
lammps-stable\_290ct2020/examples/USER/misc/kolmogorov\_crespi\_full/CH.rebo  
lammps-stable\_290ct2020/examples/USER/misc/kolmogorov\_crespi\_full/CH\_taper.KC  
lammps-stable\_290ct2020/examples/USER/misc/kolmogorov\_crespi\_full/in.bilayer-graphene  
lammps-stable\_290ct2020/examples/USER/misc/kolmogorov\_crespi\_full/log.5Jun19.bilayer-graphene.g++.1  
lammps-stable\_290ct2020/examples/USER/misc/kolmogorov\_crespi\_full/log.5Jun19.bilayer-graphene.g++.4  
lammps-stable\_290ct2020/examples/USER/misc/kolmogorov\_crespi\_full/log.5Jun19.

bilayer-graphene.icc.1  
lammps-stable\_290ct2020/examples/USER/misc/kolmogorov\_crespi\_full/log.5Jun19.  
bilayer-graphene.icc.4  
lammps-stable\_290ct2020/examples/USER/misc/kolmogorov\_crespi\_z/  
lammps-stable\_290ct2020/examples/USER/misc/kolmogorov\_crespi\_z/CC.KC  
lammps-stable\_290ct2020/examples/USER/misc/kolmogorov\_crespi\_z/CH.rebo  
lammps-stable\_290ct2020/examples/USER/misc/kolmogorov\_crespi\_z/data.bilayer-g  
raphene  
lammps-stable\_290ct2020/examples/USER/misc/kolmogorov\_crespi\_z/data.graphene-  
adsorbant  
lammps-stable\_290ct2020/examples/USER/misc/kolmogorov\_crespi\_z/in.atom-diffus  
ion  
lammps-stable\_290ct2020/examples/USER/misc/kolmogorov\_crespi\_z/in.bilayer-gra  
phene  
lammps-stable\_290ct2020/examples/USER/misc/kolmogorov\_crespi\_z/log.16Mar18.at  
om-diffusion.g++.1  
lammps-stable\_290ct2020/examples/USER/misc/kolmogorov\_crespi\_z/log.16Mar18.at  
om-diffusion.g++.4  
lammps-stable\_290ct2020/examples/USER/misc/kolmogorov\_crespi\_z/log.30Apr19.bi  
layer-graphene.g++.1  
lammps-stable\_290ct2020/examples/USER/misc/kolmogorov\_crespi\_z/log.30Apr19.bi  
layer-graphene.g++.4  
lammps-stable\_290ct2020/examples/USER/misc/lebedeva/  
lammps-stable\_290ct2020/examples/USER/misc/lebedeva/2particles.dat  
lammps-stable\_290ct2020/examples/USER/misc/lebedeva/2particles.in  
lammps-stable\_290ct2020/examples/USER/misc/lebedeva/CC.Lebedeva  
lammps-stable\_290ct2020/examples/USER/misc/lebedeva/LammpsResult.dat  
lammps-stable\_290ct2020/examples/USER/misc/lebedeva/LebDer.pl  
lammps-stable\_290ct2020/examples/USER/misc/lebedeva/lebedeva00.plot  
lammps-stable\_290ct2020/examples/USER/misc/local\_density/  
lammps-stable\_290ct2020/examples/USER/misc/local\_density/benzene\_water/  
lammps-stable\_290ct2020/examples/USER/misc/local\_density/benzene\_water/benzen  
e\_water.data  
lammps-stable\_290ct2020/examples/USER/misc/local\_density/benzene\_water/benzen  
e\_water.in  
lammps-stable\_290ct2020/examples/USER/misc/local\_density/benzene\_water/benzen  
e\_water.localdensity.table  
lammps-stable\_290ct2020/examples/USER/misc/local\_density/benzene\_water/benzen  
e\_water.pair.table  
lammps-stable\_290ct2020/examples/USER/misc/local\_density/benzene\_water/log.04  
Sep19.g++.1  
lammps-stable\_290ct2020/examples/USER/misc/local\_density/methanol\_implicit\_wa  
ter/  
lammps-stable\_290ct2020/examples/USER/misc/local\_density/methanol\_implicit\_wa  
ter/log.04Sep19.g++.1  
lammps-stable\_290ct2020/examples/USER/misc/local\_density/methanol\_implicit\_wa  
ter/methanol\_implicit\_water.data  
lammps-stable\_290ct2020/examples/USER/misc/local\_density/methanol\_implicit\_wa  
ter/methanol\_implicit\_water.in  
lammps-stable\_290ct2020/examples/USER/misc/local\_density/methanol\_implicit\_wa  
ter/methanol\_implicit\_water.localdensity.table  
lammps-stable\_290ct2020/examples/USER/misc/local\_density/methanol\_implicit\_wa  
ter/methanol\_implicit\_water.pair.table  
lammps-stable\_290ct2020/examples/USER/misc/meam\_spline/  
lammps-stable\_290ct2020/examples/USER/misc/meam\_spline/Si\_1.meam.spline  
lammps-stable\_290ct2020/examples/USER/misc/meam\_spline/Ti0.meam.spline  
lammps-stable\_290ct2020/examples/USER/misc/meam\_spline/in.meam-spline.Si  
lammps-stable\_290ct2020/examples/USER/misc/meam\_spline/in.meam-spline.Ti02  
lammps-stable\_290ct2020/examples/USER/misc/meam\_spline/log.4May2017.meam-spli  
ne.Si.g++.1

lammps-stable\_290ct2020/examples/USER/misc/meam\_spline/log.4May2017.meam-spline.Si.g++.4  
lammps-stable\_290ct2020/examples/USER/misc/meam\_spline/log.4May2017.meam-spline.TiO2.g++.1  
lammps-stable\_290ct2020/examples/USER/misc/meam\_spline/log.4May2017.meam-spline.TiO2.g++.4  
lammps-stable\_290ct2020/examples/USER/misc/meam\_sw\_spline/  
lammps-stable\_290ct2020/examples/USER/misc/meam\_sw\_spline/Si/  
lammps-stable\_290ct2020/examples/USER/misc/meam\_sw\_spline/Si/bcc.in  
lammps-stable\_290ct2020/examples/USER/misc/meam\_sw\_spline/Si/bcc\_relax.in  
lammps-stable\_290ct2020/examples/USER/misc/meam\_sw\_spline/Si/dc.in  
lammps-stable\_290ct2020/examples/USER/misc/meam\_sw\_spline/Si/dc\_relax.in  
lammps-stable\_290ct2020/examples/USER/misc/meam\_sw\_spline/Si/energy\_conservation.meam.sw.in  
lammps-stable\_290ct2020/examples/USER/misc/meam\_sw\_spline/Si/fcc.in  
lammps-stable\_290ct2020/examples/USER/misc/meam\_sw\_spline/Si/fcc\_relax.in  
lammps-stable\_290ct2020/examples/USER/misc/meam\_sw\_spline/Si/hcp\_relax.in  
lammps-stable\_290ct2020/examples/USER/misc/meam\_sw\_spline/Si/sc.in  
lammps-stable\_290ct2020/examples/USER/misc/meam\_sw\_spline/Si/sc\_relax.in  
lammps-stable\_290ct2020/examples/USER/misc/meam\_sw\_spline/Si/single\_atom.in  
lammps-stable\_290ct2020/examples/USER/misc/meam\_sw\_spline/Ti/  
lammps-stable\_290ct2020/examples/USER/misc/meam\_sw\_spline/Ti/alpha.in  
lammps-stable\_290ct2020/examples/USER/misc/meam\_sw\_spline/Ti/alpha\_relaxation.in  
lammps-stable\_290ct2020/examples/USER/misc/meam\_sw\_spline/Ti/beta.in  
lammps-stable\_290ct2020/examples/USER/misc/meam\_sw\_spline/Ti/energy\_conservation.meam.sw.in  
lammps-stable\_290ct2020/examples/USER/misc/meam\_sw\_spline/Ti/fcc.in  
lammps-stable\_290ct2020/examples/USER/misc/meam\_sw\_spline/Ti/hexagonal.in  
lammps-stable\_290ct2020/examples/USER/misc/meam\_sw\_spline/Ti/omega.in  
lammps-stable\_290ct2020/examples/USER/misc/meam\_sw\_spline/Ti/single\_atom.in  
lammps-stable\_290ct2020/examples/USER/misc/momb/  
lammps-stable\_290ct2020/examples/USER/misc/momb/Ag\_01X5.5\_02X0.55.eam.fs  
lammps-stable\_290ct2020/examples/USER/misc/momb/README  
lammps-stable\_290ct2020/examples/USER/misc/momb/in.system  
lammps-stable\_290ct2020/examples/USER/misc/momb/log.17Mar2017.system.g++.1  
lammps-stable\_290ct2020/examples/USER/misc/momb/log.17Mar2017.system.g++.4  
lammps-stable\_290ct2020/examples/USER/misc/momb/system.data  
lammps-stable\_290ct2020/examples/USER/misc/momentum/  
lammps-stable\_290ct2020/examples/USER/misc/momentum/in.momentum  
lammps-stable\_290ct2020/examples/USER/misc/mop/  
lammps-stable\_290ct2020/examples/USER/misc/mop/data.mop  
lammps-stable\_290ct2020/examples/USER/misc/mop/in.compute\_stress\_mop  
lammps-stable\_290ct2020/examples/USER/misc/mop/log.5Sep18.compute\_stress\_mop.g++.1  
lammps-stable\_290ct2020/examples/USER/misc/mop/log.5Sep18.compute\_stress\_mop.g++.4  
lammps-stable\_290ct2020/examples/USER/misc/mop/moppz.time.reference  
lammps-stable\_290ct2020/examples/USER/misc/mop/mopz0.time.reference  
lammps-stable\_290ct2020/examples/USER/misc/orient\_eco/  
lammps-stable\_290ct2020/examples/USER/misc/orient\_eco/Ni\_u3.eam  
lammps-stable\_290ct2020/examples/USER/misc/orient\_eco/data.sigma5  
lammps-stable\_290ct2020/examples/USER/misc/orient\_eco/in.orient\_eco  
lammps-stable\_290ct2020/examples/USER/misc/orient\_eco/log.2Jun2020.orient\_eco.g++.1  
lammps-stable\_290ct2020/examples/USER/misc/orient\_eco/log.2Jun2020.orient\_eco.g++.4  
lammps-stable\_290ct2020/examples/USER/misc/orient\_eco/sigma5.ori  
lammps-stable\_290ct2020/examples/USER/misc/pafi/  
lammps-stable\_290ct2020/examples/USER/misc/pafi/README

```
lammps-stable_290ct2020/examples/USER/misc/pafi/in.pafi
lammps-stable_290ct2020/examples/USER/misc/pafi/log.15Apr20.pafi.g++.1
lammps-stable_290ct2020/examples/USER/misc/pafi/log.15Apr20.pafi.g++.4
lammps-stable_290ct2020/examples/USER/misc/pafi/pafipath.4.data
lammps-stable_290ct2020/examples/USER/misc/pimd/
lammps-stable_290ct2020/examples/USER/misc/pimd/para-h2/
lammps-stable_290ct2020/examples/USER/misc/pimd/para-h2/H2.data
lammps-stable_290ct2020/examples/USER/misc/pimd/para-h2/H2.xyz
lammps-stable_290ct2020/examples/USER/misc/pimd/para-h2/NM.info
lammps-stable_290ct2020/examples/USER/misc/pimd/para-h2/in.scp
lammps-stable_290ct2020/examples/USER/misc/pimd/para-h2/pair.table
lammps-stable_290ct2020/examples/USER/misc/pimd/para-h2/run.sh
lammps-stable_290ct2020/examples/USER/misc/pimd/para-h2/vmd.src
lammps-stable_290ct2020/examples/USER/misc/pimd/prot-hairpin/
lammps-stable_290ct2020/examples/USER/misc/pimd/prot-hairpin/in.scp
lammps-stable_290ct2020/examples/USER/misc/pimd/prot-hairpin/run.sh
lammps-stable_290ct2020/examples/USER/misc/pimd/prot-hairpin/system.data
lammps-stable_290ct2020/examples/USER/misc/propel_self/
lammps-stable_290ct2020/examples/USER/misc/propel_self/2d_velocity/
lammps-stable_290ct2020/examples/USER/misc/propel_self/2d_velocity/in.2d_lang
evin
lammps-stable_290ct2020/examples/USER/misc/propel_self/2d_velocity/in.2d_visc
ous
lammps-stable_290ct2020/examples/USER/misc/propel_self/3d_quaternion/
lammps-stable_290ct2020/examples/USER/misc/propel_self/3d_quaternion/in.3d_qu
aternion
lammps-stable_290ct2020/examples/USER/misc/rhok/
lammps-stable_290ct2020/examples/USER/misc/rhok/README.md
lammps-stable_290ct2020/examples/USER/misc/rhok/in.crystal
lammps-stable_290ct2020/examples/USER/misc/rhok/in.pinning
lammps-stable_290ct2020/examples/USER/misc/rhok/in.setup
lammps-stable_290ct2020/examples/USER/misc/rhok/log.22Sep2017.crystal.g++.1
lammps-stable_290ct2020/examples/USER/misc/rhok/log.22Sep2017.crystal.g++.4
lammps-stable_290ct2020/examples/USER/misc/rhok/log.22Sep2017.pinning.g++.1
lammps-stable_290ct2020/examples/USER/misc/rhok/log.22Sep2017.pinning.g++.4
lammps-stable_290ct2020/examples/USER/misc/rhok/log.22Sep2017.setup.g++.1
lammps-stable_290ct2020/examples/USER/misc/rhok/log.22Sep2017.setup.g++.4
lammps-stable_290ct2020/examples/USER/misc/slater/
lammps-stable_290ct2020/examples/USER/misc/slater/data.after_equilibration
lammps-stable_290ct2020/examples/USER/misc/slater/data.after_production_run
lammps-stable_290ct2020/examples/USER/misc/slater/in.slater
lammps-stable_290ct2020/examples/USER/misc/slater/log.lammps
lammps-stable_290ct2020/examples/USER/misc/slater/tmp_1_1.rdf
lammps-stable_290ct2020/examples/USER/misc/slater/tmp_1_2.rdf
lammps-stable_290ct2020/examples/USER/misc/slater/tmp_1_3.rdf
lammps-stable_290ct2020/examples/USER/misc/slater/tmp_2_2.rdf
lammps-stable_290ct2020/examples/USER/misc/slater/tmp_2_3.rdf
lammps-stable_290ct2020/examples/USER/misc/slater/tmp_3_3.rdf
lammps-stable_290ct2020/examples/USER/misc/srp/
lammps-stable_290ct2020/examples/USER/misc/srp/data.chain
lammps-stable_290ct2020/examples/USER/misc/srp/in.srp
lammps-stable_290ct2020/examples/USER/misc/temper_npt/
lammps-stable_290ct2020/examples/USER/misc/temper_npt/data.peptide
lammps-stable_290ct2020/examples/USER/misc/temper_npt/in.temper_npt
lammps-stable_290ct2020/examples/USER/misc/temper_npt/log.temper_npt-17Aug17.
g++.8
lammps-stable_290ct2020/examples/USER/misc/temper_npt/log.temper_npt-17Aug17.
g++.8.0
lammps-stable_290ct2020/examples/USER/misc/temper_npt/log.temper_npt-17Aug17.
g++.8.1
```



```
lammps-stable_290ct2020/examples/USER/misc/temper_npt/log.temper_npt-17Aug17.
g++.8.2
lammps-stable_290ct2020/examples/USER/misc/temper_npt/log.temper_npt-17Aug17.
g++.8.3
lammps-stable_290ct2020/examples/USER/misc/temper_npt/log.temper_npt-17Aug17.
g++.8.4
lammps-stable_290ct2020/examples/USER/misc/temper_npt/log.temper_npt-17Aug17.
g++.8.5
lammps-stable_290ct2020/examples/USER/misc/temper_npt/log.temper_npt-17Aug17.
g++.8.6
lammps-stable_290ct2020/examples/USER/misc/temper_npt/log.temper_npt-17Aug17.
g++.8.7
lammps-stable_290ct2020/examples/USER/misc/ti/
lammps-stable_290ct2020/examples/USER/misc/ti/in.ti_spring
lammps-stable_290ct2020/examples/USER/mofff/
lammps-stable_290ct2020/examples/USER/mofff/hkust1.data
lammps-stable_290ct2020/examples/USER/mofff/in.hkust1
lammps-stable_290ct2020/examples/USER/mofff/in.hkust1_long
lammps-stable_290ct2020/examples/USER/mofff/log.27Nov18.hkust1.g++.1
lammps-stable_290ct2020/examples/USER/mofff/log.27Nov18.hkust1.g++.4
lammps-stable_290ct2020/examples/USER/mofff/log.27Nov18.hkust1_long.g++.1
lammps-stable_290ct2020/examples/USER/mofff/log.27Nov18.hkust1_long.g++.4
lammps-stable_290ct2020/examples/USER/phonon/
lammps-stable_290ct2020/examples/USER/phonon/1-1D-mono/
lammps-stable_290ct2020/examples/USER/phonon/1-1D-mono/README
lammps-stable_290ct2020/examples/USER/phonon/1-1D-mono/data.pos
lammps-stable_290ct2020/examples/USER/phonon/1-1D-mono/disp.dat
lammps-stable_290ct2020/examples/USER/phonon/1-1D-mono/in.Ana
lammps-stable_290ct2020/examples/USER/phonon/1-1D-mono/in.disp
lammps-stable_290ct2020/examples/USER/phonon/1-1D-mono/log.lammps
lammps-stable_290ct2020/examples/USER/phonon/1-1D-mono/map.in
lammps-stable_290ct2020/examples/USER/phonon/1-1D-mono/pdisp.eps
lammps-stable_290ct2020/examples/USER/phonon/1-1D-mono/pdisp.gnuplot
lammps-stable_290ct2020/examples/USER/phonon/1-1D-mono/phonon.bin.2000000
lammps-stable_290ct2020/examples/USER/phonon/1-1D-mono/phonon.log
lammps-stable_290ct2020/examples/USER/phonon/1-1D-mono/plot.disp
lammps-stable_290ct2020/examples/USER/phonon/2-1D-diatomic/
lammps-stable_290ct2020/examples/USER/phonon/2-1D-diatomic/README
lammps-stable_290ct2020/examples/USER/phonon/2-1D-diatomic/data.pos
lammps-stable_290ct2020/examples/USER/phonon/2-1D-diatomic/disp.dat
lammps-stable_290ct2020/examples/USER/phonon/2-1D-diatomic/in.Ana
lammps-stable_290ct2020/examples/USER/phonon/2-1D-diatomic/in.disp
lammps-stable_290ct2020/examples/USER/phonon/2-1D-diatomic/log.lammps
lammps-stable_290ct2020/examples/USER/phonon/2-1D-diatomic/map.in
lammps-stable_290ct2020/examples/USER/phonon/2-1D-diatomic/pdisp.eps
lammps-stable_290ct2020/examples/USER/phonon/2-1D-diatomic/pdisp.gnuplot
lammps-stable_290ct2020/examples/USER/phonon/2-1D-diatomic/phonon.bin.2000000
lammps-stable_290ct2020/examples/USER/phonon/2-1D-diatomic/phonon.log
lammps-stable_290ct2020/examples/USER/phonon/2-1D-diatomic/plot.disp
lammps-stable_290ct2020/examples/USER/phonon/3-3D-FCC-Cu-EAM/
lammps-stable_290ct2020/examples/USER/phonon/3-3D-FCC-Cu-EAM/CuPhonon.bin.650
0000
lammps-stable_290ct2020/examples/USER/phonon/3-3D-FCC-Cu-EAM/CuPhonon.log
lammps-stable_290ct2020/examples/USER/phonon/3-3D-FCC-Cu-EAM/README
lammps-stable_290ct2020/examples/USER/phonon/3-3D-FCC-Cu-EAM/cuu3.eam
lammps-stable_290ct2020/examples/USER/phonon/3-3D-FCC-Cu-EAM/data.pos
lammps-stable_290ct2020/examples/USER/phonon/3-3D-FCC-Cu-EAM/disp-expr.dat
lammps-stable_290ct2020/examples/USER/phonon/3-3D-FCC-Cu-EAM/disp-ld.dat
lammps-stable_290ct2020/examples/USER/phonon/3-3D-FCC-Cu-EAM/disp.dat
lammps-stable_290ct2020/examples/USER/phonon/3-3D-FCC-Cu-EAM/dos-expr.dat
```

```
lammps-stable_290ct2020/examples/USER/phonon/3-3D-FCC-Cu-EAM/dos-ld.dat
lammps-stable_290ct2020/examples/USER/phonon/3-3D-FCC-Cu-EAM/dos.dat
lammps-stable_290ct2020/examples/USER/phonon/3-3D-FCC-Cu-EAM/in.EAM3D
lammps-stable_290ct2020/examples/USER/phonon/3-3D-FCC-Cu-EAM/in.disp
lammps-stable_290ct2020/examples/USER/phonon/3-3D-FCC-Cu-EAM/in.disp2
lammps-stable_290ct2020/examples/USER/phonon/3-3D-FCC-Cu-EAM/in.dos
lammps-stable_290ct2020/examples/USER/phonon/3-3D-FCC-Cu-EAM/map.in
lammps-stable_290ct2020/examples/USER/phonon/3-3D-FCC-Cu-EAM/pdisp.eps
lammps-stable_290ct2020/examples/USER/phonon/3-3D-FCC-Cu-EAM/pdisp.gnuplot
lammps-stable_290ct2020/examples/USER/phonon/3-3D-FCC-Cu-EAM/pdos.eps
lammps-stable_290ct2020/examples/USER/phonon/3-3D-FCC-Cu-EAM/plot.disp
lammps-stable_290ct2020/examples/USER/phonon/3-3D-FCC-Cu-EAM/plot.dos
lammps-stable_290ct2020/examples/USER/phonon/4-Graphene/
lammps-stable_290ct2020/examples/USER/phonon/4-Graphene/Graphene.bin.6000000
lammps-stable_290ct2020/examples/USER/phonon/4-Graphene/Graphene.log
lammps-stable_290ct2020/examples/USER/phonon/4-Graphene/README
lammps-stable_290ct2020/examples/USER/phonon/4-Graphene/SiC.tersoff
lammps-stable_290ct2020/examples/USER/phonon/4-Graphene/data.pos
lammps-stable_290ct2020/examples/USER/phonon/4-Graphene/in.disp
lammps-stable_290ct2020/examples/USER/phonon/4-Graphene/in.graphene
lammps-stable_290ct2020/examples/USER/phonon/4-Graphene/map.in
lammps-stable_290ct2020/examples/USER/phonon/4-Graphene/pdisp.dat
lammps-stable_290ct2020/examples/USER/phonon/4-Graphene/pdisp.eps
lammps-stable_290ct2020/examples/USER/phonon/4-Graphene/pdisp.gnuplot
lammps-stable_290ct2020/examples/USER/phonon/4-Graphene/plot.disp
lammps-stable_290ct2020/examples/USER/phonon/dynamical_matrix_command/
lammps-stable_290ct2020/examples/USER/phonon/dynamical_matrix_command/Silicon
/
lammps-stable_290ct2020/examples/USER/phonon/dynamical_matrix_command/Silicon
/README.md
lammps-stable_290ct2020/examples/USER/phonon/dynamical_matrix_command/Silicon
/SiCGe.tersoff
lammps-stable_290ct2020/examples/USER/phonon/dynamical_matrix_command/Silicon
/ff-silicon.lmp
lammps-stable_290ct2020/examples/USER/phonon/dynamical_matrix_command/Silicon
/in.silicon
lammps-stable_290ct2020/examples/USER/phonon/dynamical_matrix_command/Silicon
/lmp_bank/
lammps-stable_290ct2020/examples/USER/phonon/dynamical_matrix_command/Silicon
/lmp_bank/amorphous_silicon.lmp
lammps-stable_290ct2020/examples/USER/phonon/dynamical_matrix_command/Silicon
/lmp_bank/silicon_216.lmp
lammps-stable_290ct2020/examples/USER/phonon/dynamical_matrix_command/Silicon
/lmp_bank/silicon_512.lmp
lammps-stable_290ct2020/examples/USER/phonon/dynamical_matrix_command/Silicon
/lmp_bank/silicon_8.lmp
lammps-stable_290ct2020/examples/USER/phonon/dynamical_matrix_command/Silicon
/results/
lammps-stable_290ct2020/examples/USER/phonon/dynamical_matrix_command/Silicon
/results/dynmat.dat
lammps-stable_290ct2020/examples/USER/phonon/dynamical_matrix_command/Silicon
/results/out.silicon
lammps-stable_290ct2020/examples/USER/phonon/dynamical_matrix_command/Silicon
/silicon_input_file.lmp
lammps-stable_290ct2020/examples/USER/phonon/dynamical_matrix_command/python/
lammps-stable_290ct2020/examples/USER/phonon/dynamical_matrix_command/python/
README.md
lammps-stable_290ct2020/examples/USER/phonon/dynamical_matrix_command/python/
SiCGe.tersoff
lammps-stable_290ct2020/examples/USER/phonon/dynamical_matrix_command/python/
```

```
dynmat.py
lammps-stable_290ct2020/examples/USER/phonon/dynamical_matrix_command/python/
ff-silicon.lmp
lammps-stable_290ct2020/examples/USER/phonon/dynamical_matrix_command/python/
results/
lammps-stable_290ct2020/examples/USER/phonon/dynamical_matrix_command/python/
results/dynmat.dat
lammps-stable_290ct2020/examples/USER/phonon/dynamical_matrix_command/python/
results/out.dynamt
lammps-stable_290ct2020/examples/USER/phonon/dynamical_matrix_command/python/
silicon_input_file.lmp
lammps-stable_290ct2020/examples/USER/plumed/
lammps-stable_290ct2020/examples/USER/plumed/data.peptide
lammps-stable_290ct2020/examples/USER/plumed/in.peptide-plumed
lammps-stable_290ct2020/examples/USER/plumed/log.4Feb20.peptide-plumed.g++.1
lammps-stable_290ct2020/examples/USER/plumed/log.4Feb20.peptide-plumed.g++.4
lammps-stable_290ct2020/examples/USER/plumed/plumed.dat
lammps-stable_290ct2020/examples/USER/plumed/reference/
lammps-stable_290ct2020/examples/USER/plumed/reference/colvar
lammps-stable_290ct2020/examples/USER/plumed/reference/p.log
lammps-stable_290ct2020/examples/USER/ptm/
lammps-stable_290ct2020/examples/USER/ptm/ptm_example.in
lammps-stable_290ct2020/examples/USER/qtb/
lammps-stable_290ct2020/examples/USER/qtb/README
lammps-stable_290ct2020/examples/USER/qtb/alpha_quartz_qbmsst/
lammps-stable_290ct2020/examples/USER/qtb/alpha_quartz_qbmsst/alpha_quartz_po
tential.mod
lammps-stable_290ct2020/examples/USER/qtb/alpha_quartz_qbmsst/alpha_quartz_qt
b.mod
lammps-stable_290ct2020/examples/USER/qtb/alpha_quartz_qbmsst/in.alpha_quartz
_qbmsst
lammps-stable_290ct2020/examples/USER/qtb/alpha_quartz_qbmsst/log.15Jun20.alp
ha_quartz_qbmsst.g++.1
lammps-stable_290ct2020/examples/USER/qtb/alpha_quartz_qbmsst/log.15Jun20.alp
ha_quartz_qbmsst.g++.4
lammps-stable_290ct2020/examples/USER/qtb/alpha_quartz_qbmsst/potential_SiO2.
TPF
lammps-stable_290ct2020/examples/USER/qtb/alpha_quartz_qtb/
lammps-stable_290ct2020/examples/USER/qtb/alpha_quartz_qtb/in.alpha_quartz_qt
b
lammps-stable_290ct2020/examples/USER/qtb/alpha_quartz_qtb/log.15Jun20.alpha_
quartz_qtb.g++.1
lammps-stable_290ct2020/examples/USER/qtb/alpha_quartz_qtb/log.15Jun20.alpha_
quartz_qtb.g++.4
lammps-stable_290ct2020/examples/USER/qtb/methane_qbmsst/
lammps-stable_290ct2020/examples/USER/qtb/methane_qbmsst/ffield.reax
lammps-stable_290ct2020/examples/USER/qtb/methane_qbmsst/methane_qbmsst.in
lammps-stable_290ct2020/examples/USER/qtb/methane_qbmsst/methane_qtb.mod
lammps-stable_290ct2020/examples/USER/qtb/methane_qtb/
lammps-stable_290ct2020/examples/USER/qtb/methane_qtb/ffield.reax
lammps-stable_290ct2020/examples/USER/qtb/methane_qtb/methane_qtb.in
lammps-stable_290ct2020/examples/USER/quip/
lammps-stable_290ct2020/examples/USER/quip/data_gap
lammps-stable_290ct2020/examples/USER/quip/data_sw
lammps-stable_290ct2020/examples/USER/quip/gap_example.xml
lammps-stable_290ct2020/examples/USER/quip/gap_example_sparse.dat
lammps-stable_290ct2020/examples/USER/quip/in.gap
lammps-stable_290ct2020/examples/USER/quip/in.molecular
lammps-stable_290ct2020/examples/USER/quip/in.sw
lammps-stable_290ct2020/examples/USER/quip/log.24Jul17.gap.g++.1
```

lammps-stable\_290ct2020/examples/USER/quip/log.24Jul17.gap.g++.4  
lammps-stable\_290ct2020/examples/USER/quip/log.24Jul17.molecular.g++.1  
lammps-stable\_290ct2020/examples/USER/quip/log.24Jul17.molecular.g++.4  
lammps-stable\_290ct2020/examples/USER/quip/log.24Jul17.sw.g++.1  
lammps-stable\_290ct2020/examples/USER/quip/log.24Jul17.sw.g++.4  
lammps-stable\_290ct2020/examples/USER/quip/methane-box-8.data  
lammps-stable\_290ct2020/examples/USER/quip/out.molecular  
lammps-stable\_290ct2020/examples/USER/quip/sw\_example.xml  
lammps-stable\_290ct2020/examples/USER/reaction/  
lammps-stable\_290ct2020/examples/USER/reaction/nylon,6-6\_melt/  
lammps-stable\_290ct2020/examples/USER/reaction/nylon,6-6\_melt/in.large\_nylon\_  
melt  
lammps-stable\_290ct2020/examples/USER/reaction/nylon,6-6\_melt/large\_nylon\_mel  
t.data.gz  
lammps-stable\_290ct2020/examples/USER/reaction/nylon,6-6\_melt/log.20Apr18.lar  
ge\_nylon\_melt.g++.1  
lammps-stable\_290ct2020/examples/USER/reaction/nylon,6-6\_melt/log.20Apr18.lar  
ge\_nylon\_melt.g++.4  
lammps-stable\_290ct2020/examples/USER/reaction/nylon,6-6\_melt/rxn1\_stp1\_map  
lammps-stable\_290ct2020/examples/USER/reaction/nylon,6-6\_melt/rxn1\_stp1\_react  
ed.data\_template  
lammps-stable\_290ct2020/examples/USER/reaction/nylon,6-6\_melt/rxn1\_stp1\_unrea  
cted.data\_template  
lammps-stable\_290ct2020/examples/USER/reaction/nylon,6-6\_melt/rxn1\_stp2\_map  
lammps-stable\_290ct2020/examples/USER/reaction/nylon,6-6\_melt/rxn1\_stp2\_react  
ed.data\_template  
lammps-stable\_290ct2020/examples/USER/reaction/nylon,6-6\_melt/rxn1\_stp2\_unrea  
cted.data\_template  
lammps-stable\_290ct2020/examples/USER/reaction/tiny\_epoxy/  
lammps-stable\_290ct2020/examples/USER/reaction/tiny\_epoxy/in.tiny\_epoxy.stabi  
lized  
lammps-stable\_290ct2020/examples/USER/reaction/tiny\_epoxy/log.20Nov19.tiny\_ep  
oxy.stabilized.g++.1  
lammps-stable\_290ct2020/examples/USER/reaction/tiny\_epoxy/log.20Nov19.tiny\_ep  
oxy.stabilized.g++.4  
lammps-stable\_290ct2020/examples/USER/reaction/tiny\_epoxy/rxn1\_stp1.map  
lammps-stable\_290ct2020/examples/USER/reaction/tiny\_epoxy/rxn1\_stp1\_post.data\_  
template  
lammps-stable\_290ct2020/examples/USER/reaction/tiny\_epoxy/rxn1\_stp1\_pre.data\_  
template  
lammps-stable\_290ct2020/examples/USER/reaction/tiny\_epoxy/rxn1\_stp2.map  
lammps-stable\_290ct2020/examples/USER/reaction/tiny\_epoxy/rxn1\_stp2\_post.data\_  
template  
lammps-stable\_290ct2020/examples/USER/reaction/tiny\_epoxy/rxn2\_stp1.map  
lammps-stable\_290ct2020/examples/USER/reaction/tiny\_epoxy/rxn2\_stp1\_post.data\_  
template  
lammps-stable\_290ct2020/examples/USER/reaction/tiny\_epoxy/rxn2\_stp1\_pre.data\_  
template  
lammps-stable\_290ct2020/examples/USER/reaction/tiny\_epoxy/rxn2\_stp2.map  
lammps-stable\_290ct2020/examples/USER/reaction/tiny\_epoxy/rxn2\_stp2\_post.data\_  
template  
lammps-stable\_290ct2020/examples/USER/reaction/tiny\_epoxy/tiny\_epoxy.data  
lammps-stable\_290ct2020/examples/USER/reaction/tiny\_nylon/  
lammps-stable\_290ct2020/examples/USER/reaction/tiny\_nylon/in.tiny\_nylon.stabi  
lized  
lammps-stable\_290ct2020/examples/USER/reaction/tiny\_nylon/in.tiny\_nylon.stabi  
lized\_variable\_probability  
lammps-stable\_290ct2020/examples/USER/reaction/tiny\_nylon/in.tiny\_nylon.unsta  
bilized  
lammps-stable\_290ct2020/examples/USER/reaction/tiny\_nylon/log.22Apr20.tiny\_ny

```
lon.stabilized_variable_probability.g++.1
lammps-stable_290ct2020/examples/USER/reaction/tiny_nylon/log.22Apr20.tiny_ny
lon.stabilized_variable_probability.g++.4
lammps-stable_290ct2020/examples/USER/reaction/tiny_nylon/log.5Jun19.tiny_nyl
on.stabilized.g++.1
lammps-stable_290ct2020/examples/USER/reaction/tiny_nylon/log.5Jun19.tiny_nyl
on.stabilized.g++.4
lammps-stable_290ct2020/examples/USER/reaction/tiny_nylon/log.5Jun19.tiny_nyl
on.unstabilized.g++.1
lammps-stable_290ct2020/examples/USER/reaction/tiny_nylon/log.5Jun19.tiny_nyl
on.unstabilized.g++.4
lammps-stable_290ct2020/examples/USER/reaction/tiny_nylon/rxn1_stp1_map
lammps-stable_290ct2020/examples/USER/reaction/tiny_nylon/rxn1_stp1_reacted.d
ata_template
lammps-stable_290ct2020/examples/USER/reaction/tiny_nylon/rxn1_stp1_unreacte
d.data_template
lammps-stable_290ct2020/examples/USER/reaction/tiny_nylon/rxn1_stp2_map
lammps-stable_290ct2020/examples/USER/reaction/tiny_nylon/rxn1_stp2_reacted.d
ata_template
lammps-stable_290ct2020/examples/USER/reaction/tiny_nylon/rxn1_stp2_unreacte
d.data_template
lammps-stable_290ct2020/examples/USER/reaction/tiny_nylon/tiny_nylon.data
lammps-stable_290ct2020/examples/USER/reaction/tiny_polystyrene/
lammps-stable_290ct2020/examples/USER/reaction/tiny_polystyrene/2styrene_map
lammps-stable_290ct2020/examples/USER/reaction/tiny_polystyrene/2styrene_reac
ted.data_template
lammps-stable_290ct2020/examples/USER/reaction/tiny_polystyrene/2styrene_unre
acted.data_template
lammps-stable_290ct2020/examples/USER/reaction/tiny_polystyrene/chain_chain_m
ap
lammps-stable_290ct2020/examples/USER/reaction/tiny_polystyrene/chain_chain_r
eacted.data_template
lammps-stable_290ct2020/examples/USER/reaction/tiny_polystyrene/chain_chain_u
nreacted.data_template
lammps-stable_290ct2020/examples/USER/reaction/tiny_polystyrene/chain_plus_st
yrene_map
lammps-stable_290ct2020/examples/USER/reaction/tiny_polystyrene/chain_plus_st
yrene_reacted.data_template
lammps-stable_290ct2020/examples/USER/reaction/tiny_polystyrene/chain_plus_st
yrene_unreacted.data_template
lammps-stable_290ct2020/examples/USER/reaction/tiny_polystyrene/in.tiny_polys
tyrene.stabilized
lammps-stable_290ct2020/examples/USER/reaction/tiny_polystyrene/log.20Nov19.t
iny_polystyrene.stabilized.g++.1
lammps-stable_290ct2020/examples/USER/reaction/tiny_polystyrene/log.20Nov19.t
iny_polystyrene.stabilized.g++.4
lammps-stable_290ct2020/examples/USER/reaction/tiny_polystyrene/tiny_polystyr
ene.data
lammps-stable_290ct2020/examples/USER/scafacos/
lammps-stable_290ct2020/examples/USER/scafacos/data.NaCl
lammps-stable_290ct2020/examples/USER/scafacos/data.cloud_wall
lammps-stable_290ct2020/examples/USER/scafacos/data.hammersley_sphere
lammps-stable_290ct2020/examples/USER/scafacos/in.scafacos
lammps-stable_290ct2020/examples/USER/scafacos/in.scafacos.cw.ewald
lammps-stable_290ct2020/examples/USER/scafacos/in.scafacos.cw.fmm
lammps-stable_290ct2020/examples/USER/scafacos/in.scafacos.cw.p2nfft
lammps-stable_290ct2020/examples/USER/scafacos/in.scafacos.cw.p3m
lammps-stable_290ct2020/examples/USER/scafacos/in.scafacos.ewald
lammps-stable_290ct2020/examples/USER/scafacos/in.scafacos.fmm
lammps-stable_290ct2020/examples/USER/scafacos/in.scafacos.hsph.direct
```

```
lammps-stable_290ct2020/examples/USER/scafacos/in.scafacos.hsph.fmm
lammps-stable_290ct2020/examples/USER/scafacos/in.scafacos.hsph.p2nfft
lammps-stable_290ct2020/examples/USER/scafacos/in.scafacos.p2nfft
lammps-stable_290ct2020/examples/USER/scafacos/in.scafacos.p3m
lammps-stable_290ct2020/examples/USER/scafacos/log.27Nov18.scafacos.cw.ewald.
g++.1
lammps-stable_290ct2020/examples/USER/scafacos/log.27Nov18.scafacos.cw.ewald.
g++.4
lammps-stable_290ct2020/examples/USER/scafacos/log.27Nov18.scafacos.cw.fmm.
g++.1
lammps-stable_290ct2020/examples/USER/scafacos/log.27Nov18.scafacos.cw.fmm.
g++.4
lammps-stable_290ct2020/examples/USER/scafacos/log.27Nov18.scafacos.cw.p2nff
t.g++.1
lammps-stable_290ct2020/examples/USER/scafacos/log.27Nov18.scafacos.cw.p2nff
t.g++.4
lammps-stable_290ct2020/examples/USER/scafacos/log.27Nov18.scafacos.cw.p3m.
g++.1
lammps-stable_290ct2020/examples/USER/scafacos/log.27Nov18.scafacos.cw.p3m.
g++.4
lammps-stable_290ct2020/examples/USER/scafacos/log.27Nov18.scafacos.ewald.
g++.1
lammps-stable_290ct2020/examples/USER/scafacos/log.27Nov18.scafacos.ewald.
g++.4
lammps-stable_290ct2020/examples/USER/scafacos/log.27Nov18.scafacos.fmm.g++.1
lammps-stable_290ct2020/examples/USER/scafacos/log.27Nov18.scafacos.fmm.g++.4
lammps-stable_290ct2020/examples/USER/scafacos/log.27Nov18.scafacos.g++.1
lammps-stable_290ct2020/examples/USER/scafacos/log.27Nov18.scafacos.g++.4
lammps-stable_290ct2020/examples/USER/scafacos/log.27Nov18.scafacos.hsph.dire
ct.g++.1
lammps-stable_290ct2020/examples/USER/scafacos/log.27Nov18.scafacos.hsph.dire
ct.g++.4
lammps-stable_290ct2020/examples/USER/scafacos/log.27Nov18.scafacos.hsph.fmm.
g++.1
lammps-stable_290ct2020/examples/USER/scafacos/log.27Nov18.scafacos.hsph.fmm.
g++.4
lammps-stable_290ct2020/examples/USER/scafacos/log.27Nov18.scafacos.hsph.p2nf
ft.g++.1
lammps-stable_290ct2020/examples/USER/scafacos/log.27Nov18.scafacos.hsph.p2nf
ft.g++.4
lammps-stable_290ct2020/examples/USER/scafacos/log.27Nov18.scafacos.p2nfft.
g++.1
lammps-stable_290ct2020/examples/USER/scafacos/log.27Nov18.scafacos.p2nfft.
g++.4
lammps-stable_290ct2020/examples/USER/scafacos/log.27Nov18.scafacos.p3m.g++.1
lammps-stable_290ct2020/examples/USER/scafacos/log.27Nov18.scafacos.p3m.g++.4
lammps-stable_290ct2020/examples/USER/sdpd/
lammps-stable_290ct2020/examples/USER/sdpd/2d-diffusion-in-shear-flow/
lammps-stable_290ct2020/examples/USER/sdpd/2d-diffusion-in-shear-flow/in.lamm
ps
lammps-stable_290ct2020/examples/USER/sdpd/2d-diffusion-in-shear-flow/log.240
ct18.2d-diffusion-in-shear-flow.g++.1
lammps-stable_290ct2020/examples/USER/sdpd/2d-diffusion-in-shear-flow/log.240
ct18.2d-diffusion-in-shear-flow.g++.4
lammps-stable_290ct2020/examples/USER/sdpd/2d-diffusion/
lammps-stable_290ct2020/examples/USER/sdpd/2d-diffusion/in.lammps
lammps-stable_290ct2020/examples/USER/sdpd/2d-diffusion/log.240ct18.2d-diffus
ion.g++.1
lammps-stable_290ct2020/examples/USER/sdpd/2d-diffusion/log.240ct18.2d-diffus
ion.g++.4
```

```
lammps-stable_290ct2020/examples/USER/sdpd/README
lammps-stable_290ct2020/examples/USER/sdpd/equipartition-verification/
lammps-stable_290ct2020/examples/USER/sdpd/equipartition-verification/in.lammps
lammps-stable_290ct2020/examples/USER/sdpd/equipartition-verification/log.240
ct18.equipartition.g++.1
lammps-stable_290ct2020/examples/USER/sdpd/equipartition-verification/log.240
ct18.equipartition.g++.4
lammps-stable_290ct2020/examples/USER/smd/
lammps-stable_290ct2020/examples/USER/smd/README
lammps-stable_290ct2020/examples/USER/smd/aluminum_strip_pull/
lammps-stable_290ct2020/examples/USER/smd/aluminum_strip_pull/in.aluminum_str
ip_pull
lammps-stable_290ct2020/examples/USER/smd/aluminum_strip_pull/log.90ct20.alum
inum_strip_pull.g++.1
lammps-stable_290ct2020/examples/USER/smd/aluminum_strip_pull/log.90ct20.alum
inum_strip_pull.g++.4
lammps-stable_290ct2020/examples/USER/smd/fluid_structure_interaction/
lammps-stable_290ct2020/examples/USER/smd/fluid_structure_interaction/in.flui
d_structure_interaction
lammps-stable_290ct2020/examples/USER/smd/fluid_structure_interaction/log.90c
t20.fluid_structure_interaction.g++.1
lammps-stable_290ct2020/examples/USER/smd/fluid_structure_interaction/log.90c
t20.fluid_structure_interaction.g++.4
lammps-stable_290ct2020/examples/USER/smd/funnel_flow/
lammps-stable_290ct2020/examples/USER/smd/funnel_flow/boundary.stl
lammps-stable_290ct2020/examples/USER/smd/funnel_flow/in.funnel_flow
lammps-stable_290ct2020/examples/USER/smd/funnel_flow/log.90ct20.funnel_flow.
g++.1
lammps-stable_290ct2020/examples/USER/smd/funnel_flow/log.90ct20.funnel_flow.
g++.4
lammps-stable_290ct2020/examples/USER/smd/rubber_rings_3d/
lammps-stable_290ct2020/examples/USER/smd/rubber_rings_3d/in.rubber_rings_3d
lammps-stable_290ct2020/examples/USER/smd/rubber_rings_3d/log.90ct20.rubber_r
ings_3d.g++.1
lammps-stable_290ct2020/examples/USER/smd/rubber_rings_3d/log.90ct20.rubber_r
ings_3d.g++.4
lammps-stable_290ct2020/examples/USER/smd/rubber_rings_3d/washer_hex_adjuste
d.data
lammps-stable_290ct2020/examples/USER/smd/rubber_strip_pull/
lammps-stable_290ct2020/examples/USER/smd/rubber_strip_pull/in.rubber_strip_p
ull
lammps-stable_290ct2020/examples/USER/smd/rubber_strip_pull/log.90ct20.rubber
_strip_pull.g++.1
lammps-stable_290ct2020/examples/USER/smd/rubber_strip_pull/log.90ct20.rubber
_strip_pull.g++.4
lammps-stable_290ct2020/examples/USER/smd/rubber_strip_pull/plot.gpl
lammps-stable_290ct2020/examples/USER/smtbq/
lammps-stable_290ct2020/examples/USER/smtbq/data.Alpha
lammps-stable_290ct2020/examples/USER/smtbq/ffield.smtbq.Al
lammps-stable_290ct2020/examples/USER/smtbq/ffield.smtbq.Al203
lammps-stable_290ct2020/examples/USER/smtbq/ffield.smtbq.Ti02
lammps-stable_290ct2020/examples/USER/smtbq/in.smtbq.Al
lammps-stable_290ct2020/examples/USER/smtbq/in.smtbq.Al203
lammps-stable_290ct2020/examples/USER/smtbq/in.smtbq.Ti02
lammps-stable_290ct2020/examples/USER/smtbq/log.smtbq.Al.g++.1
lammps-stable_290ct2020/examples/USER/smtbq/log.smtbq.Al.g++.4
lammps-stable_290ct2020/examples/USER/smtbq/log.smtbq.Al203.g++.1
lammps-stable_290ct2020/examples/USER/smtbq/log.smtbq.Al203.g++.4
lammps-stable_290ct2020/examples/USER/smtbq/log.smtbq.Ti02.g++.1
```

```
lammps-stable_290ct2020/examples/USER/smtbq/log.smtbq.TiO2.g++.4
lammps-stable_290ct2020/examples/USER/sph/
lammps-stable_290ct2020/examples/USER/sph/README
lammps-stable_290ct2020/examples/USER/sph/cavity_flow/
lammps-stable_290ct2020/examples/USER/sph/cavity_flow/cavity_flow.lmp
lammps-stable_290ct2020/examples/USER/sph/heatconduction/
lammps-stable_290ct2020/examples/USER/sph/heatconduction/compare_analytic.gpl
lammps-stable_290ct2020/examples/USER/sph/heatconduction/sph_heat_conduction_
2d.lmp
lammps-stable_290ct2020/examples/USER/sph/heatconduction/sph_heat_conduction_
3d.lmp
lammps-stable_290ct2020/examples/USER/sph/shock_tube/
lammps-stable_290ct2020/examples/USER/sph/shock_tube/compare_exact.gpl
lammps-stable_290ct2020/examples/USER/sph/shock_tube/exact_solution.dat
lammps-stable_290ct2020/examples/USER/sph/shock_tube/shock2d.lmp
lammps-stable_290ct2020/examples/USER/sph/shock_tube/shock3d.lmp
lammps-stable_290ct2020/examples/USER/sph/water_collapse/
lammps-stable_290ct2020/examples/USER/sph/water_collapse/data.initial
lammps-stable_290ct2020/examples/USER/sph/water_collapse/water_collapse.lmp
lammps-stable_290ct2020/examples/USER/tally/
lammps-stable_290ct2020/examples/USER/tally/README
lammps-stable_290ct2020/examples/USER/tally/data.spce
lammps-stable_290ct2020/examples/USER/tally/in.force
lammps-stable_290ct2020/examples/USER/tally/in.pe
lammps-stable_290ct2020/examples/USER/tally/in.stress
lammps-stable_290ct2020/examples/USER/tally/log.12Jun17.force.1
lammps-stable_290ct2020/examples/USER/tally/log.12Jun17.force.4
lammps-stable_290ct2020/examples/USER/tally/log.12Jun17.pe.1
lammps-stable_290ct2020/examples/USER/tally/log.12Jun17.pe.4
lammps-stable_290ct2020/examples/USER/tally/log.12Jun17.stress.1
lammps-stable_290ct2020/examples/USER/tally/log.12Jun17.stress.4
lammps-stable_290ct2020/examples/USER/uef/
lammps-stable_290ct2020/examples/USER/uef/README
lammps-stable_290ct2020/examples/USER/uef/npt_biaxial/
lammps-stable_290ct2020/examples/USER/uef/npt_biaxial/data.wca
lammps-stable_290ct2020/examples/USER/uef/npt_biaxial/in.npt_biaxial
lammps-stable_290ct2020/examples/USER/uef/npt_biaxial/log.27Nov18.npt_biaxia
l.g++.1
lammps-stable_290ct2020/examples/USER/uef/npt_biaxial/log.27Nov18.npt_biaxia
l.g++.4
lammps-stable_290ct2020/examples/USER/uef/nvt_uniaxial/
lammps-stable_290ct2020/examples/USER/uef/nvt_uniaxial/data.wca
lammps-stable_290ct2020/examples/USER/uef/nvt_uniaxial/in.nvt_uniaxial
lammps-stable_290ct2020/examples/USER/uef/nvt_uniaxial/log.27Nov18.nvt_uniaki
al.g++.1
lammps-stable_290ct2020/examples/USER/uef/nvt_uniaxial/log.27Nov18.nvt_uniaki
al.g++.4
lammps-stable_290ct2020/examples/USER/vtk/
lammps-stable_290ct2020/examples/USER/vtk/in.vtk
lammps-stable_290ct2020/examples/USER/vtk/in.vtp
lammps-stable_290ct2020/examples/USER/yaff/
lammps-stable_290ct2020/examples/USER/yaff/README
lammps-stable_290ct2020/examples/USER/yaff/mil53al/
lammps-stable_290ct2020/examples/USER/yaff/mil53al/lammps.data
lammps-stable_290ct2020/examples/USER/yaff/mil53al/lammps.in
lammps-stable_290ct2020/examples/USER/yaff/mof5/
lammps-stable_290ct2020/examples/USER/yaff/mof5/lammps.data
lammps-stable_290ct2020/examples/USER/yaff/mof5/lammps.in
lammps-stable_290ct2020/examples/VISCOSITY/
lammps-stable_290ct2020/examples/VISCOSITY/README
```



lammps-stable\_290ct2020/examples/VISCOSITY/data.cos.1000SPCE  
lammps-stable\_290ct2020/examples/VISCOSITY/in.cos.1000SPCE  
lammps-stable\_290ct2020/examples/VISCOSITY/in.einstein.2d  
lammps-stable\_290ct2020/examples/VISCOSITY/in.gk.2d  
lammps-stable\_290ct2020/examples/VISCOSITY/in.mp.2d  
lammps-stable\_290ct2020/examples/VISCOSITY/in.nemd.2d  
lammps-stable\_290ct2020/examples/VISCOSITY/in.wall.2d  
lammps-stable\_290ct2020/examples/VISCOSITY/log.130ct16.einstein.2d.g++.1  
lammps-stable\_290ct2020/examples/VISCOSITY/log.130ct16.gk.2d.g++.1  
lammps-stable\_290ct2020/examples/VISCOSITY/log.130ct16.mp.2d.g++.1  
lammps-stable\_290ct2020/examples/VISCOSITY/log.130ct16.nemd.2d.g++.1  
lammps-stable\_290ct2020/examples/VISCOSITY/log.130ct16.wall.2d.g++.1  
lammps-stable\_290ct2020/examples/VISCOSITY/log.30Apr20.cos.1000SPCE.g++.1  
lammps-stable\_290ct2020/examples/VISCOSITY/profile.130ct16.einstein.2d.g++.1  
lammps-stable\_290ct2020/examples/VISCOSITY/profile.130ct16.gk.2d.g++.1  
lammps-stable\_290ct2020/examples/VISCOSITY/profile.130ct16.mp.2d.g++.1  
lammps-stable\_290ct2020/examples/VISCOSITY/profile.130ct16.nemd.2d.g++.1  
lammps-stable\_290ct2020/examples/VISCOSITY/profile.130ct16.wall.2d.g++.1  
lammps-stable\_290ct2020/examples/airebo/  
lammps-stable\_290ct2020/examples/airebo/CH.airebo  
lammps-stable\_290ct2020/examples/airebo/CH.airebo-m  
lammps-stable\_290ct2020/examples/airebo/CH.rebo  
lammps-stable\_290ct2020/examples/airebo/data.airebo  
lammps-stable\_290ct2020/examples/airebo/in.airebo  
lammps-stable\_290ct2020/examples/airebo/in.airebo-0-0  
lammps-stable\_290ct2020/examples/airebo/in.airebo-m  
lammps-stable\_290ct2020/examples/airebo/in.rebo2  
lammps-stable\_290ct2020/examples/airebo/log.30Apr2019.airebo-0-0.g++.1  
lammps-stable\_290ct2020/examples/airebo/log.30Apr2019.airebo-0-0.g++.4  
lammps-stable\_290ct2020/examples/airebo/log.30Apr2019.airebo-m.g++.1  
lammps-stable\_290ct2020/examples/airebo/log.30Apr2019.airebo-m.g++.4  
lammps-stable\_290ct2020/examples/airebo/log.30Apr2019.airebo.g++.1  
lammps-stable\_290ct2020/examples/airebo/log.30Apr2019.airebo.g++.4  
lammps-stable\_290ct2020/examples/airebo/log.30Apr2019.rebo2.g++.1  
lammps-stable\_290ct2020/examples/airebo/log.30Apr2019.rebo2.g++.4  
lammps-stable\_290ct2020/examples/atm/  
lammps-stable\_290ct2020/examples/atm/in.atm  
lammps-stable\_290ct2020/examples/atm/log.27Nov18.atm.g++.1  
lammps-stable\_290ct2020/examples/atm/log.27Nov18.atm.g++.4  
lammps-stable\_290ct2020/examples/balance/  
lammps-stable\_290ct2020/examples/balance/in.balance  
lammps-stable\_290ct2020/examples/balance/in.balance.bond.fast  
lammps-stable\_290ct2020/examples/balance/in.balance.bond.slow  
lammps-stable\_290ct2020/examples/balance/in.balance.clock.dynamic  
lammps-stable\_290ct2020/examples/balance/in.balance.clock.static  
lammps-stable\_290ct2020/examples/balance/in.balance.group.dynamic  
lammps-stable\_290ct2020/examples/balance/in.balance.group.static  
lammps-stable\_290ct2020/examples/balance/in.balance.kspace  
lammps-stable\_290ct2020/examples/balance/in.balance.neigh.dynamic  
lammps-stable\_290ct2020/examples/balance/in.balance.neigh.rcb  
lammps-stable\_290ct2020/examples/balance/in.balance.neigh.static  
lammps-stable\_290ct2020/examples/balance/in.balance.var.dynamic  
lammps-stable\_290ct2020/examples/balance/log.27Nov18.balance.bond.fast.g++.2  
lammps-stable\_290ct2020/examples/balance/log.27Nov18.balance.bond.fast.g++.4  
lammps-stable\_290ct2020/examples/balance/log.27Nov18.balance.bond.slow.g++.2  
lammps-stable\_290ct2020/examples/balance/log.27Nov18.balance.bond.slow.g++.4  
lammps-stable\_290ct2020/examples/balance/log.27Nov18.balance.clock.dynamic.  
g++.2  
lammps-stable\_290ct2020/examples/balance/log.27Nov18.balance.clock.dynamic.  
g++.4

```
lammps-stable_290ct2020/examples/balance/log.27Nov18.balance.clock.static.  
g++.2  
lammps-stable_290ct2020/examples/balance/log.27Nov18.balance.clock.static.  
g++.4  
lammps-stable_290ct2020/examples/balance/log.27Nov18.balance.g++.2  
lammps-stable_290ct2020/examples/balance/log.27Nov18.balance.g++.4  
lammps-stable_290ct2020/examples/balance/log.27Nov18.balance.group.dynamic.  
g++.2  
lammps-stable_290ct2020/examples/balance/log.27Nov18.balance.group.dynamic.  
g++.4  
lammps-stable_290ct2020/examples/balance/log.27Nov18.balance.group.static.  
g++.2  
lammps-stable_290ct2020/examples/balance/log.27Nov18.balance.group.static.  
g++.4  
lammps-stable_290ct2020/examples/balance/log.27Nov18.balance.kspace.g++.2  
lammps-stable_290ct2020/examples/balance/log.27Nov18.balance.kspace.g++.4  
lammps-stable_290ct2020/examples/balance/log.27Nov18.balance.neigh.dynamic.  
g++.2  
lammps-stable_290ct2020/examples/balance/log.27Nov18.balance.neigh.dynamic.  
g++.4  
lammps-stable_290ct2020/examples/balance/log.27Nov18.balance.neigh.rcb.g++.2  
lammps-stable_290ct2020/examples/balance/log.27Nov18.balance.neigh.rcb.g++.4  
lammps-stable_290ct2020/examples/balance/log.27Nov18.balance.neigh.static.  
g++.2  
lammps-stable_290ct2020/examples/balance/log.27Nov18.balance.neigh.static.  
g++.4  
lammps-stable_290ct2020/examples/balance/log.27Nov18.balance.var.dynamic.g++.  
2  
lammps-stable_290ct2020/examples/balance/log.27Nov18.balance.var.dynamic.g++.  
4  
lammps-stable_290ct2020/examples/body/  
lammps-stable_290ct2020/examples/body/data.body  
lammps-stable_290ct2020/examples/body/data.cubes  
lammps-stable_290ct2020/examples/body/data.squares  
lammps-stable_290ct2020/examples/body/in.body  
lammps-stable_290ct2020/examples/body/in.cubes  
lammps-stable_290ct2020/examples/body/in.pour3d  
lammps-stable_290ct2020/examples/body/in.squares  
lammps-stable_290ct2020/examples/body/in.wall2d  
lammps-stable_290ct2020/examples/body/log.27Nov18.body.g++.1  
lammps-stable_290ct2020/examples/body/log.27Nov18.body.g++.4  
lammps-stable_290ct2020/examples/body/log.27Nov18.cubes.g++.1  
lammps-stable_290ct2020/examples/body/log.27Nov18.cubes.g++.4  
lammps-stable_290ct2020/examples/body/log.27Nov18.pour3d.g++.1  
lammps-stable_290ct2020/examples/body/log.27Nov18.pour3d.g++.4  
lammps-stable_290ct2020/examples/body/log.27Nov18.squares.g++.1  
lammps-stable_290ct2020/examples/body/log.27Nov18.squares.g++.4  
lammps-stable_290ct2020/examples/body/log.27Nov18.wall2d.g++.1  
lammps-stable_290ct2020/examples/body/log.27Nov18.wall2d.g++.4  
lammps-stable_290ct2020/examples/body/molecule.cube  
lammps-stable_290ct2020/examples/body/molecule.point3d  
lammps-stable_290ct2020/examples/body/molecule.rod3d  
lammps-stable_290ct2020/examples/body/molecule.tetra  
lammps-stable_290ct2020/examples/cmap/  
lammps-stable_290ct2020/examples/cmap/charmm22.cmap  
lammps-stable_290ct2020/examples/cmap/gagg.data  
lammps-stable_290ct2020/examples/cmap/in.cmap  
lammps-stable_290ct2020/examples/cmap/log.27Nov18.cmap.g++.1  
lammps-stable_290ct2020/examples/cmap/log.27Nov18.cmap.g++.4  
lammps-stable_290ct2020/examples/colloid/
```

```
lammps-stable_290ct2020/examples/colloid/in.colloid
lammps-stable_290ct2020/examples/colloid/log.27Nov18.colloid.g++.1
lammps-stable_290ct2020/examples/colloid/log.27Nov18.colloid.g++.4
lammps-stable_290ct2020/examples/comb/
lammps-stable_290ct2020/examples/comb/README
lammps-stable_290ct2020/examples/comb/data.Cu20
lammps-stable_290ct2020/examples/comb/data.CuS
lammps-stable_290ct2020/examples/comb/data.c-Hf02
lammps-stable_290ct2020/examples/comb/data.comb3-0HCCu
lammps-stable_290ct2020/examples/comb/data.m-Hf02
lammps-stable_290ct2020/examples/comb/data.t-Hf02
lammps-stable_290ct2020/examples/comb/elastic.f90
lammps-stable_290ct2020/examples/comb/ffield.comb
lammps-stable_290ct2020/examples/comb/ffield.comb3
lammps-stable_290ct2020/examples/comb/in.comb.Cu
lammps-stable_290ct2020/examples/comb/in.comb.Cu20.elastic
lammps-stable_290ct2020/examples/comb/in.comb.Hf02
lammps-stable_290ct2020/examples/comb/in.comb.Si
lammps-stable_290ct2020/examples/comb/in.comb.Si.elastic
lammps-stable_290ct2020/examples/comb/in.comb3
lammps-stable_290ct2020/examples/comb/lib.comb3
lammps-stable_290ct2020/examples/comb/log.27Nov18.comb.Cu.g++.1
lammps-stable_290ct2020/examples/comb/log.27Nov18.comb.Cu.g++.4
lammps-stable_290ct2020/examples/comb/log.27Nov18.comb.Cu20.elastic.g++.1
lammps-stable_290ct2020/examples/comb/log.27Nov18.comb.Cu20.elastic.g++.4
lammps-stable_290ct2020/examples/comb/log.27Nov18.comb.Hf02.g++.1
lammps-stable_290ct2020/examples/comb/log.27Nov18.comb.Hf02.g++.4
lammps-stable_290ct2020/examples/comb/log.27Nov18.comb.Si.elastic.g++.1
lammps-stable_290ct2020/examples/comb/log.27Nov18.comb.Si.elastic.g++.4
lammps-stable_290ct2020/examples/comb/log.27Nov18.comb.Si.g++.1
lammps-stable_290ct2020/examples/comb/log.27Nov18.comb.Si.g++.4
lammps-stable_290ct2020/examples/comb/log.27Nov18.comb3.g++.1
lammps-stable_290ct2020/examples/comb/log.27Nov18.comb3.g++.4
lammps-stable_290ct2020/examples/controller/
lammps-stable_290ct2020/examples/controller/in.controller.temp
lammps-stable_290ct2020/examples/controller/in.controller.wall
lammps-stable_290ct2020/examples/controller/log.27Nov18.controller.temp.g++.1
lammps-stable_290ct2020/examples/controller/log.27Nov18.controller.temp.g++.4
lammps-stable_290ct2020/examples/controller/log.27Nov18.controller.wall.g++.1
lammps-stable_290ct2020/examples/controller/log.27Nov18.controller.wall.g++.2
lammps-stable_290ct2020/examples/coreshell/
lammps-stable_290ct2020/examples/coreshell/data.coreshell
lammps-stable_290ct2020/examples/coreshell/in.coreshell
lammps-stable_290ct2020/examples/coreshell/in.coreshell.dsf
lammps-stable_290ct2020/examples/coreshell/in.coreshell.thermostats
lammps-stable_290ct2020/examples/coreshell/in.coreshell.wolf
lammps-stable_290ct2020/examples/coreshell/log.27Nov18.coreshell.dsf.g++.1
lammps-stable_290ct2020/examples/coreshell/log.27Nov18.coreshell.dsf.g++.4
lammps-stable_290ct2020/examples/coreshell/log.27Nov18.coreshell.g++.1
lammps-stable_290ct2020/examples/coreshell/log.27Nov18.coreshell.g++.4
lammps-stable_290ct2020/examples/coreshell/log.27Nov18.coreshell.thermostats.g++.1
lammps-stable_290ct2020/examples/coreshell/log.27Nov18.coreshell.thermostats.g++.4
lammps-stable_290ct2020/examples/coreshell/log.27Nov18.coreshell.wolf.g++.1
lammps-stable_290ct2020/examples/coreshell/log.27Nov18.coreshell.wolf.g++.4
lammps-stable_290ct2020/examples/crack/
lammps-stable_290ct2020/examples/crack/in.crack
lammps-stable_290ct2020/examples/crack/log.27Nov18.crack.g++.1
lammps-stable_290ct2020/examples/crack/log.27Nov18.crack.g++.4
```

lammps-stable\_290ct2020/examples/deposit/  
lammps-stable\_290ct2020/examples/deposit/in.deposit.atom  
lammps-stable\_290ct2020/examples/deposit/in.deposit.molecule  
lammps-stable\_290ct2020/examples/deposit/in.deposit.molecule.shake  
lammps-stable\_290ct2020/examples/deposit/log.27Nov18.deposit.atom.g++.1  
lammps-stable\_290ct2020/examples/deposit/log.27Nov18.deposit.atom.g++.4  
lammps-stable\_290ct2020/examples/deposit/log.27Nov18.deposit.molecule.g++.1  
lammps-stable\_290ct2020/examples/deposit/log.27Nov18.deposit.molecule.g++.4  
lammps-stable\_290ct2020/examples/deposit/log.27Nov18.deposit.molecule.shake.g++.1  
lammps-stable\_290ct2020/examples/deposit/log.27Nov18.deposit.molecule.shake.g++.4  
lammps-stable\_290ct2020/examples/deposit/molecule.dimer  
lammps-stable\_290ct2020/examples/deposit/molecule.dimer.shake  
lammps-stable\_290ct2020/examples/dipole/  
lammps-stable\_290ct2020/examples/dipole/in.dipole  
lammps-stable\_290ct2020/examples/dipole/log.27Nov18.dipole.g++.1  
lammps-stable\_290ct2020/examples/dipole/log.27Nov18.dipole.g++.4  
lammps-stable\_290ct2020/examples/dreiding/  
lammps-stable\_290ct2020/examples/dreiding/README  
lammps-stable\_290ct2020/examples/dreiding/ch3oh.box.dreiding.bgf  
lammps-stable\_290ct2020/examples/dreiding/ch3oh.box.dreiding.cerius2.eng.dat  
lammps-stable\_290ct2020/examples/dreiding/data.dreiding  
lammps-stable\_290ct2020/examples/dreiding/in.dreiding  
lammps-stable\_290ct2020/examples/dreiding/log.27Nov18.dreiding.g++.1  
lammps-stable\_290ct2020/examples/dreiding/log.27Nov18.dreiding.g++.4  
lammps-stable\_290ct2020/examples/eim/  
lammps-stable\_290ct2020/examples/eim/data.eim  
lammps-stable\_290ct2020/examples/eim/ffield.eim  
lammps-stable\_290ct2020/examples/eim/in.eim  
lammps-stable\_290ct2020/examples/eim/log.27Nov18.eim.g++.1  
lammps-stable\_290ct2020/examples/eim/log.27Nov18.eim.g++.4  
lammps-stable\_290ct2020/examples/ellipse/  
lammps-stable\_290ct2020/examples/ellipse/in.ellipse.gayberne  
lammps-stable\_290ct2020/examples/ellipse/in.ellipse.resquared  
lammps-stable\_290ct2020/examples/ellipse/log.27Nov18.ellipse.gayberne.g++.1  
lammps-stable\_290ct2020/examples/ellipse/log.27Nov18.ellipse.gayberne.g++.4  
lammps-stable\_290ct2020/examples/ellipse/log.27Nov18.ellipse.resquared.g++.1  
lammps-stable\_290ct2020/examples/ellipse/log.27Nov18.ellipse.resquared.g++.4  
lammps-stable\_290ct2020/examples/fire/  
lammps-stable\_290ct2020/examples/fire/README  
lammps-stable\_290ct2020/examples/fire/Si.sw  
lammps-stable\_290ct2020/examples/fire/final.sivac  
lammps-stable\_290ct2020/examples/fire/in.cg  
lammps-stable\_290ct2020/examples/fire/in.fire  
lammps-stable\_290ct2020/examples/fire/in.fire\_mod  
lammps-stable\_290ct2020/examples/fire/in.fire\_mod\_old  
lammps-stable\_290ct2020/examples/fire/in.fire\_old  
lammps-stable\_290ct2020/examples/fire/in.neb.sivac.fire  
lammps-stable\_290ct2020/examples/fire/in.neb.sivac.fire\_mod  
lammps-stable\_290ct2020/examples/fire/in.neb.sivac.fire\_mod\_old  
lammps-stable\_290ct2020/examples/fire/in.neb.sivac.fire\_old  
lammps-stable\_290ct2020/examples/fire/in.neb.sivac.qm  
lammps-stable\_290ct2020/examples/fire/initial.sivac  
lammps-stable\_290ct2020/examples/fire/log.09Janv20.cg.g++.1  
lammps-stable\_290ct2020/examples/fire/log.09Janv20.fire.g++.1  
lammps-stable\_290ct2020/examples/fire/log.09Janv20.fire\_mod.g++.1  
lammps-stable\_290ct2020/examples/fire/log.09Janv20.fire\_mod\_old.g++.1  
lammps-stable\_290ct2020/examples/fire/log.09Janv20.fire\_old.g++.1  
lammps-stable\_290ct2020/examples/fire/log.09Janv20.neb.fire.g++.4

```
lammps-stable_290ct2020/examples/fire/log.09Janv20.neb.fire.g++.8
lammps-stable_290ct2020/examples/fire/log.09Janv20.neb.fire_mod.g++.4
lammps-stable_290ct2020/examples/fire/log.09Janv20.neb.fire_mod.g++.8
lammps-stable_290ct2020/examples/fire/log.09Janv20.neb.fire_mod_old.g++.4
lammps-stable_290ct2020/examples/fire/log.09Janv20.neb.fire_mod_old.g++.8
lammps-stable_290ct2020/examples/fire/log.09Janv20.neb.fire_old.g++.4
lammps-stable_290ct2020/examples/fire/log.09Janv20.neb.fire_old.g++.8
lammps-stable_290ct2020/examples/fire/log.09Janv20.neb.qm.g++.4
lammps-stable_290ct2020/examples/fire/log.09Janv20.neb.qm.g++.8
lammps-stable_290ct2020/examples/flow/
lammps-stable_290ct2020/examples/flow/in.flow.couette
lammps-stable_290ct2020/examples/flow/in.flow.pois
lammps-stable_290ct2020/examples/flow/log.27Nov18.flow.couette.g++.1
lammps-stable_290ct2020/examples/flow/log.27Nov18.flow.couette.g++.4
lammps-stable_290ct2020/examples/flow/log.27Nov18.flow.pois.g++.1
lammps-stable_290ct2020/examples/flow/log.27Nov18.flow.pois.g++.4
lammps-stable_290ct2020/examples/friction/
lammps-stable_290ct2020/examples/friction/in.friction
lammps-stable_290ct2020/examples/friction/log.27Nov18.friction.g++.1
lammps-stable_290ct2020/examples/friction/log.27Nov18.friction.g++.4
lammps-stable_290ct2020/examples/gcmc/
lammps-stable_290ct2020/examples/gcmc/CO2.txt
lammps-stable_290ct2020/examples/gcmc/H2O.txt
lammps-stable_290ct2020/examples/gcmc/data.spce
lammps-stable_290ct2020/examples/gcmc/data.widom.lj
lammps-stable_290ct2020/examples/gcmc/in.gcmc.co2
lammps-stable_290ct2020/examples/gcmc/in.gcmc.h2o
lammps-stable_290ct2020/examples/gcmc/in.gcmc.lj
lammps-stable_290ct2020/examples/gcmc/in.widom.lj
lammps-stable_290ct2020/examples/gcmc/in.widom.spce
lammps-stable_290ct2020/examples/gcmc/log.27Nov18.gcmc.co2.g++.1
lammps-stable_290ct2020/examples/gcmc/log.27Nov18.gcmc.h2o.g++.1
lammps-stable_290ct2020/examples/gcmc/log.27Nov18.gcmc.lj.g++.1
lammps-stable_290ct2020/examples/gcmc/log.27Nov18.gcmc.lj.g++.4
lammps-stable_290ct2020/examples/gcmc/log.30Jun20.widom.lj.g++.1
lammps-stable_290ct2020/examples/gcmc/log.30Jun20.widom.lj.g++.4
lammps-stable_290ct2020/examples/gcmc/log.30Jun20.widom.spce.g++.1
lammps-stable_290ct2020/examples/gjff/
lammps-stable_290ct2020/examples/gjff/README.md
lammps-stable_290ct2020/examples/gjff/argon.lmp
lammps-stable_290ct2020/examples/gjff/ff-argon.lmp
lammps-stable_290ct2020/examples/gjff/in.gjff.vfull
lammps-stable_290ct2020/examples/gjff/in.gjff.vhalf
lammps-stable_290ct2020/examples/gjff/log.150ct19.gjff.vfull.g++.1
lammps-stable_290ct2020/examples/gjff/log.150ct19.gjff.vfull.g++.4
lammps-stable_290ct2020/examples/gjff/log.150ct19.gjff.vhalf.g++.1
lammps-stable_290ct2020/examples/gjff/log.150ct19.gjff.vhalf.g++.4
lammps-stable_290ct2020/examples/granregion/
lammps-stable_290ct2020/examples/granregion/in.granregion.box
lammps-stable_290ct2020/examples/granregion/in.granregion.funnel
lammps-stable_290ct2020/examples/granregion/in.granregion.mixer
lammps-stable_290ct2020/examples/granregion/log.27Nov18.granregion.box.g++.1
lammps-stable_290ct2020/examples/granregion/log.27Nov18.granregion.box.g++.4
lammps-stable_290ct2020/examples/granregion/log.27Nov18.granregion.funnel.
g++.1
lammps-stable_290ct2020/examples/granregion/log.27Nov18.granregion.funnel.
g++.4
lammps-stable_290ct2020/examples/granregion/log.27Nov18.granregion.mixer.g++.
1
lammps-stable_290ct2020/examples/granregion/log.27Nov18.granregion.mixer.g++.
```

4

lammps-stable\_290ct2020/examples/granular/  
lammps-stable\_290ct2020/examples/granular/in.pour.drum  
lammps-stable\_290ct2020/examples/granular/in.pour.flatwall  
lammps-stable\_290ct2020/examples/granular/log.29Mar19.pour.drum.g++.1  
lammps-stable\_290ct2020/examples/granular/log.29Mar19.pour.drum.g++.4  
lammps-stable\_290ct2020/examples/granular/log.29Mar19.pour.flatwall.g++.1  
lammps-stable\_290ct2020/examples/granular/log.29Mar19.pour.flatwall.g++.4  
lammps-stable\_290ct2020/examples/hugoniostat/  
lammps-stable\_290ct2020/examples/hugoniostat/in.hugoniostat  
lammps-stable\_290ct2020/examples/hugoniostat/log.27Nov18.hugoniostat.g++.1  
lammps-stable\_290ct2020/examples/hugoniostat/log.27Nov18.hugoniostat.g++.4  
lammps-stable\_290ct2020/examples/hugoniostat/log.50ct16.hugoniostat.g++.1  
lammps-stable\_290ct2020/examples/hugoniostat/log.50ct16.hugoniostat.g++.4  
lammps-stable\_290ct2020/examples/hyper/  
lammps-stable\_290ct2020/examples/hyper/adatoms.list.50  
lammps-stable\_290ct2020/examples/hyper/global.000000.jpg  
lammps-stable\_290ct2020/examples/hyper/global.041000.jpg  
lammps-stable\_290ct2020/examples/hyper/global.045000.jpg  
lammps-stable\_290ct2020/examples/hyper/global.048000.jpg  
lammps-stable\_290ct2020/examples/hyper/global.089000.jpg  
lammps-stable\_290ct2020/examples/hyper/in.hyper.global  
lammps-stable\_290ct2020/examples/hyper/in.hyper.local  
lammps-stable\_290ct2020/examples/hyper/local.000000.jpg  
lammps-stable\_290ct2020/examples/hyper/local.000400.jpg  
lammps-stable\_290ct2020/examples/hyper/local.001300.jpg  
lammps-stable\_290ct2020/examples/hyper/log.2Jun2020.hyper.global.g++.4  
lammps-stable\_290ct2020/examples/hyper/log.2Jun2020.hyper.local.g++.4  
lammps-stable\_290ct2020/examples/hyper/ptvoterlammps.eam  
lammps-stable\_290ct2020/examples/indent/  
lammps-stable\_290ct2020/examples/indent/in.indent  
lammps-stable\_290ct2020/examples/indent/in.indent.min  
lammps-stable\_290ct2020/examples/indent/log.27Nov18.indent.g++.1  
lammps-stable\_290ct2020/examples/indent/log.27Nov18.indent.g++.4  
lammps-stable\_290ct2020/examples/indent/log.27Nov18.indent.min.g++.1  
lammps-stable\_290ct2020/examples/indent/log.27Nov18.indent.min.g++.4  
lammps-stable\_290ct2020/examples/kim/  
lammps-stable\_290ct2020/examples/kim/in.kim-ex.melt  
lammps-stable\_290ct2020/examples/kim/in.kim-pm-property  
lammps-stable\_290ct2020/examples/kim/in.kim-pm-query.melt  
lammps-stable\_290ct2020/examples/kim/in.kim-pm.melt  
lammps-stable\_290ct2020/examples/kim/in.kim-sm.melt  
lammps-stable\_290ct2020/examples/kim/in.lammps.melt  
lammps-stable\_290ct2020/examples/kim/log.7Aug19.in.kim-ex.melt.clang.1  
lammps-stable\_290ct2020/examples/kim/log.7Aug19.in.kim-ex.melt.clang.4  
lammps-stable\_290ct2020/examples/kim/log.7Aug19.in.kim-pm-query.melt.clang.1  
lammps-stable\_290ct2020/examples/kim/log.7Aug19.in.kim-pm-query.melt.clang.4  
lammps-stable\_290ct2020/examples/kim/log.7Aug19.in.kim-pm.melt.clang.1  
lammps-stable\_290ct2020/examples/kim/log.7Aug19.in.kim-pm.melt.clang.4  
lammps-stable\_290ct2020/examples/kim/log.7Aug19.in.kim-sm.melt.clang.1  
lammps-stable\_290ct2020/examples/kim/log.7Aug19.in.kim-sm.melt.clang.4  
lammps-stable\_290ct2020/examples/kim/log.7Aug19.in.lammps.melt.clang.1  
lammps-stable\_290ct2020/examples/kim/log.7Aug19.in.lammps.melt.clang.4  
lammps-stable\_290ct2020/examples/latte/  
lammps-stable\_290ct2020/examples/latte/TBparam/  
lammps-stable\_290ct2020/examples/latte/TBparam/bondints.nonortho  
lammps-stable\_290ct2020/examples/latte/TBparam/electrons.dat  
lammps-stable\_290ct2020/examples/latte/TBparam/ppots.nonortho  
lammps-stable\_290ct2020/examples/latte/data.ch4  
lammps-stable\_290ct2020/examples/latte/data.graphene

```
lammps-stable_290ct2020/examples/latte/data.sucrose
lammps-stable_290ct2020/examples/latte/data.water
lammps-stable_290ct2020/examples/latte/in.graphene.boxrel
lammps-stable_290ct2020/examples/latte/in.latte.multiple
lammps-stable_290ct2020/examples/latte/in.latte.sucrose
lammps-stable_290ct2020/examples/latte/in.latte.sucrose.md
lammps-stable_290ct2020/examples/latte/in.latte.water
lammps-stable_290ct2020/examples/latte/in.latte.water.md
lammps-stable_290ct2020/examples/latte/in.latte.water.min
lammps-stable_290ct2020/examples/latte/latte.in
lammps-stable_290ct2020/examples/latte/log.19Sep17.latte.sucrose.md.g++.1
lammps-stable_290ct2020/examples/latte/log.19Sep17.latte.water.md.g++.1
lammps-stable_290ct2020/examples/latte/log.21Jun18.latte.graphene.boxrelax.
g++.1
lammps-stable_290ct2020/examples/latte/log.21Jun18.latte.multiple.g++.1
lammps-stable_290ct2020/examples/latte/log.21Jun18.latte.sucrose.g++.1
lammps-stable_290ct2020/examples/latte/log.21Jun18.latte.water.g++.1
lammps-stable_290ct2020/examples/latte/log.21Jun18.latte.water.min.g++.1
lammps-stable_290ct2020/examples/meam/
lammps-stable_290ct2020/examples/meam/Ni.meam
lammps-stable_290ct2020/examples/meam/SiC.meam
lammps-stable_290ct2020/examples/meam/data.meam
lammps-stable_290ct2020/examples/meam/in.meam.shear
lammps-stable_290ct2020/examples/meam/in.meamc
lammps-stable_290ct2020/examples/meam/in.meamc.shear
lammps-stable_290ct2020/examples/meam/library.meam
lammps-stable_290ct2020/examples/meam/log.27Nov18.meamc.g++.1
lammps-stable_290ct2020/examples/meam/log.27Nov18.meamc.g++.4
lammps-stable_290ct2020/examples/meam/log.27Nov18.meamc.shear.g++.1
lammps-stable_290ct2020/examples/meam/log.27Nov18.meamc.shear.g++.4
lammps-stable_290ct2020/examples/melt/
lammps-stable_290ct2020/examples/melt/in.melt
lammps-stable_290ct2020/examples/melt/log.27Nov18.melt.g++.1
lammps-stable_290ct2020/examples/melt/log.27Nov18.melt.g++.4
lammps-stable_290ct2020/examples/message/
lammps-stable_290ct2020/examples/message/README
lammps-stable_290ct2020/examples/message/Script.sh
lammps-stable_290ct2020/examples/message/in.message
lammps-stable_290ct2020/examples/message/in.message.client
lammps-stable_290ct2020/examples/message/in.message.server
lammps-stable_290ct2020/examples/message/in.message.tilt
lammps-stable_290ct2020/examples/message/in.message.tilt.client
lammps-stable_290ct2020/examples/message/in.message.tilt.server
lammps-stable_290ct2020/examples/message/log.28Aug18.message.client.file.g++.
1
lammps-stable_290ct2020/examples/message/log.28Aug18.message.client.file.g++.
2
lammps-stable_290ct2020/examples/message/log.28Aug18.message.client.mpione.
g++.1
lammps-stable_290ct2020/examples/message/log.28Aug18.message.client.mpione.
g++.2
lammps-stable_290ct2020/examples/message/log.28Aug18.message.client.mpitwo.
g++.1
lammps-stable_290ct2020/examples/message/log.28Aug18.message.client.mpitwo.
g++.2
lammps-stable_290ct2020/examples/message/log.28Aug18.message.client.zmq.g++.1
lammps-stable_290ct2020/examples/message/log.28Aug18.message.client.zmq.g++.2
lammps-stable_290ct2020/examples/message/log.28Aug18.message.g++.1
lammps-stable_290ct2020/examples/message/log.28Aug18.message.g++.4
lammps-stable_290ct2020/examples/message/log.28Aug18.message.server.file.g++.
```

```
1
lammps-stable_290ct2020/examples/message/log.28Aug18.message.server.file.g++.
4
lammps-stable_290ct2020/examples/message/log.28Aug18.message.server.mpione.
g++.1
lammps-stable_290ct2020/examples/message/log.28Aug18.message.server.mpione.
g++.4
lammps-stable_290ct2020/examples/message/log.28Aug18.message.server.mpitwo.
g++.1
lammps-stable_290ct2020/examples/message/log.28Aug18.message.server.mpitwo.
g++.4
lammps-stable_290ct2020/examples/message/log.28Aug18.message.server.zmq.g++.1
lammps-stable_290ct2020/examples/message/log.28Aug18.message.server.zmq.g++.4
lammps-stable_290ct2020/examples/message/log.28Aug18.message.tilt.client.mpio
ne.g++.1
lammps-stable_290ct2020/examples/message/log.28Aug18.message.tilt.client.mpio
ne.g++.2
lammps-stable_290ct2020/examples/message/log.28Aug18.message.tilt.client.mpit
wo.g++.1
lammps-stable_290ct2020/examples/message/log.28Aug18.message.tilt.client.mpit
wo.g++.2
lammps-stable_290ct2020/examples/message/log.28Aug18.message.tilt.client.zmq.
g++.1
lammps-stable_290ct2020/examples/message/log.28Aug18.message.tilt.client.zmq.
g++.2
lammps-stable_290ct2020/examples/message/log.28Aug18.message.tilt.g++.1
lammps-stable_290ct2020/examples/message/log.28Aug18.message.tilt.g++.4
lammps-stable_290ct2020/examples/message/log.28Aug18.message.tilt.server.mpio
ne.g++.1
lammps-stable_290ct2020/examples/message/log.28Aug18.message.tilt.server.mpio
ne.g++.4
lammps-stable_290ct2020/examples/message/log.28Aug18.message.tilt.server.mpit
wo.g++.1
lammps-stable_290ct2020/examples/message/log.28Aug18.message.tilt.server.mpit
wo.g++.4
lammps-stable_290ct2020/examples/message/log.28Aug18.message.tilt.server.zmq.
g++.1
lammps-stable_290ct2020/examples/message/log.28Aug18.message.tilt.server.zmq.
g++.4
lammps-stable_290ct2020/examples/micelle/
lammps-stable_290ct2020/examples/micelle/data.micelle
lammps-stable_290ct2020/examples/micelle/def.micelle
lammps-stable_290ct2020/examples/micelle/in.micelle
lammps-stable_290ct2020/examples/micelle/in.micelle-rigid
lammps-stable_290ct2020/examples/micelle/log.29Mar2019.micelle-rigid.g++.1
lammps-stable_290ct2020/examples/micelle/log.29Mar2019.micelle-rigid.g++.4
lammps-stable_290ct2020/examples/micelle/log.29Mar2019.micelle.g++.1
lammps-stable_290ct2020/examples/micelle/log.29Mar2019.micelle.g++.4
lammps-stable_290ct2020/examples/min/
lammps-stable_290ct2020/examples/min/in.min
lammps-stable_290ct2020/examples/min/in.min.box
lammps-stable_290ct2020/examples/min/log.27Nov18.min.box.g++.1
lammps-stable_290ct2020/examples/min/log.27Nov18.min.box.g++.4
lammps-stable_290ct2020/examples/min/log.27Nov18.min.g++.1
lammps-stable_290ct2020/examples/min/log.27Nov18.min.g++.4
lammps-stable_290ct2020/examples/mliap/
lammps-stable_290ct2020/examples/mliap/InP_JCPA2020.mliap
lammps-stable_290ct2020/examples/mliap/InP_JCPA2020.mliap.descriptor
lammps-stable_290ct2020/examples/mliap/InP_JCPA2020.mliap.model
lammps-stable_290ct2020/examples/mliap/Ta06A.mliap
```



lammps-stable\_290ct2020/examples/mliap/Ta06A.mliap.descriptor  
lammps-stable\_290ct2020/examples/mliap/Ta06A.mliap.model  
lammps-stable\_290ct2020/examples/mliap/W.quadratic.mliap  
lammps-stable\_290ct2020/examples/mliap/W.quadratic.mliap.descriptor  
lammps-stable\_290ct2020/examples/mliap/W.quadratic.mliap.model  
lammps-stable\_290ct2020/examples/mliap/WBe\_Wood\_PRB2019.mliap  
lammps-stable\_290ct2020/examples/mliap/WBe\_Wood\_PRB2019.mliap.descriptor  
lammps-stable\_290ct2020/examples/mliap/WBe\_Wood\_PRB2019.mliap.model  
lammps-stable\_290ct2020/examples/mliap/compute.mliap.descriptor  
lammps-stable\_290ct2020/examples/mliap/in.mliap.quadratic.compute  
lammps-stable\_290ct2020/examples/mliap/in.mliap.snap.Ta06A  
lammps-stable\_290ct2020/examples/mliap/in.mliap.snap.WBe.PR2019  
lammps-stable\_290ct2020/examples/mliap/in.mliap.snap.chem  
lammps-stable\_290ct2020/examples/mliap/in.mliap.snap.compute  
lammps-stable\_290ct2020/examples/mliap/in.mliap.snap.quadratic  
lammps-stable\_290ct2020/examples/mliap/log.03Jul20.mliap.quadratic.compute.  
g++.1  
lammps-stable\_290ct2020/examples/mliap/log.03Jul20.mliap.quadratic.compute.  
g++.4  
lammps-stable\_290ct2020/examples/mliap/log.03Jul20.mliap.snap.compute.g++.1  
lammps-stable\_290ct2020/examples/mliap/log.03Jul20.mliap.snap.compute.g++.4  
lammps-stable\_290ct2020/examples/mliap/log.21Jun20.mliap.snap.Ta06A.g++.1  
lammps-stable\_290ct2020/examples/mliap/log.21Jun20.mliap.snap.Ta06A.g++.4  
lammps-stable\_290ct2020/examples/mliap/log.21Jun20.mliap.snap.WBe.PR2019.  
g++.1  
lammps-stable\_290ct2020/examples/mliap/log.21Jun20.mliap.snap.WBe.PR2019.  
g++.4  
lammps-stable\_290ct2020/examples/mliap/log.21Jun20.mliap.snap.chem.g++.1  
lammps-stable\_290ct2020/examples/mliap/log.21Jun20.mliap.snap.chem.g++.4  
lammps-stable\_290ct2020/examples/mliap/log.21Jun20.mliap.snap.quadratic.g++.1  
lammps-stable\_290ct2020/examples/mliap/log.21Jun20.mliap.snap.quadratic.g++.4  
lammps-stable\_290ct2020/examples/mliap/log.snap.Ta06A.ref  
lammps-stable\_290ct2020/examples/mscg/  
lammps-stable\_290ct2020/examples/mscg/README  
lammps-stable\_290ct2020/examples/mscg/control.in  
lammps-stable\_290ct2020/examples/mscg/data.meoh  
lammps-stable\_290ct2020/examples/mscg/dump.meoh  
lammps-stable\_290ct2020/examples/mscg/in.mscg  
lammps-stable\_290ct2020/examples/mscg/log.31Mar17.g++.1  
lammps-stable\_290ct2020/examples/mscg/output\_9Jan17/  
lammps-stable\_290ct2020/examples/mscg/output\_9Jan17/1\_1.dat  
lammps-stable\_290ct2020/examples/mscg/output\_9Jan17/1\_1.table  
lammps-stable\_290ct2020/examples/mscg/output\_9Jan17/b-spline.out  
lammps-stable\_290ct2020/examples/mscg/output\_9Jan17/rmin.in  
lammps-stable\_290ct2020/examples/mscg/output\_9Jan17/rmin\_b.in  
lammps-stable\_290ct2020/examples/mscg/output\_9Jan17/sol\_info.out  
lammps-stable\_290ct2020/examples/mscg/output\_9Jan17/x.out  
lammps-stable\_290ct2020/examples/msst/  
lammps-stable\_290ct2020/examples/msst/in.msst  
lammps-stable\_290ct2020/examples/msst/log.30Jun20.msst.g++.1  
lammps-stable\_290ct2020/examples/msst/log.30Jun20.msst.g++.4  
lammps-stable\_290ct2020/examples/nb3b/  
lammps-stable\_290ct2020/examples/nb3b/MOH.nb3b.harmonic  
lammps-stable\_290ct2020/examples/nb3b/data.nb3b  
lammps-stable\_290ct2020/examples/nb3b/in.nb3b  
lammps-stable\_290ct2020/examples/nb3b/log.27Nov18.nb3b.g++.1  
lammps-stable\_290ct2020/examples/nb3b/log.27Nov18.nb3b.g++.4  
lammps-stable\_290ct2020/examples/neb/  
lammps-stable\_290ct2020/examples/neb/README  
lammps-stable\_290ct2020/examples/neb/Si.sw

lammps-stable\_290ct2020/examples/neb/final.hop1  
lammps-stable\_290ct2020/examples/neb/final.hop2  
lammps-stable\_290ct2020/examples/neb/final.sivac  
lammps-stable\_290ct2020/examples/neb/in.neb.hop1  
lammps-stable\_290ct2020/examples/neb/in.neb.hop1.end  
lammps-stable\_290ct2020/examples/neb/in.neb.hop2  
lammps-stable\_290ct2020/examples/neb/in.neb.sivac  
lammps-stable\_290ct2020/examples/neb/initial.hop1  
lammps-stable\_290ct2020/examples/neb/initial.hop1.end  
lammps-stable\_290ct2020/examples/neb/initial.hop2  
lammps-stable\_290ct2020/examples/neb/initial.sivac  
lammps-stable\_290ct2020/examples/neb/log.19Jun17.neb.hop1.end.g++.4  
lammps-stable\_290ct2020/examples/neb/log.19Jun17.neb.hop1.end.g++.8  
lammps-stable\_290ct2020/examples/neb/log.19Jun17.neb.hop1.g++.4  
lammps-stable\_290ct2020/examples/neb/log.19Jun17.neb.hop1.g++.8  
lammps-stable\_290ct2020/examples/neb/log.19Jun17.neb.hop2.g++.4  
lammps-stable\_290ct2020/examples/neb/log.19Jun17.neb.hop2.g++.8  
lammps-stable\_290ct2020/examples/neb/log.19Jun17.neb.sivac.g++.4  
lammps-stable\_290ct2020/examples/neb/log.19Jun17.neb.sivac.g++.8  
lammps-stable\_290ct2020/examples/nemd/  
lammps-stable\_290ct2020/examples/nemd/in.nemd  
lammps-stable\_290ct2020/examples/nemd/log.27Nov18.nemd.g++.1  
lammps-stable\_290ct2020/examples/nemd/log.27Nov18.nemd.g++.4  
lammps-stable\_290ct2020/examples/numdiff/  
lammps-stable\_290ct2020/examples/numdiff/README.md  
lammps-stable\_290ct2020/examples/numdiff/in.numdiff  
lammps-stable\_290ct2020/examples/obstacle/  
lammps-stable\_290ct2020/examples/obstacle/in.obstacle  
lammps-stable\_290ct2020/examples/obstacle/log.27Nov18.obstacle.g++.1  
lammps-stable\_290ct2020/examples/obstacle/log.27Nov18.obstacle.g++.4  
lammps-stable\_290ct2020/examples/peptide/  
lammps-stable\_290ct2020/examples/peptide/data.peptide  
lammps-stable\_290ct2020/examples/peptide/in.peptide  
lammps-stable\_290ct2020/examples/peptide/log.27Nov18.peptide.g++.1  
lammps-stable\_290ct2020/examples/peptide/log.27Nov18.peptide.g++.4  
lammps-stable\_290ct2020/examples/peri/  
lammps-stable\_290ct2020/examples/peri/in.peri-pmb  
lammps-stable\_290ct2020/examples/peri/in.peri.eps  
lammps-stable\_290ct2020/examples/peri/in.peri.lps  
lammps-stable\_290ct2020/examples/peri/in.peri.pmb  
lammps-stable\_290ct2020/examples/peri/in.peri.ves  
lammps-stable\_290ct2020/examples/peri/log.27Nov18.peri.eps.g++.1  
lammps-stable\_290ct2020/examples/peri/log.27Nov18.peri.eps.g++.4  
lammps-stable\_290ct2020/examples/peri/log.27Nov18.peri.lps.g++.1  
lammps-stable\_290ct2020/examples/peri/log.27Nov18.peri.lps.g++.4  
lammps-stable\_290ct2020/examples/peri/log.27Nov18.peri.pmb.g++.1  
lammps-stable\_290ct2020/examples/peri/log.27Nov18.peri.pmb.g++.4  
lammps-stable\_290ct2020/examples/peri/log.27Nov18.peri.ves.g++.1  
lammps-stable\_290ct2020/examples/peri/log.27Nov18.peri.ves.g++.4  
lammps-stable\_290ct2020/examples/pour/  
lammps-stable\_290ct2020/examples/pour/in.pour  
lammps-stable\_290ct2020/examples/pour/in.pour.2d  
lammps-stable\_290ct2020/examples/pour/in.pour.2d.molecule  
lammps-stable\_290ct2020/examples/pour/log.27Nov18.pour.2d.g++.1  
lammps-stable\_290ct2020/examples/pour/log.27Nov18.pour.2d.g++.4  
lammps-stable\_290ct2020/examples/pour/log.27Nov18.pour.2d.molecule.g++.1  
lammps-stable\_290ct2020/examples/pour/log.27Nov18.pour.2d.molecule.g++.4  
lammps-stable\_290ct2020/examples/pour/log.27Nov18.pour.g++.1  
lammps-stable\_290ct2020/examples/pour/log.27Nov18.pour.g++.4  
lammps-stable\_290ct2020/examples/pour/molecule.vshape

lammps-stable\_290ct2020/examples/prd/  
lammps-stable\_290ct2020/examples/prd/README  
lammps-stable\_290ct2020/examples/prd/Si.sw  
lammps-stable\_290ct2020/examples/prd/in.prd  
lammps-stable\_290ct2020/examples/prd/log.50ct16.prd.g++.4  
lammps-stable\_290ct2020/examples/prd/log.50ct16.prd.g++.8  
lammps-stable\_290ct2020/examples/prd/screen.50ct16.prd.g++.4.0  
lammps-stable\_290ct2020/examples/prd/screen.50ct16.prd.g++.4.1  
lammps-stable\_290ct2020/examples/prd/screen.50ct16.prd.g++.4.2  
lammps-stable\_290ct2020/examples/prd/screen.50ct16.prd.g++.4.3  
lammps-stable\_290ct2020/examples/prd/screen.50ct16.prd.g++.8.0  
lammps-stable\_290ct2020/examples/prd/screen.50ct16.prd.g++.8.1  
lammps-stable\_290ct2020/examples/prd/screen.50ct16.prd.g++.8.2  
lammps-stable\_290ct2020/examples/prd/screen.50ct16.prd.g++.8.3  
lammps-stable\_290ct2020/examples/python/  
lammps-stable\_290ct2020/examples/python/README.fix\_python\_move  
lammps-stable\_290ct2020/examples/python/README.pair\_python  
lammps-stable\_290ct2020/examples/python/data.spce  
lammps-stable\_290ct2020/examples/python/funcs.py  
lammps-stable\_290ct2020/examples/python/in.fix\_python\_invoke  
lammps-stable\_290ct2020/examples/python/in.fix\_python\_invoke\_neighlist  
lammps-stable\_290ct2020/examples/python/in.fix\_python\_move\_nve\_melt  
lammps-stable\_290ct2020/examples/python/in.fix\_python\_move\_nve\_melt\_opt  
lammps-stable\_290ct2020/examples/python/in.pair\_python\_coulomb  
lammps-stable\_290ct2020/examples/python/in.pair\_python\_hybrid  
lammps-stable\_290ct2020/examples/python/in.pair\_python\_long  
lammps-stable\_290ct2020/examples/python/in.pair\_python\_melt  
lammps-stable\_290ct2020/examples/python/in.pair\_python\_spce  
lammps-stable\_290ct2020/examples/python/in.pair\_python\_table  
lammps-stable\_290ct2020/examples/python/in.python  
lammps-stable\_290ct2020/examples/python/log.27Nov18.fix\_python\_invoke.g++.1  
lammps-stable\_290ct2020/examples/python/log.27Nov18.fix\_python\_invoke.g++.4  
lammps-stable\_290ct2020/examples/python/log.27Nov18.fix\_python\_move\_nve\_melt.g++.1  
lammps-stable\_290ct2020/examples/python/log.27Nov18.fix\_python\_move\_nve\_melt.g++.4  
lammps-stable\_290ct2020/examples/python/log.27Nov18.fix\_python\_move\_nve\_melt\_opt.g++.1  
lammps-stable\_290ct2020/examples/python/log.27Nov18.fix\_python\_move\_nve\_melt\_opt.g++.4  
lammps-stable\_290ct2020/examples/python/log.27Nov18.pair\_python\_coulomb.g++.1  
lammps-stable\_290ct2020/examples/python/log.27Nov18.pair\_python\_coulomb.g++.4  
lammps-stable\_290ct2020/examples/python/log.27Nov18.pair\_python\_hybrid.g++.1  
lammps-stable\_290ct2020/examples/python/log.27Nov18.pair\_python\_hybrid.g++.4  
lammps-stable\_290ct2020/examples/python/log.27Nov18.pair\_python\_long.g++.1  
lammps-stable\_290ct2020/examples/python/log.27Nov18.pair\_python\_long.g++.4  
lammps-stable\_290ct2020/examples/python/log.27Nov18.pair\_python\_melt.g++.1  
lammps-stable\_290ct2020/examples/python/log.27Nov18.pair\_python\_melt.g++.4  
lammps-stable\_290ct2020/examples/python/log.27Nov18.pair\_python\_spce.g++.1  
lammps-stable\_290ct2020/examples/python/log.27Nov18.pair\_python\_spce.g++.4  
lammps-stable\_290ct2020/examples/python/log.27Nov18.pair\_python\_table.g++.1  
lammps-stable\_290ct2020/examples/python/log.27Nov18.pair\_python\_table.g++.4  
lammps-stable\_290ct2020/examples/python/log.27Nov18.python.g++.1  
lammps-stable\_290ct2020/examples/python/log.27Nov18.python.g++.4  
lammps-stable\_290ct2020/examples/python/py\_nve.py  
lammps-stable\_290ct2020/examples/python/py\_pot.py  
lammps-stable\_290ct2020/examples/qqq/  
lammps-stable\_290ct2020/examples/qqq/data.CH0  
lammps-stable\_290ct2020/examples/qqq/data.aC  
lammps-stable\_290ct2020/examples/qqq/ffield.reax.cho

lammps-stable\_290ct2020/examples/qqq/in.qqq.buck  
lammps-stable\_290ct2020/examples/qqq/in.qqq.reaxc  
lammps-stable\_290ct2020/examples/qqq/log.27Nov18.qqq.buck.g++.1  
lammps-stable\_290ct2020/examples/qqq/log.27Nov18.qqq.buck.g++.4  
lammps-stable\_290ct2020/examples/qqq/log.27Nov18.qqq.reaxc.g++.1  
lammps-stable\_290ct2020/examples/qqq/log.27Nov18.qqq.reaxc.g++.4  
lammps-stable\_290ct2020/examples/qqq/param.qqq.reax  
lammps-stable\_290ct2020/examples/qqq/param.qqq1  
lammps-stable\_290ct2020/examples/qqq/param.qqq2  
lammps-stable\_290ct2020/examples/rdf-adf/  
lammps-stable\_290ct2020/examples/rdf-adf/data.spce  
lammps-stable\_290ct2020/examples/rdf-adf/in.spce  
lammps-stable\_290ct2020/examples/rdf-adf/log.27Nov18.spce.g++.1  
lammps-stable\_290ct2020/examples/rdf-adf/log.27Nov18.spce.g++.4  
lammps-stable\_290ct2020/examples/rdf-adf/spce-adf.dat.ref  
lammps-stable\_290ct2020/examples/rdf-adf/spce-rdf.dat.ref  
lammps-stable\_290ct2020/examples/reax/  
lammps-stable\_290ct2020/examples/reax/AB/  
lammps-stable\_290ct2020/examples/reax/AB/README  
lammps-stable\_290ct2020/examples/reax/AB/data.AB  
lammps-stable\_290ct2020/examples/reax/AB/ffield.reax.AB  
lammps-stable\_290ct2020/examples/reax/AB/in.AB  
lammps-stable\_290ct2020/examples/reax/AB/lmp\_control  
lammps-stable\_290ct2020/examples/reax/AB/log.8Mar18.AB.g++.1  
lammps-stable\_290ct2020/examples/reax/AB/log.8Mar18.AB.g++.4  
lammps-stable\_290ct2020/examples/reax/AB/param.qqq  
lammps-stable\_290ct2020/examples/reax/Au0/  
lammps-stable\_290ct2020/examples/reax/Au0/README  
lammps-stable\_290ct2020/examples/reax/Au0/data.Au0  
lammps-stable\_290ct2020/examples/reax/Au0/ffield.reax.Au0  
lammps-stable\_290ct2020/examples/reax/Au0/in.Au0  
lammps-stable\_290ct2020/examples/reax/Au0/lmp\_control  
lammps-stable\_290ct2020/examples/reax/Au0/log.8Mar18.Au0.g++.1  
lammps-stable\_290ct2020/examples/reax/Au0/log.8Mar18.Au0.g++.4  
lammps-stable\_290ct2020/examples/reax/Au0/param.qqq  
lammps-stable\_290ct2020/examples/reax/CH0/  
lammps-stable\_290ct2020/examples/reax/CH0/README  
lammps-stable\_290ct2020/examples/reax/CH0/data.CH0  
lammps-stable\_290ct2020/examples/reax/CH0/ffield.reax.cho  
lammps-stable\_290ct2020/examples/reax/CH0/in.CH0  
lammps-stable\_290ct2020/examples/reax/CH0/lmp\_control  
lammps-stable\_290ct2020/examples/reax/CH0/log.8Mar18.CH0.g++.1  
lammps-stable\_290ct2020/examples/reax/CH0/log.8Mar18.CH0.g++.4  
lammps-stable\_290ct2020/examples/reax/CH0/param.qqq  
lammps-stable\_290ct2020/examples/reax/FC/  
lammps-stable\_290ct2020/examples/reax/FC/README  
lammps-stable\_290ct2020/examples/reax/FC/data.FC  
lammps-stable\_290ct2020/examples/reax/FC/ffield.reax.FC  
lammps-stable\_290ct2020/examples/reax/FC/in.FC  
lammps-stable\_290ct2020/examples/reax/FC/log.8Mar18.FC.g++.1  
lammps-stable\_290ct2020/examples/reax/FC/log.8Mar18.FC.g++.4  
lammps-stable\_290ct2020/examples/reax/FeOH3/  
lammps-stable\_290ct2020/examples/reax/FeOH3/README  
lammps-stable\_290ct2020/examples/reax/FeOH3/data.FeOH3  
lammps-stable\_290ct2020/examples/reax/FeOH3/ffield.reax.Fe\_0\_C\_H  
lammps-stable\_290ct2020/examples/reax/FeOH3/in.FeOH3  
lammps-stable\_290ct2020/examples/reax/FeOH3/lmp\_control  
lammps-stable\_290ct2020/examples/reax/FeOH3/log.50ct16.FeOH3.g++.1  
lammps-stable\_290ct2020/examples/reax/FeOH3/log.50ct16.FeOH3.g++.4  
lammps-stable\_290ct2020/examples/reax/FeOH3/param.qqq

lammps-stable\_290ct2020/examples/reax/HNS/  
lammps-stable\_290ct2020/examples/reax/HNS/README.txt  
lammps-stable\_290ct2020/examples/reax/HNS/data.hns-equil  
lammps-stable\_290ct2020/examples/reax/HNS/ffield.reax.hns  
lammps-stable\_290ct2020/examples/reax/HNS/in.reaxc.hns  
lammps-stable\_290ct2020/examples/reax/HNS/log.8Mar18.reaxc.hns.g++.1  
lammps-stable\_290ct2020/examples/reax/HNS/log.8Mar18.reaxc.hns.g++.4  
lammps-stable\_290ct2020/examples/reax/RDX/  
lammps-stable\_290ct2020/examples/reax/RDX/README  
lammps-stable\_290ct2020/examples/reax/RDX/data.RDX  
lammps-stable\_290ct2020/examples/reax/RDX/ffield.reax.rdx  
lammps-stable\_290ct2020/examples/reax/RDX/in.RDX  
lammps-stable\_290ct2020/examples/reax/RDX/lmp\_control  
lammps-stable\_290ct2020/examples/reax/RDX/log.8Mar18.RDX.g++.1  
lammps-stable\_290ct2020/examples/reax/RDX/log.8Mar18.RDX.g++.4  
lammps-stable\_290ct2020/examples/reax/RDX/param.qeq  
lammps-stable\_290ct2020/examples/reax/README  
lammps-stable\_290ct2020/examples/reax/VOH/  
lammps-stable\_290ct2020/examples/reax/VOH/README  
lammps-stable\_290ct2020/examples/reax/VOH/data.VOH  
lammps-stable\_290ct2020/examples/reax/VOH/ffield.reax.V\_0\_C\_H  
lammps-stable\_290ct2020/examples/reax/VOH/in.VOH  
lammps-stable\_290ct2020/examples/reax/VOH/lmp\_control  
lammps-stable\_290ct2020/examples/reax/VOH/log.8Mar18.VOH.g++.1  
lammps-stable\_290ct2020/examples/reax/VOH/log.8Mar18.VOH.g++.4  
lammps-stable\_290ct2020/examples/reax/VOH/param.qeq  
lammps-stable\_290ct2020/examples/reax/ZnOH2/  
lammps-stable\_290ct2020/examples/reax/ZnOH2/README  
lammps-stable\_290ct2020/examples/reax/ZnOH2/data.ZnOH2  
lammps-stable\_290ct2020/examples/reax/ZnOH2/ffield.reax.ZnOH  
lammps-stable\_290ct2020/examples/reax/ZnOH2/in.ZnOH2  
lammps-stable\_290ct2020/examples/reax/ZnOH2/lmp\_control  
lammps-stable\_290ct2020/examples/reax/ZnOH2/log.8Mar18.ZnOH2.g++.1  
lammps-stable\_290ct2020/examples/reax/ZnOH2/log.8Mar18.ZnOH2.g++.4  
lammps-stable\_290ct2020/examples/reax/ZnOH2/param.qeq  
lammps-stable\_290ct2020/examples/reax/ci-reaxFF/  
lammps-stable\_290ct2020/examples/reax/ci-reaxFF/CH4.dat  
lammps-stable\_290ct2020/examples/reax/ci-reaxFF/ci-reaxFF\_ZBL.dat  
lammps-stable\_290ct2020/examples/reax/ci-reaxFF/control  
lammps-stable\_290ct2020/examples/reax/ci-reaxFF/ffield.ci-reax.CH  
lammps-stable\_290ct2020/examples/reax/ci-reaxFF/in.ci-reax.CH  
lammps-stable\_290ct2020/examples/reax/ci-reaxFF/log.8Mar18.ci-reax.CH.g++.1  
lammps-stable\_290ct2020/examples/reax/ci-reaxFF/log.8Mar18.ci-reax.CH.g++.4  
lammps-stable\_290ct2020/examples/reax/control.reax\_c.rdx  
lammps-stable\_290ct2020/examples/reax/control.reax\_c.tatb  
lammps-stable\_290ct2020/examples/reax/data.rdx  
lammps-stable\_290ct2020/examples/reax/data.tatb  
lammps-stable\_290ct2020/examples/reax/ffield.reax  
lammps-stable\_290ct2020/examples/reax/in.reaxc.rdx  
lammps-stable\_290ct2020/examples/reax/in.reaxc.rdx-shielded  
lammps-stable\_290ct2020/examples/reax/in.reaxc.tatb  
lammps-stable\_290ct2020/examples/reax/in.reaxc.tatb-shielded  
lammps-stable\_290ct2020/examples/reax/log.4Jan19.reaxc.rdx-shielded.g++.1  
lammps-stable\_290ct2020/examples/reax/log.4Jan19.reaxc.rdx-shielded.g++.4  
lammps-stable\_290ct2020/examples/reax/log.4Jan19.reaxc.tatb-shielded.g++.1  
lammps-stable\_290ct2020/examples/reax/log.4Jan19.reaxc.tatb-shielded.g++.4  
lammps-stable\_290ct2020/examples/reax/log.8March18.reaxc.rdx.g++.1  
lammps-stable\_290ct2020/examples/reax/log.8March18.reaxc.rdx.g++.4  
lammps-stable\_290ct2020/examples/reax/log.8March18.reaxc.tatb.g++.1  
lammps-stable\_290ct2020/examples/reax/log.8March18.reaxc.tatb.g++.4

lammps-stable\_290ct2020/examples/rerun/  
lammps-stable\_290ct2020/examples/rerun/README  
lammps-stable\_290ct2020/examples/rerun/in.first  
lammps-stable\_290ct2020/examples/rerun/in.rdf.first  
lammps-stable\_290ct2020/examples/rerun/in.rdf.rerun  
lammps-stable\_290ct2020/examples/rerun/in.read\_dump  
lammps-stable\_290ct2020/examples/rerun/in.rerun  
lammps-stable\_290ct2020/examples/rerun/log.09Jan20.first.g++.4  
lammps-stable\_290ct2020/examples/rerun/log.09Jan20.rdf.first.g++.4  
lammps-stable\_290ct2020/examples/rerun/log.09Jan20.rdf.rerun.g++.4  
lammps-stable\_290ct2020/examples/rerun/log.09Jan20.read\_dump.g++.4  
lammps-stable\_290ct2020/examples/rerun/log.09Jan20.rerun.g++.4  
lammps-stable\_290ct2020/examples/rerun/rdf.09Jan20.first.g++.4  
lammps-stable\_290ct2020/examples/rerun/rdf.09Jan20.rerun.g++.4  
lammps-stable\_290ct2020/examples/rigid/  
lammps-stable\_290ct2020/examples/rigid/bodies.txt  
lammps-stable\_290ct2020/examples/rigid/data.rigid  
lammps-stable\_290ct2020/examples/rigid/data.rigid-property  
lammps-stable\_290ct2020/examples/rigid/data.rigid.tnr  
lammps-stable\_290ct2020/examples/rigid/in.rigid  
lammps-stable\_290ct2020/examples/rigid/in.rigid.atomfile  
lammps-stable\_290ct2020/examples/rigid/in.rigid.atomvar  
lammps-stable\_290ct2020/examples/rigid/in.rigid.early  
lammps-stable\_290ct2020/examples/rigid/in.rigid.gravity  
lammps-stable\_290ct2020/examples/rigid/in.rigid.nve  
lammps-stable\_290ct2020/examples/rigid/in.rigid.nve.early  
lammps-stable\_290ct2020/examples/rigid/in.rigid.poems  
lammps-stable\_290ct2020/examples/rigid/in.rigid.poems2  
lammps-stable\_290ct2020/examples/rigid/in.rigid.property  
lammps-stable\_290ct2020/examples/rigid/in.rigid.tnr  
lammps-stable\_290ct2020/examples/rigid/log.27Nov18.rigid.atomfile.g++.1  
lammps-stable\_290ct2020/examples/rigid/log.27Nov18.rigid.atomfile.g++.4  
lammps-stable\_290ct2020/examples/rigid/log.27Nov18.rigid.atomvar.g++.1  
lammps-stable\_290ct2020/examples/rigid/log.27Nov18.rigid.atomvar.g++.4  
lammps-stable\_290ct2020/examples/rigid/log.27Nov18.rigid.early.g++.1  
lammps-stable\_290ct2020/examples/rigid/log.27Nov18.rigid.early.g++.4  
lammps-stable\_290ct2020/examples/rigid/log.27Nov18.rigid.g++.1  
lammps-stable\_290ct2020/examples/rigid/log.27Nov18.rigid.g++.4  
lammps-stable\_290ct2020/examples/rigid/log.27Nov18.rigid.nve.early.g++.1  
lammps-stable\_290ct2020/examples/rigid/log.27Nov18.rigid.nve.early.g++.4  
lammps-stable\_290ct2020/examples/rigid/log.27Nov18.rigid.nve.g++.1  
lammps-stable\_290ct2020/examples/rigid/log.27Nov18.rigid.nve.g++.4  
lammps-stable\_290ct2020/examples/rigid/log.27Nov18.rigid.poems.g++.1  
lammps-stable\_290ct2020/examples/rigid/log.27Nov18.rigid.poems.g++.4  
lammps-stable\_290ct2020/examples/rigid/log.27Nov18.rigid.poems2.g++.1  
lammps-stable\_290ct2020/examples/rigid/log.27Nov18.rigid.poems2.g++.4  
lammps-stable\_290ct2020/examples/rigid/log.27Nov18.rigid.property.g++.1  
lammps-stable\_290ct2020/examples/rigid/log.27Nov18.rigid.property.g++.4  
lammps-stable\_290ct2020/examples/rigid/log.27Nov18.rigid.tnr.g++.1  
lammps-stable\_290ct2020/examples/rigid/log.27Nov18.rigid.tnr.g++.4  
lammps-stable\_290ct2020/examples/rigid/molecule.data  
lammps-stable\_290ct2020/examples/shear/  
lammps-stable\_290ct2020/examples/shear/Ni\_u3.eam  
lammps-stable\_290ct2020/examples/shear/in.shear  
lammps-stable\_290ct2020/examples/shear/in.shear.void  
lammps-stable\_290ct2020/examples/shear/log.27Nov18.shear.g++.1  
lammps-stable\_290ct2020/examples/shear/log.27Nov18.shear.g++.4  
lammps-stable\_290ct2020/examples/shear/log.27Nov18.shear.void.g++.1  
lammps-stable\_290ct2020/examples/shear/log.27Nov18.shear.void.g++.4  
lammps-stable\_290ct2020/examples/snap/

lammps-stable\_290ct2020/examples/snap/He\_He\_JW2013.table  
lammps-stable\_290ct2020/examples/snap/InP\_JCPA2020.snap  
lammps-stable\_290ct2020/examples/snap/InP\_JCPA2020.snapcoeff  
lammps-stable\_290ct2020/examples/snap/InP\_JCPA2020.snapparam  
lammps-stable\_290ct2020/examples/snap/Mo\_Chén\_PRM2017.snap  
lammps-stable\_290ct2020/examples/snap/Mo\_Chén\_PRM2017.snapcoeff  
lammps-stable\_290ct2020/examples/snap/Mo\_Chén\_PRM2017.snapparam  
lammps-stable\_290ct2020/examples/snap/Ta06A.snap  
lammps-stable\_290ct2020/examples/snap/Ta06A.snapcoeff  
lammps-stable\_290ct2020/examples/snap/Ta06A.snapparam  
lammps-stable\_290ct2020/examples/snap/WBe\_Wood\_PRB2019.snap  
lammps-stable\_290ct2020/examples/snap/WBe\_Wood\_PRB2019.snapcoeff  
lammps-stable\_290ct2020/examples/snap/WBe\_Wood\_PRB2019.snapparam  
lammps-stable\_290ct2020/examples/snap/W\_2940\_2017\_2.snap  
lammps-stable\_290ct2020/examples/snap/W\_2940\_2017\_2.snapcoeff  
lammps-stable\_290ct2020/examples/snap/W\_2940\_2017\_2.snapparam  
lammps-stable\_290ct2020/examples/snap/W\_2940\_2017\_2\_He\_JW2013.snap  
lammps-stable\_290ct2020/examples/snap/W\_He\_JW2013.table  
lammps-stable\_290ct2020/examples/snap/in.snap.InP.JCPA2020  
lammps-stable\_290ct2020/examples/snap/in.snap.Mo\_Chén  
lammps-stable\_290ct2020/examples/snap/in.snap.Ta06A  
lammps-stable\_290ct2020/examples/snap/in.snap.W.2940  
lammps-stable\_290ct2020/examples/snap/in.snap.WBe.PRB2019  
lammps-stable\_290ct2020/examples/snap/in.snap.compute  
lammps-stable\_290ct2020/examples/snap/in.snap.compute.quadratic  
lammps-stable\_290ct2020/examples/snap/in.snap.hybrid.WSNAP.HePair  
lammps-stable\_290ct2020/examples/snap/log.03Jul20.snap.compute.g++.1  
lammps-stable\_290ct2020/examples/snap/log.03Jul20.snap.compute.g++.4  
lammps-stable\_290ct2020/examples/snap/log.03Jul20.snap.compute.quadratic.g++.1  
lammps-stable\_290ct2020/examples/snap/log.03Jul20.snap.compute.quadratic.g++.4  
lammps-stable\_290ct2020/examples/snap/log.15Jun20.snap.InP.JCPA2020.g++.1  
lammps-stable\_290ct2020/examples/snap/log.15Jun20.snap.InP.JCPA2020.g++.4  
lammps-stable\_290ct2020/examples/snap/log.15Jun20.snap.Mo\_Chén.g++.1  
lammps-stable\_290ct2020/examples/snap/log.15Jun20.snap.Mo\_Chén.g++.4  
lammps-stable\_290ct2020/examples/snap/log.15Jun20.snap.Ta06A.g++.1  
lammps-stable\_290ct2020/examples/snap/log.15Jun20.snap.Ta06A.g++.4  
lammps-stable\_290ct2020/examples/snap/log.15Jun20.snap.W.2940.g++.1  
lammps-stable\_290ct2020/examples/snap/log.15Jun20.snap.W.2940.g++.4  
lammps-stable\_290ct2020/examples/snap/log.15Jun20.snap.WBe.PRB2019.g++.1  
lammps-stable\_290ct2020/examples/snap/log.15Jun20.snap.WBe.PRB2019.g++.4  
lammps-stable\_290ct2020/examples/snap/log.15Jun20.snap.hybrid.WSNAP.HePair.g++.1  
lammps-stable\_290ct2020/examples/snap/log.15Jun20.snap.hybrid.WSNAP.HePair.g++.4  
lammps-stable\_290ct2020/examples/srd/  
lammps-stable\_290ct2020/examples/srd/in.srd.mixture  
lammps-stable\_290ct2020/examples/srd/in.srd.pure  
lammps-stable\_290ct2020/examples/srd/log.27Nov18.srd.mixture.g++.1  
lammps-stable\_290ct2020/examples/srd/log.27Nov18.srd.mixture.g++.4  
lammps-stable\_290ct2020/examples/srd/log.27Nov18.srd.pure.g++.1  
lammps-stable\_290ct2020/examples/srd/log.27Nov18.srd.pure.g++.4  
lammps-stable\_290ct2020/examples/steinhardt/  
lammps-stable\_290ct2020/examples/steinhardt/in.bcc  
lammps-stable\_290ct2020/examples/steinhardt/in.fcc  
lammps-stable\_290ct2020/examples/steinhardt/in.icos  
lammps-stable\_290ct2020/examples/steinhardt/log.13Sept18.bcc.g++.1  
lammps-stable\_290ct2020/examples/steinhardt/log.13Sept18.bcc.g++.4  
lammps-stable\_290ct2020/examples/steinhardt/log.13Sept18.fcc.g++.1

lammps-stable\_290ct2020/examples/steinhardt/log.13Sept18.fcc.g++.4  
lammps-stable\_290ct2020/examples/steinhardt/log.13Sept18.icos.g++.1  
lammps-stable\_290ct2020/examples/steinhardt/log.13Sept18.icos.g++.4  
lammps-stable\_290ct2020/examples/streitz/  
lammps-stable\_290ct2020/examples/streitz/Al0.eam.alloy  
lammps-stable\_290ct2020/examples/streitz/Al0.streitz  
lammps-stable\_290ct2020/examples/streitz/data.streitz  
lammps-stable\_290ct2020/examples/streitz/in.streitz.ewald  
lammps-stable\_290ct2020/examples/streitz/in.streitz.wolf  
lammps-stable\_290ct2020/examples/streitz/log.27Nov18.streitz.ewald.g++.1  
lammps-stable\_290ct2020/examples/streitz/log.27Nov18.streitz.ewald.g++.4  
lammps-stable\_290ct2020/examples/streitz/log.27Nov18.streitz.wolf.g++.1  
lammps-stable\_290ct2020/examples/streitz/log.27Nov18.streitz.wolf.g++.4  
lammps-stable\_290ct2020/examples/tad/  
lammps-stable\_290ct2020/examples/tad/README  
lammps-stable\_290ct2020/examples/tad/Si.sw  
lammps-stable\_290ct2020/examples/tad/in.tad  
lammps-stable\_290ct2020/examples/tad/log.50ct16.tad.g++.3  
lammps-stable\_290ct2020/examples/template/  
lammps-stable\_290ct2020/examples/template/co2.mol  
lammps-stable\_290ct2020/examples/template/cyclohexane.mol  
lammps-stable\_290ct2020/examples/template/h2o-co2.data  
lammps-stable\_290ct2020/examples/template/h2o.mol  
lammps-stable\_290ct2020/examples/template/in.hybrid  
lammps-stable\_290ct2020/examples/template/in.mol-data-mix  
lammps-stable\_290ct2020/examples/template/in.mol-restart-mix  
lammps-stable\_290ct2020/examples/template/in.molecular-mix  
lammps-stable\_290ct2020/examples/template/in.template-mix  
lammps-stable\_290ct2020/examples/template/in.tmpl-data-mix  
lammps-stable\_290ct2020/examples/template/in.tmpl-restart-mix  
lammps-stable\_290ct2020/examples/template/log.220ct20.hybrid.g++.1  
lammps-stable\_290ct2020/examples/template/log.220ct20.hybrid.g++.4  
lammps-stable\_290ct2020/examples/template/log.220ct20.mol-data-mix.g++.1  
lammps-stable\_290ct2020/examples/template/log.220ct20.mol-data-mix.g++.4  
lammps-stable\_290ct2020/examples/template/log.220ct20.mol-restart-mix.g++.1  
lammps-stable\_290ct2020/examples/template/log.220ct20.mol-restart-mix.g++.4  
lammps-stable\_290ct2020/examples/template/log.220ct20.molecular-mix.g++.1  
lammps-stable\_290ct2020/examples/template/log.220ct20.molecular-mix.g++.4  
lammps-stable\_290ct2020/examples/template/log.220ct20.template-mix.g++.1  
lammps-stable\_290ct2020/examples/template/log.220ct20.template-mix.g++.4  
lammps-stable\_290ct2020/examples/template/log.220ct20.tmpl-data-mix.g++.1  
lammps-stable\_290ct2020/examples/template/log.220ct20.tmpl-data-mix.g++.4  
lammps-stable\_290ct2020/examples/template/log.220ct20.tmpl-restart-mix.g++.1  
lammps-stable\_290ct2020/examples/template/log.220ct20.tmpl-restart-mix.g++.4  
lammps-stable\_290ct2020/examples/template/molecular-mix.data  
lammps-stable\_290ct2020/examples/template/template-mix.data  
lammps-stable\_290ct2020/examples/threebody/  
lammps-stable\_290ct2020/examples/threebody/BNC.tersoff  
lammps-stable\_290ct2020/examples/threebody/CdTeZnSeHgS0.sw  
lammps-stable\_290ct2020/examples/threebody/InP.vashishta  
lammps-stable\_290ct2020/examples/threebody/Si.sw  
lammps-stable\_290ct2020/examples/threebody/Si.tersoff.mod  
lammps-stable\_290ct2020/examples/threebody/Si.tersoff.modc  
lammps-stable\_290ct2020/examples/threebody/in.threebody  
lammps-stable\_290ct2020/examples/threebody/log.27Nov18.threebody.g++.1  
lammps-stable\_290ct2020/examples/threebody/log.27Nov18.threebody.g++.4  
lammps-stable\_290ct2020/examples/vashishta/  
lammps-stable\_290ct2020/examples/vashishta/InP.vashishta  
lammps-stable\_290ct2020/examples/vashishta/Si0.1990.vashishta  
lammps-stable\_290ct2020/examples/vashishta/data.quartz



```
lammps-stable_290ct2020/examples/vashishta/in.vashishta.inp
lammps-stable_290ct2020/examples/vashishta/in.vashishta.sio2
lammps-stable_290ct2020/examples/vashishta/in.vashishta.table.inp
lammps-stable_290ct2020/examples/vashishta/in.vashishta.table.sio2
lammps-stable_290ct2020/examples/vashishta/log.27Nov18.vashishta.inp.g++.1
lammps-stable_290ct2020/examples/vashishta/log.27Nov18.vashishta.inp.g++.4
lammps-stable_290ct2020/examples/vashishta/log.27Nov18.vashishta.sio2.g++.1
lammps-stable_290ct2020/examples/vashishta/log.27Nov18.vashishta.sio2.g++.4
lammps-stable_290ct2020/examples/vashishta/log.27Nov18.vashishta.table.inp.g++.1
lammps-stable_290ct2020/examples/vashishta/log.27Nov18.vashishta.table.inp.g++.4
lammps-stable_290ct2020/examples/vashishta/log.27Nov18.vashishta.table.sio2.g++.1
lammps-stable_290ct2020/examples/vashishta/log.27Nov18.vashishta.table.sio2.g++.4
lammps-stable_290ct2020/examples/voronoi/
lammps-stable_290ct2020/examples/voronoi/README
lammps-stable_290ct2020/examples/voronoi/in.voronoi
lammps-stable_290ct2020/examples/voronoi/in.voronoi.2d
lammps-stable_290ct2020/examples/voronoi/in.voronoi.data
lammps-stable_290ct2020/examples/voronoi/log.27Nov18.voronoi.2d.g++.1
lammps-stable_290ct2020/examples/voronoi/log.27Nov18.voronoi.2d.g++.4
lammps-stable_290ct2020/examples/voronoi/log.27Nov18.voronoi.data.g++.1
lammps-stable_290ct2020/examples/voronoi/log.27Nov18.voronoi.data.g++.4
lammps-stable_290ct2020/examples/voronoi/log.27Nov18.voronoi.g++.1
lammps-stable_290ct2020/examples/voronoi/log.27Nov18.voronoi.g++.4
lammps-stable_290ct2020/examples/wall/
lammps-stable_290ct2020/examples/wall/in.wall.ccl
lammps-stable_290ct2020/examples/wall/in.wall.diffusive
lammps-stable_290ct2020/examples/wall/in.wall.maxwell
lammps-stable_290ct2020/examples/wall/in.wall.specular
lammps-stable_290ct2020/examples/wall/log.9Jan20.wall.ccl.g++.1
lammps-stable_290ct2020/examples/wall/log.9Jan20.wall.ccl.g++.4
lammps-stable_290ct2020/examples/wall/log.9Jan20.wall.diffusive.g++.1
lammps-stable_290ct2020/examples/wall/log.9Jan20.wall.diffusive.g++.4
lammps-stable_290ct2020/examples/wall/log.9Jan20.wall.maxwell.g++.1
lammps-stable_290ct2020/examples/wall/log.9Jan20.wall.maxwell.g++.4
lammps-stable_290ct2020/examples/wall/log.9Jan20.wall.specular.g++.1
lammps-stable_290ct2020/examples/wall/log.9Jan20.wall.specular.g++.4
lammps-stable_290ct2020/fortran/
lammps-stable_290ct2020/fortran/README
lammps-stable_290ct2020/fortran/lammps.f90
lammps-stable_290ct2020/lib/
lammps-stable_290ct2020/lib/Install.py
lammps-stable_290ct2020/lib/README
lammps-stable_290ct2020/lib/atc/
lammps-stable_290ct2020/lib/atc/ATC_Coupling.cpp
lammps-stable_290ct2020/lib/atc/ATC_Coupling.h
lammps-stable_290ct2020/lib/atc/ATC_CouplingEnergy.cpp
lammps-stable_290ct2020/lib/atc/ATC_CouplingEnergy.h
lammps-stable_290ct2020/lib/atc/ATC_CouplingMass.cpp
lammps-stable_290ct2020/lib/atc/ATC_CouplingMass.h
lammps-stable_290ct2020/lib/atc/ATC_CouplingMomentum.cpp
lammps-stable_290ct2020/lib/atc/ATC_CouplingMomentum.h
lammps-stable_290ct2020/lib/atc/ATC_CouplingMomentumEnergy.cpp
lammps-stable_290ct2020/lib/atc/ATC_CouplingMomentumEnergy.h
lammps-stable_290ct2020/lib/atc/ATC_Error.h
lammps-stable_290ct2020/lib/atc/ATC_Method.cpp
lammps-stable_290ct2020/lib/atc/ATC_Method.h
```

lammps-stable\_290ct2020/lib/atc/ATC\_Transfer.cpp  
lammps-stable\_290ct2020/lib/atc/ATC\_Transfer.h  
lammps-stable\_290ct2020/lib/atc/ATC\_TransferKernel.cpp  
lammps-stable\_290ct2020/lib/atc/ATC\_TransferKernel.h  
lammps-stable\_290ct2020/lib/atc/ATC\_TransferPartitionOfUnity.cpp  
lammps-stable\_290ct2020/lib/atc/ATC\_TransferPartitionOfUnity.h  
lammps-stable\_290ct2020/lib/atc/ATC\_TypeDefs.h  
lammps-stable\_290ct2020/lib/atc/Array.h  
lammps-stable\_290ct2020/lib/atc/Array2D.h  
lammps-stable\_290ct2020/lib/atc/AtomToMoleculeTransfer.cpp  
lammps-stable\_290ct2020/lib/atc/AtomToMoleculeTransfer.h  
lammps-stable\_290ct2020/lib/atc/AtomicRegulator.cpp  
lammps-stable\_290ct2020/lib/atc/AtomicRegulator.h  
lammps-stable\_290ct2020/lib/atc/BodyForce.cpp  
lammps-stable\_290ct2020/lib/atc/BodyForce.h  
lammps-stable\_290ct2020/lib/atc/CBLattice.cpp  
lammps-stable\_290ct2020/lib/atc/CBLattice.h  
lammps-stable\_290ct2020/lib/atc/CG.h  
lammps-stable\_290ct2020/lib/atc/CauchyBorn.cpp  
lammps-stable\_290ct2020/lib/atc/CauchyBorn.h  
lammps-stable\_290ct2020/lib/atc/CbEam.h  
lammps-stable\_290ct2020/lib/atc/CbLjCut.h  
lammps-stable\_290ct2020/lib/atc/CbLjSmoothLinear.h  
lammps-stable\_290ct2020/lib/atc/CbPotential.cpp  
lammps-stable\_290ct2020/lib/atc/CbPotential.h  
lammps-stable\_290ct2020/lib/atc/ChargeRegulator.cpp  
lammps-stable\_290ct2020/lib/atc/ChargeRegulator.h  
lammps-stable\_290ct2020/lib/atc/CloneVector.h  
lammps-stable\_290ct2020/lib/atc/ConcentrationRegulator.cpp  
lammps-stable\_290ct2020/lib/atc/ConcentrationRegulator.h  
lammps-stable\_290ct2020/lib/atc/DenseMatrix.h  
lammps-stable\_290ct2020/lib/atc/DenseVector.h  
lammps-stable\_290ct2020/lib/atc/DependencyManager.h  
lammps-stable\_290ct2020/lib/atc/DiagonalMatrix.h  
lammps-stable\_290ct2020/lib/atc/DislocationExtractor.h  
lammps-stable\_290ct2020/lib/atc/ElasticTimeIntegrator.cpp  
lammps-stable\_290ct2020/lib/atc/ElasticTimeIntegrator.h  
lammps-stable\_290ct2020/lib/atc/ElectronChargeDensity.cpp  
lammps-stable\_290ct2020/lib/atc/ElectronChargeDensity.h  
lammps-stable\_290ct2020/lib/atc/ElectronDragPower.cpp  
lammps-stable\_290ct2020/lib/atc/ElectronDragPower.h  
lammps-stable\_290ct2020/lib/atc/ElectronFlux.cpp  
lammps-stable\_290ct2020/lib/atc/ElectronFlux.h  
lammps-stable\_290ct2020/lib/atc/ElectronHeatCapacity.cpp  
lammps-stable\_290ct2020/lib/atc/ElectronHeatCapacity.h  
lammps-stable\_290ct2020/lib/atc/ElectronHeatFlux.cpp  
lammps-stable\_290ct2020/lib/atc/ElectronHeatFlux.h  
lammps-stable\_290ct2020/lib/atc/ElectronPhononExchange.cpp  
lammps-stable\_290ct2020/lib/atc/ElectronPhononExchange.h  
lammps-stable\_290ct2020/lib/atc/ExtrinsicModel.cpp  
lammps-stable\_290ct2020/lib/atc/ExtrinsicModel.h  
lammps-stable\_290ct2020/lib/atc/ExtrinsicModelDriftDiffusion.cpp  
lammps-stable\_290ct2020/lib/atc/ExtrinsicModelDriftDiffusion.h  
lammps-stable\_290ct2020/lib/atc/ExtrinsicModelElectrostatic.cpp  
lammps-stable\_290ct2020/lib/atc/ExtrinsicModelElectrostatic.h  
lammps-stable\_290ct2020/lib/atc/ExtrinsicModelTwoTemperature.cpp  
lammps-stable\_290ct2020/lib/atc/ExtrinsicModelTwoTemperature.h  
lammps-stable\_290ct2020/lib/atc/FE\_Element.cpp  
lammps-stable\_290ct2020/lib/atc/FE\_Element.h  
lammps-stable\_290ct2020/lib/atc/FE\_Engine.cpp

```
lammps-stable_290ct2020/lib/atc/FE_Engine.h
lammps-stable_290ct2020/lib/atc/FE_Interpolate.cpp
lammps-stable_290ct2020/lib/atc/FE_Interpolate.h
lammps-stable_290ct2020/lib/atc/FE_Mesh.cpp
lammps-stable_290ct2020/lib/atc/FE_Mesh.h
lammps-stable_290ct2020/lib/atc/FE_Quadrature.h
lammps-stable_290ct2020/lib/atc/FieldEulerIntegrator.cpp
lammps-stable_290ct2020/lib/atc/FieldEulerIntegrator.h
lammps-stable_290ct2020/lib/atc/FieldManager.cpp
lammps-stable_290ct2020/lib/atc/FieldManager.h
lammps-stable_290ct2020/lib/atc/Function.cpp
lammps-stable_290ct2020/lib/atc/Function.h
lammps-stable_290ct2020/lib/atc/FundamentalAtomicQuantity.cpp
lammps-stable_290ct2020/lib/atc/FundamentalAtomicQuantity.h
lammps-stable_290ct2020/lib/atc/GMRES.h
lammps-stable_290ct2020/lib/atc/GhostManager.cpp
lammps-stable_290ct2020/lib/atc/GhostManager.h
lammps-stable_290ct2020/lib/atc/ImplicitSolveOperator.cpp
lammps-stable_290ct2020/lib/atc/ImplicitSolveOperator.h
lammps-stable_290ct2020/lib/atc/Install.py
lammps-stable_290ct2020/lib/atc/InterscaleOperators.cpp
lammps-stable_290ct2020/lib/atc/InterscaleOperators.h
lammps-stable_290ct2020/lib/atc/KD_Tree.cpp
lammps-stable_290ct2020/lib/atc/KD_Tree.h
lammps-stable_290ct2020/lib/atc/KernelFunction.cpp
lammps-stable_290ct2020/lib/atc/KernelFunction.h
lammps-stable_290ct2020/lib/atc/KinetoThermostat.cpp
lammps-stable_290ct2020/lib/atc/KinetoThermostat.h
lammps-stable_290ct2020/lib/atc/Kinetostat.cpp
lammps-stable_290ct2020/lib/atc/Kinetostat.h
lammps-stable_290ct2020/lib/atc/LammpsInterface.cpp
lammps-stable_290ct2020/lib/atc/LammpsInterface.h
lammps-stable_290ct2020/lib/atc/LinearSolver.cpp
lammps-stable_290ct2020/lib/atc/LinearSolver.h
lammps-stable_290ct2020/lib/atc/MPI_Wrappers.cpp
lammps-stable_290ct2020/lib/atc/MPI_Wrappers.h
lammps-stable_290ct2020/lib/atc/Makefile.g++
lammps-stable_290ct2020/lib/atc/Makefile.icc
lammps-stable_290ct2020/lib/atc/Makefile.lammps.empty
lammps-stable_290ct2020/lib/atc/Makefile.lammps.installed
lammps-stable_290ct2020/lib/atc/Makefile.lammps.linalg
lammps-stable_290ct2020/lib/atc/Makefile.mpi
lammps-stable_290ct2020/lib/atc/Makefile.mpic++
lammps-stable_290ct2020/lib/atc/Makefile.serial
lammps-stable_290ct2020/lib/atc/Material.cpp
lammps-stable_290ct2020/lib/atc/Material.h
lammps-stable_290ct2020/lib/atc/Matrix.cpp
lammps-stable_290ct2020/lib/atc/Matrix.h
lammps-stable_290ct2020/lib/atc/MatrixDef.h
lammps-stable_290ct2020/lib/atc/MatrixLibrary.h
lammps-stable_290ct2020/lib/atc/MeshReader.cpp
lammps-stable_290ct2020/lib/atc/MeshReader.h
lammps-stable_290ct2020/lib/atc/MoleculeSet.cpp
lammps-stable_290ct2020/lib/atc/MoleculeSet.h
lammps-stable_290ct2020/lib/atc/NonLinearSolver.cpp
lammps-stable_290ct2020/lib/atc/NonLinearSolver.h
lammps-stable_290ct2020/lib/atc/OutputManager.cpp
lammps-stable_290ct2020/lib/atc/OutputManager.h
lammps-stable_290ct2020/lib/atc/PaqAtcUtility.cpp
lammps-stable_290ct2020/lib/atc/PaqAtcUtility.h
```

lammps-stable\_290ct2020/lib/atc/ParDenseMatrix.h  
lammps-stable\_290ct2020/lib/atc/ParDiagonalMatrix.cpp  
lammps-stable\_290ct2020/lib/atc/ParDiagonalMatrix.h  
lammps-stable\_290ct2020/lib/atc/ParSparseMatrix.cpp  
lammps-stable\_290ct2020/lib/atc/ParSparseMatrix.h  
lammps-stable\_290ct2020/lib/atc/PerAtomQuantity-inl.h  
lammps-stable\_290ct2020/lib/atc/PerAtomQuantity.h  
lammps-stable\_290ct2020/lib/atc/PerAtomQuantityLibrary.cpp  
lammps-stable\_290ct2020/lib/atc/PerAtomQuantityLibrary.h  
lammps-stable\_290ct2020/lib/atc/PerPairQuantity.cpp  
lammps-stable\_290ct2020/lib/atc/PerPairQuantity.h  
lammps-stable\_290ct2020/lib/atc/PhysicsModel.cpp  
lammps-stable\_290ct2020/lib/atc/PhysicsModel.h  
lammps-stable\_290ct2020/lib/atc/PoissonSolver.cpp  
lammps-stable\_290ct2020/lib/atc/PoissonSolver.h  
lammps-stable\_290ct2020/lib/atc/PolynomialSolver.cpp  
lammps-stable\_290ct2020/lib/atc/PolynomialSolver.h  
lammps-stable\_290ct2020/lib/atc/PrescribedDataManager.cpp  
lammps-stable\_290ct2020/lib/atc/PrescribedDataManager.h  
lammps-stable\_290ct2020/lib/atc/Quadrature.cpp  
lammps-stable\_290ct2020/lib/atc/Quadrature.h  
lammps-stable\_290ct2020/lib/atc/README  
lammps-stable\_290ct2020/lib/atc/SchrodingerSolver.cpp  
lammps-stable\_290ct2020/lib/atc/SchrodingerSolver.h  
lammps-stable\_290ct2020/lib/atc/ShapeFunction.h  
lammps-stable\_290ct2020/lib/atc/SparseMatrix-inl.h  
lammps-stable\_290ct2020/lib/atc/SparseMatrix.h  
lammps-stable\_290ct2020/lib/atc/SparseVector-inl.h  
lammps-stable\_290ct2020/lib/atc/SparseVector.h  
lammps-stable\_290ct2020/lib/atc/SpeciesTimeIntegrator.cpp  
lammps-stable\_290ct2020/lib/atc/SpeciesTimeIntegrator.h  
lammps-stable\_290ct2020/lib/atc/Stress.cpp  
lammps-stable\_290ct2020/lib/atc/Stress.h  
lammps-stable\_290ct2020/lib/atc/ThermalTimeIntegrator.cpp  
lammps-stable\_290ct2020/lib/atc/ThermalTimeIntegrator.h  
lammps-stable\_290ct2020/lib/atc/Thermostat.cpp  
lammps-stable\_290ct2020/lib/atc/Thermostat.h  
lammps-stable\_290ct2020/lib/atc/TimeFilter.cpp  
lammps-stable\_290ct2020/lib/atc/TimeFilter.h  
lammps-stable\_290ct2020/lib/atc/TimeIntegrator.cpp  
lammps-stable\_290ct2020/lib/atc/TimeIntegrator.h  
lammps-stable\_290ct2020/lib/atc/TransferLibrary.cpp  
lammps-stable\_290ct2020/lib/atc/TransferLibrary.h  
lammps-stable\_290ct2020/lib/atc/TransferOperator.cpp  
lammps-stable\_290ct2020/lib/atc/TransferOperator.h  
lammps-stable\_290ct2020/lib/atc/Utility.h  
lammps-stable\_290ct2020/lib/atc/Vector.cpp  
lammps-stable\_290ct2020/lib/atc/Vector.h  
lammps-stable\_290ct2020/lib/atc/ViscousStress.cpp  
lammps-stable\_290ct2020/lib/atc/ViscousStress.h  
lammps-stable\_290ct2020/lib/atc/VoigtOperations.h  
lammps-stable\_290ct2020/lib/atc/WeakEquation.h  
lammps-stable\_290ct2020/lib/atc/WeakEquationChargeDiffusion.cpp  
lammps-stable\_290ct2020/lib/atc/WeakEquationChargeDiffusion.h  
lammps-stable\_290ct2020/lib/atc/WeakEquationDiffusion.cpp  
lammps-stable\_290ct2020/lib/atc/WeakEquationDiffusion.h  
lammps-stable\_290ct2020/lib/atc/WeakEquationElectronContinuity.cpp  
lammps-stable\_290ct2020/lib/atc/WeakEquationElectronContinuity.h  
lammps-stable\_290ct2020/lib/atc/WeakEquationElectronMomentum.cpp  
lammps-stable\_290ct2020/lib/atc/WeakEquationElectronMomentum.h

```
lammps-stable_290ct2020/lib/atc/WeakEquationElectronTemperature.cpp
lammps-stable_290ct2020/lib/atc/WeakEquationElectronTemperature.h
lammps-stable_290ct2020/lib/atc/WeakEquationMassDiffusion.cpp
lammps-stable_290ct2020/lib/atc/WeakEquationMassDiffusion.h
lammps-stable_290ct2020/lib/atc/WeakEquationMomentum.cpp
lammps-stable_290ct2020/lib/atc/WeakEquationMomentum.h
lammps-stable_290ct2020/lib/atc/WeakEquationPhononTemperature.cpp
lammps-stable_290ct2020/lib/atc/WeakEquationPhononTemperature.h
lammps-stable_290ct2020/lib/atc/WeakEquationPoisson.cpp
lammps-stable_290ct2020/lib/atc/WeakEquationPoisson.h
lammps-stable_290ct2020/lib/atc/WeakEquationSchrodinger.cpp
lammps-stable_290ct2020/lib/atc/WeakEquationSchrodinger.h
lammps-stable_290ct2020/lib/awpmd/
lammps-stable_290ct2020/lib/awpmd/Install.py
lammps-stable_290ct2020/lib/awpmd/Makefile.lammps.empty
lammps-stable_290ct2020/lib/awpmd/Makefile.lammps.installed
lammps-stable_290ct2020/lib/awpmd/Makefile.lammps.linalg
lammps-stable_290ct2020/lib/awpmd/Makefile.mpi
lammps-stable_290ct2020/lib/awpmd/Makefile.mpicc
lammps-stable_290ct2020/lib/awpmd/Makefile.serial
lammps-stable_290ct2020/lib/awpmd/README
lammps-stable_290ct2020/lib/awpmd/ivutils/
lammps-stable_290ct2020/lib/awpmd/ivutils/include/
lammps-stable_290ct2020/lib/awpmd/ivutils/include/cerf.h
lammps-stable_290ct2020/lib/awpmd/ivutils/include/cvector_3.h
lammps-stable_290ct2020/lib/awpmd/ivutils/include/erf.h
lammps-stable_290ct2020/lib/awpmd/ivutils/include/lapack_inter.h
lammps-stable_290ct2020/lib/awpmd/ivutils/include/logexc.h
lammps-stable_290ct2020/lib/awpmd/ivutils/include/pairhash.h
lammps-stable_290ct2020/lib/awpmd/ivutils/include/refobj.h
lammps-stable_290ct2020/lib/awpmd/ivutils/include/vector_3.h
lammps-stable_290ct2020/lib/awpmd/ivutils/include/wavepacket.h
lammps-stable_290ct2020/lib/awpmd/ivutils/src/
lammps-stable_290ct2020/lib/awpmd/ivutils/src/logexc.cpp
lammps-stable_290ct2020/lib/awpmd/license/
lammps-stable_290ct2020/lib/awpmd/license/COPYING
lammps-stable_290ct2020/lib/awpmd/license/awpmd_license.txt
lammps-stable_290ct2020/lib/awpmd/license/wx_license.txt
lammps-stable_290ct2020/lib/awpmd/systems/
lammps-stable_290ct2020/lib/awpmd/systems/interact/
lammps-stable_290ct2020/lib/awpmd/systems/interact/TCP/
lammps-stable_290ct2020/lib/awpmd/systems/interact/TCP/tcpdefs.h
lammps-stable_290ct2020/lib/awpmd/systems/interact/TCP/wpmd.cpp
lammps-stable_290ct2020/lib/awpmd/systems/interact/TCP/wpmd.h
lammps-stable_290ct2020/lib/awpmd/systems/interact/TCP/wpmd_split.cpp
lammps-stable_290ct2020/lib/awpmd/systems/interact/TCP/wpmd_split.h
lammps-stable_290ct2020/lib/colvars/
lammps-stable_290ct2020/lib/colvars/Install.py
lammps-stable_290ct2020/lib/colvars/Makefile.common
lammps-stable_290ct2020/lib/colvars/Makefile.deps
lammps-stable_290ct2020/lib/colvars/Makefile.g++
lammps-stable_290ct2020/lib/colvars/Makefile.g++-debug
lammps-stable_290ct2020/lib/colvars/Makefile.g++-no-lepton
lammps-stable_290ct2020/lib/colvars/Makefile.lammps.debug
lammps-stable_290ct2020/lib/colvars/Makefile.lammps.empty
lammps-stable_290ct2020/lib/colvars/Makefile.lepton.deps
lammps-stable_290ct2020/lib/colvars/Makefile.mpi
lammps-stable_290ct2020/lib/colvars/Makefile.serial
lammps-stable_290ct2020/lib/colvars/README
lammps-stable_290ct2020/lib/colvars/colvar.cpp
```

```
lammps-stable_290ct2020/lib/colvars/colvar.h
lammps-stable_290ct2020/lib/colvars/colvar_UIestimator.h
lammps-stable_290ct2020/lib/colvars/colvar_arithmeticpath.h
lammps-stable_290ct2020/lib/colvars/colvar_geometricpath.h
lammps-stable_290ct2020/lib/colvars/colvaratoms.cpp
lammps-stable_290ct2020/lib/colvars/colvaratoms.h
lammps-stable_290ct2020/lib/colvars/colvarbias.cpp
lammps-stable_290ct2020/lib/colvars/colvarbias.h
lammps-stable_290ct2020/lib/colvars/colvarbias_abf.cpp
lammps-stable_290ct2020/lib/colvars/colvarbias_abf.h
lammps-stable_290ct2020/lib/colvars/colvarbias_alb.cpp
lammps-stable_290ct2020/lib/colvars/colvarbias_alb.h
lammps-stable_290ct2020/lib/colvars/colvarbias_histogram.cpp
lammps-stable_290ct2020/lib/colvars/colvarbias_histogram.h
lammps-stable_290ct2020/lib/colvars/colvarbias_meta.cpp
lammps-stable_290ct2020/lib/colvars/colvarbias_meta.h
lammps-stable_290ct2020/lib/colvars/colvarbias_restraint.cpp
lammps-stable_290ct2020/lib/colvars/colvarbias_restraint.h
lammps-stable_290ct2020/lib/colvars/colvarcomp.cpp
lammps-stable_290ct2020/lib/colvars/colvarcomp.h
lammps-stable_290ct2020/lib/colvars/colvarcomp_angles.cpp
lammps-stable_290ct2020/lib/colvars/colvarcomp_aphath.cpp
lammps-stable_290ct2020/lib/colvars/colvarcomp_coordnums.cpp
lammps-stable_290ct2020/lib/colvars/colvarcomp_distances.cpp
lammps-stable_290ct2020/lib/colvars/colvarcomp_gpath.cpp
lammps-stable_290ct2020/lib/colvars/colvarcomp_protein.cpp
lammps-stable_290ct2020/lib/colvars/colvarcomp_rotations.cpp
lammps-stable_290ct2020/lib/colvars/colvarcomp_volmaps.cpp
lammps-stable_290ct2020/lib/colvars/colvardeps.cpp
lammps-stable_290ct2020/lib/colvars/colvardeps.h
lammps-stable_290ct2020/lib/colvars/colvargrid.cpp
lammps-stable_290ct2020/lib/colvars/colvargrid.h
lammps-stable_290ct2020/lib/colvars/colvarmodule.cpp
lammps-stable_290ct2020/lib/colvars/colvarmodule.h
lammps-stable_290ct2020/lib/colvars/colvarparams.cpp
lammps-stable_290ct2020/lib/colvars/colvarparams.h
lammps-stable_290ct2020/lib/colvars/colvarparse.cpp
lammps-stable_290ct2020/lib/colvars/colvarparse.h
lammps-stable_290ct2020/lib/colvars/colvarproxy.cpp
lammps-stable_290ct2020/lib/colvars/colvarproxy.h
lammps-stable_290ct2020/lib/colvars/colvarproxy_replicas.cpp
lammps-stable_290ct2020/lib/colvars/colvarproxy_tcl.cpp
lammps-stable_290ct2020/lib/colvars/colvarproxy_tcl.h
lammps-stable_290ct2020/lib/colvars/colvarproxy_volmaps.cpp
lammps-stable_290ct2020/lib/colvars/colvarproxy_volmaps.h
lammps-stable_290ct2020/lib/colvars/colvars_version.h
lammps-stable_290ct2020/lib/colvars/colvarscript.cpp
lammps-stable_290ct2020/lib/colvars/colvarscript.h
lammps-stable_290ct2020/lib/colvars/colvarscript_commands.cpp
lammps-stable_290ct2020/lib/colvars/colvarscript_commands.h
lammps-stable_290ct2020/lib/colvars/colvarscript_commands_bias.cpp
lammps-stable_290ct2020/lib/colvars/colvarscript_commands_bias.h
lammps-stable_290ct2020/lib/colvars/colvarscript_commands_colvar.cpp
lammps-stable_290ct2020/lib/colvars/colvarscript_commands_colvar.h
lammps-stable_290ct2020/lib/colvars/colvartypes.cpp
lammps-stable_290ct2020/lib/colvars/colvartypes.h
lammps-stable_290ct2020/lib/colvars/colvarvalue.cpp
lammps-stable_290ct2020/lib/colvars/colvarvalue.h
lammps-stable_290ct2020/lib/colvars/lepton/
lammps-stable_290ct2020/lib/colvars/lepton/include/
```

```
lammps-stable_290ct2020/lib/colvars/lepton/include/Lepton.h
lammps-stable_290ct2020/lib/colvars/lepton/include/lepton/
lammps-stable_290ct2020/lib/colvars/lepton/include/lepton/CompiledExpression.
h
lammps-stable_290ct2020/lib/colvars/lepton/include/lepton/CustomFunction.h
lammps-stable_290ct2020/lib/colvars/lepton/include/lepton/Exception.h
lammps-stable_290ct2020/lib/colvars/lepton/include/lepton/ExpressionProgram.h
lammps-stable_290ct2020/lib/colvars/lepton/include/lepton/ExpressionTreeNode.
h
lammps-stable_290ct2020/lib/colvars/lepton/include/lepton/Operation.h
lammps-stable_290ct2020/lib/colvars/lepton/include/lepton/ParsedExpression.h
lammps-stable_290ct2020/lib/colvars/lepton/include/lepton/Parser.h
lammps-stable_290ct2020/lib/colvars/lepton/include/lepton/windowsIncludes.h
lammps-stable_290ct2020/lib/colvars/lepton/src/
lammps-stable_290ct2020/lib/colvars/lepton/src/CompiledExpression.cpp
lammps-stable_290ct2020/lib/colvars/lepton/src/ExpressionProgram.cpp
lammps-stable_290ct2020/lib/colvars/lepton/src/ExpressionTreeNode.cpp
lammps-stable_290ct2020/lib/colvars/lepton/src/MSVC_erfc.h
lammps-stable_290ct2020/lib/colvars/lepton/src/Operation.cpp
lammps-stable_290ct2020/lib/colvars/lepton/src/ParsedExpression.cpp
lammps-stable_290ct2020/lib/colvars/lepton/src/Parser.cpp
lammps-stable_290ct2020/lib/compress/
lammps-stable_290ct2020/lib/compress/Makefile.lammps
lammps-stable_290ct2020/lib/compress/README
lammps-stable_290ct2020/lib/gpu/
lammps-stable_290ct2020/lib/gpu/Install.py
lammps-stable_290ct2020/lib/gpu/Makefile.fermi
lammps-stable_290ct2020/lib/gpu/Makefile.hip
lammps-stable_290ct2020/lib/gpu/Makefile.lammps.mac_osx
lammps-stable_290ct2020/lib/gpu/Makefile.lammps.mingw-cross
lammps-stable_290ct2020/lib/gpu/Makefile.lammps.openc1
lammps-stable_290ct2020/lib/gpu/Makefile.lammps.standard
lammps-stable_290ct2020/lib/gpu/Makefile.linux
lammps-stable_290ct2020/lib/gpu/Makefile.linux.double
lammps-stable_290ct2020/lib/gpu/Makefile.linux.mixed
lammps-stable_290ct2020/lib/gpu/Makefile.linux.single
lammps-stable_290ct2020/lib/gpu/Makefile.linux_multi
lammps-stable_290ct2020/lib/gpu/Makefile.linux_openc1
lammps-stable_290ct2020/lib/gpu/Makefile.mac_openc1
lammps-stable_290ct2020/lib/gpu/Makefile.mpi
lammps-stable_290ct2020/lib/gpu/Makefile.serial
lammps-stable_290ct2020/lib/gpu/Makefile.serial_openc1
lammps-stable_290ct2020/lib/gpu/Makefile.xk7
lammps-stable_290ct2020/lib/gpu/Nvidia.makefile
lammps-stable_290ct2020/lib/gpu/Nvidia.makefile_multi
lammps-stable_290ct2020/lib/gpu/Opencl.makefile
lammps-stable_290ct2020/lib/gpu/README
lammps-stable_290ct2020/lib/gpu/cudpp_mini/
lammps-stable_290ct2020/lib/gpu/cudpp_mini/README
lammps-stable_290ct2020/lib/gpu/cudpp_mini/cta/
lammps-stable_290ct2020/lib/gpu/cudpp_mini/cta/radixsort_cta.cu
lammps-stable_290ct2020/lib/gpu/cudpp_mini/cta/scan_cta.cu
lammps-stable_290ct2020/lib/gpu/cudpp_mini/cudpp.cpp
lammps-stable_290ct2020/lib/gpu/cudpp_mini/cudpp.h
lammps-stable_290ct2020/lib/gpu/cudpp_mini/cudpp_globals.h
lammps-stable_290ct2020/lib/gpu/cudpp_mini/cudpp_maximal_launch.cpp
lammps-stable_290ct2020/lib/gpu/cudpp_mini/cudpp_maximal_launch.h
lammps-stable_290ct2020/lib/gpu/cudpp_mini/cudpp_plan.cpp
lammps-stable_290ct2020/lib/gpu/cudpp_mini/cudpp_plan.h
lammps-stable_290ct2020/lib/gpu/cudpp_mini/cudpp_plan_manager.cpp
```

```
lammps-stable_290ct2020/lib/gpu/cudpp_mini/cudpp_plan_manager.h
lammps-stable_290ct2020/lib/gpu/cudpp_mini/cudpp_radixsort.h
lammps-stable_290ct2020/lib/gpu/cudpp_mini/cudpp_scan.h
lammps-stable_290ct2020/lib/gpu/cudpp_mini/cudpp_util.h
lammps-stable_290ct2020/lib/gpu/cudpp_mini/cutil.h
lammps-stable_290ct2020/lib/gpu/cudpp_mini/kernel/
lammps-stable_290ct2020/lib/gpu/cudpp_mini/kernel/radixsort_kernel.cu
lammps-stable_290ct2020/lib/gpu/cudpp_mini/kernel/scan_kernel.cu
lammps-stable_290ct2020/lib/gpu/cudpp_mini/kernel/vector_kernel.cu
lammps-stable_290ct2020/lib/gpu/cudpp_mini/license.txt
lammps-stable_290ct2020/lib/gpu/cudpp_mini/radixsort_app.cu
lammps-stable_290ct2020/lib/gpu/cudpp_mini/scan_app.cu
lammps-stable_290ct2020/lib/gpu/cudpp_mini/sharedmem.h
lammps-stable_290ct2020/lib/gpu/geryon/
lammps-stable_290ct2020/lib/gpu/geryon/README
lammps-stable_290ct2020/lib/gpu/geryon/VERSION.txt
lammps-stable_290ct2020/lib/gpu/geryon/file_to_cstr.sh
lammps-stable_290ct2020/lib/gpu/geryon/hip_device.h
lammps-stable_290ct2020/lib/gpu/geryon/hip_kernel.h
lammps-stable_290ct2020/lib/gpu/geryon/hip_macros.h
lammps-stable_290ct2020/lib/gpu/geryon/hip_mat.h
lammps-stable_290ct2020/lib/gpu/geryon/hip_memory.h
lammps-stable_290ct2020/lib/gpu/geryon/hip_texture.h
lammps-stable_290ct2020/lib/gpu/geryon/hip_timer.h
lammps-stable_290ct2020/lib/gpu/geryon/nvd_device.h
lammps-stable_290ct2020/lib/gpu/geryon/nvd_kernel.h
lammps-stable_290ct2020/lib/gpu/geryon/nvd_macros.h
lammps-stable_290ct2020/lib/gpu/geryon/nvd_mat.h
lammps-stable_290ct2020/lib/gpu/geryon/nvd_memory.h
lammps-stable_290ct2020/lib/gpu/geryon/nvd_texture.h
lammps-stable_290ct2020/lib/gpu/geryon/nvd_timer.h
lammps-stable_290ct2020/lib/gpu/geryon/ocl_device.h
lammps-stable_290ct2020/lib/gpu/geryon/ocl_kernel.h
lammps-stable_290ct2020/lib/gpu/geryon/ocl_macros.h
lammps-stable_290ct2020/lib/gpu/geryon/ocl_mat.h
lammps-stable_290ct2020/lib/gpu/geryon/ocl_memory.h
lammps-stable_290ct2020/lib/gpu/geryon/ocl_texture.h
lammps-stable_290ct2020/lib/gpu/geryon/ocl_timer.h
lammps-stable_290ct2020/lib/gpu/geryon/ucl_arg_kludge.h
lammps-stable_290ct2020/lib/gpu/geryon/ucl_basemat.h
lammps-stable_290ct2020/lib/gpu/geryon/ucl_copy.h
lammps-stable_290ct2020/lib/gpu/geryon/ucl_d_mat.h
lammps-stable_290ct2020/lib/gpu/geryon/ucl_d_vec.h
lammps-stable_290ct2020/lib/gpu/geryon/ucl_get_devices.cpp
lammps-stable_290ct2020/lib/gpu/geryon/ucl_h_mat.h
lammps-stable_290ct2020/lib/gpu/geryon/ucl_h_vec.h
lammps-stable_290ct2020/lib/gpu/geryon/ucl_matrix.h
lammps-stable_290ct2020/lib/gpu/geryon/ucl_nv_kernel.h
lammps-stable_290ct2020/lib/gpu/geryon/ucl_print.h
lammps-stable_290ct2020/lib/gpu/geryon/ucl_s_obj_help.h
lammps-stable_290ct2020/lib/gpu/geryon/ucl_types.h
lammps-stable_290ct2020/lib/gpu/geryon/ucl_vector.h
lammps-stable_290ct2020/lib/gpu/lal_answer.cpp
lammps-stable_290ct2020/lib/gpu/lal_answer.h
lammps-stable_290ct2020/lib/gpu/lal_atom.cpp
lammps-stable_290ct2020/lib/gpu/lal_atom.cu
lammps-stable_290ct2020/lib/gpu/lal_atom.h
lammps-stable_290ct2020/lib/gpu/lal_aux_fun1.h
lammps-stable_290ct2020/lib/gpu/lal_balance.h
lammps-stable_290ct2020/lib/gpu/lal_base_atomic.cpp
```



lammps-stable\_290ct2020/lib/gpu/lal\_base\_atomic.h  
lammps-stable\_290ct2020/lib/gpu/lal\_base\_charge.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_base\_charge.h  
lammps-stable\_290ct2020/lib/gpu/lal\_base\_dipole.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_base\_dipole.h  
lammps-stable\_290ct2020/lib/gpu/lal\_base\_dpd.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_base\_dpd.h  
lammps-stable\_290ct2020/lib/gpu/lal\_base\_ellipsoid.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_base\_ellipsoid.h  
lammps-stable\_290ct2020/lib/gpu/lal\_base\_three.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_base\_three.h  
lammps-stable\_290ct2020/lib/gpu/lal\_beck.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_beck.cu  
lammps-stable\_290ct2020/lib/gpu/lal\_beck.h  
lammps-stable\_290ct2020/lib/gpu/lal\_beck\_ext.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_born.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_born.cu  
lammps-stable\_290ct2020/lib/gpu/lal\_born.h  
lammps-stable\_290ct2020/lib/gpu/lal\_born\_coul\_long.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_born\_coul\_long.cu  
lammps-stable\_290ct2020/lib/gpu/lal\_born\_coul\_long.h  
lammps-stable\_290ct2020/lib/gpu/lal\_born\_coul\_long\_cs.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_born\_coul\_long\_cs.cu  
lammps-stable\_290ct2020/lib/gpu/lal\_born\_coul\_long\_cs.h  
lammps-stable\_290ct2020/lib/gpu/lal\_born\_coul\_long\_cs\_ext.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_born\_coul\_long\_ext.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_born\_coul\_wolf.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_born\_coul\_wolf.cu  
lammps-stable\_290ct2020/lib/gpu/lal\_born\_coul\_wolf.h  
lammps-stable\_290ct2020/lib/gpu/lal\_born\_coul\_wolf\_cs.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_born\_coul\_wolf\_cs.cu  
lammps-stable\_290ct2020/lib/gpu/lal\_born\_coul\_wolf\_cs.h  
lammps-stable\_290ct2020/lib/gpu/lal\_born\_coul\_wolf\_cs\_ext.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_born\_coul\_wolf\_ext.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_born\_ext.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_buck.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_buck.cu  
lammps-stable\_290ct2020/lib/gpu/lal\_buck.h  
lammps-stable\_290ct2020/lib/gpu/lal\_buck\_coul.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_buck\_coul.cu  
lammps-stable\_290ct2020/lib/gpu/lal\_buck\_coul.h  
lammps-stable\_290ct2020/lib/gpu/lal\_buck\_coul\_ext.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_buck\_coul\_long.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_buck\_coul\_long.cu  
lammps-stable\_290ct2020/lib/gpu/lal\_buck\_coul\_long.h  
lammps-stable\_290ct2020/lib/gpu/lal\_buck\_coul\_long\_ext.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_buck\_ext.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_charmm\_long.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_charmm\_long.cu  
lammps-stable\_290ct2020/lib/gpu/lal\_charmm\_long.h  
lammps-stable\_290ct2020/lib/gpu/lal\_charmm\_long\_ext.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_colloid.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_colloid.cu  
lammps-stable\_290ct2020/lib/gpu/lal\_colloid.h  
lammps-stable\_290ct2020/lib/gpu/lal\_colloid\_ext.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_coul.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_coul.cu  
lammps-stable\_290ct2020/lib/gpu/lal\_coul.h  
lammps-stable\_290ct2020/lib/gpu/lal\_coul\_debye.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_coul\_debye.cu

lammps-stable\_290ct2020/lib/gpu/lal\_coul\_debye.h  
lammps-stable\_290ct2020/lib/gpu/lal\_coul\_debye\_ext.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_coul\_dsf.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_coul\_dsf.cu  
lammps-stable\_290ct2020/lib/gpu/lal\_coul\_dsf.h  
lammps-stable\_290ct2020/lib/gpu/lal\_coul\_dsf\_ext.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_coul\_ext.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_coul\_long.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_coul\_long.cu  
lammps-stable\_290ct2020/lib/gpu/lal\_coul\_long.h  
lammps-stable\_290ct2020/lib/gpu/lal\_coul\_long\_cs.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_coul\_long\_cs.cu  
lammps-stable\_290ct2020/lib/gpu/lal\_coul\_long\_cs.h  
lammps-stable\_290ct2020/lib/gpu/lal\_coul\_long\_cs\_ext.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_coul\_long\_ext.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_device.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_device.cu  
lammps-stable\_290ct2020/lib/gpu/lal\_device.h  
lammps-stable\_290ct2020/lib/gpu/lal\_dipole\_lj.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_dipole\_lj.cu  
lammps-stable\_290ct2020/lib/gpu/lal\_dipole\_lj.h  
lammps-stable\_290ct2020/lib/gpu/lal\_dipole\_lj\_ext.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_dipole\_lj\_sf.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_dipole\_lj\_sf.cu  
lammps-stable\_290ct2020/lib/gpu/lal\_dipole\_lj\_sf.h  
lammps-stable\_290ct2020/lib/gpu/lal\_dipole\_lj\_sf\_ext.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_dipole\_long\_lj.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_dipole\_long\_lj.cu  
lammps-stable\_290ct2020/lib/gpu/lal\_dipole\_long\_lj.h  
lammps-stable\_290ct2020/lib/gpu/lal\_dipole\_long\_lj\_ext.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_dpd.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_dpd.cu  
lammps-stable\_290ct2020/lib/gpu/lal\_dpd.h  
lammps-stable\_290ct2020/lib/gpu/lal\_dpd\_ext.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_dpd\_tstat\_ext.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_eam.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_eam.cu  
lammps-stable\_290ct2020/lib/gpu/lal\_eam.h  
lammps-stable\_290ct2020/lib/gpu/lal\_eam\_alloy\_ext.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_eam\_ext.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_eam\_fs\_ext.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_ellipsoid\_extra.h  
lammps-stable\_290ct2020/lib/gpu/lal\_ellipsoid\_nbor.cu  
lammps-stable\_290ct2020/lib/gpu/lal\_gauss.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_gauss.cu  
lammps-stable\_290ct2020/lib/gpu/lal\_gauss.h  
lammps-stable\_290ct2020/lib/gpu/lal\_gauss\_ext.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_gayberne.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_gayberne.cu  
lammps-stable\_290ct2020/lib/gpu/lal\_gayberne.h  
lammps-stable\_290ct2020/lib/gpu/lal\_gayberne\_ext.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_gayberne\_lj.cu  
lammps-stable\_290ct2020/lib/gpu/lal\_lj.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_lj.cu  
lammps-stable\_290ct2020/lib/gpu/lal\_lj.h  
lammps-stable\_290ct2020/lib/gpu/lal\_lj96.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_lj96.cu  
lammps-stable\_290ct2020/lib/gpu/lal\_lj96.h  
lammps-stable\_290ct2020/lib/gpu/lal\_lj96\_ext.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_lj\_class2\_long.cpp

lammps-stable\_290ct2020/lib/gpu/lal\_lj\_class2\_long.cu  
lammps-stable\_290ct2020/lib/gpu/lal\_lj\_class2\_long.h  
lammps-stable\_290ct2020/lib/gpu/lal\_lj\_class2\_long\_ext.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_lj\_coul.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_lj\_coul.cu  
lammps-stable\_290ct2020/lib/gpu/lal\_lj\_coul.h  
lammps-stable\_290ct2020/lib/gpu/lal\_lj\_coul\_debye.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_lj\_coul\_debye.cu  
lammps-stable\_290ct2020/lib/gpu/lal\_lj\_coul\_debye.h  
lammps-stable\_290ct2020/lib/gpu/lal\_lj\_coul\_debye\_ext.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_lj\_coul\_ext.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_lj\_coul\_long.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_lj\_coul\_long.cu  
lammps-stable\_290ct2020/lib/gpu/lal\_lj\_coul\_long.h  
lammps-stable\_290ct2020/lib/gpu/lal\_lj\_coul\_long\_ext.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_lj\_coul\_msm.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_lj\_coul\_msm.cu  
lammps-stable\_290ct2020/lib/gpu/lal\_lj\_coul\_msm.h  
lammps-stable\_290ct2020/lib/gpu/lal\_lj\_coul\_msm\_ext.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_lj\_cubic.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_lj\_cubic.cu  
lammps-stable\_290ct2020/lib/gpu/lal\_lj\_cubic.h  
lammps-stable\_290ct2020/lib/gpu/lal\_lj\_cubic\_ext.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_lj\_dsf.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_lj\_dsf.cu  
lammps-stable\_290ct2020/lib/gpu/lal\_lj\_dsf.h  
lammps-stable\_290ct2020/lib/gpu/lal\_lj\_dsf\_ext.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_lj\_expand.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_lj\_expand.cu  
lammps-stable\_290ct2020/lib/gpu/lal\_lj\_expand.h  
lammps-stable\_290ct2020/lib/gpu/lal\_lj\_expand\_coul\_long.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_lj\_expand\_coul\_long.cu  
lammps-stable\_290ct2020/lib/gpu/lal\_lj\_expand\_coul\_long.h  
lammps-stable\_290ct2020/lib/gpu/lal\_lj\_expand\_coul\_long\_ext.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_lj\_expand\_ext.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_lj\_ext.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_lj\_gromacs.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_lj\_gromacs.cu  
lammps-stable\_290ct2020/lib/gpu/lal\_lj\_gromacs.h  
lammps-stable\_290ct2020/lib/gpu/lal\_lj\_gromacs\_ext.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_lj\_sdk.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_lj\_sdk.cu  
lammps-stable\_290ct2020/lib/gpu/lal\_lj\_sdk.h  
lammps-stable\_290ct2020/lib/gpu/lal\_lj\_sdk\_ext.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_lj\_sdk\_long.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_lj\_sdk\_long.cu  
lammps-stable\_290ct2020/lib/gpu/lal\_lj\_sdk\_long.h  
lammps-stable\_290ct2020/lib/gpu/lal\_lj\_sdk\_long\_ext.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_lj\_tip4p\_long.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_lj\_tip4p\_long.cu  
lammps-stable\_290ct2020/lib/gpu/lal\_lj\_tip4p\_long.h  
lammps-stable\_290ct2020/lib/gpu/lal\_lj\_tip4p\_long\_ext.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_mie.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_mie.cu  
lammps-stable\_290ct2020/lib/gpu/lal\_mie.h  
lammps-stable\_290ct2020/lib/gpu/lal\_mie\_ext.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_morse.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_morse.cu  
lammps-stable\_290ct2020/lib/gpu/lal\_morse.h  
lammps-stable\_290ct2020/lib/gpu/lal\_morse\_ext.cpp

lammps-stable\_290ct2020/lib/gpu/lal\_neighbor.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_neighbor.h  
lammps-stable\_290ct2020/lib/gpu/lal\_neighbor\_cpu.cu  
lammps-stable\_290ct2020/lib/gpu/lal\_neighbor\_gpu.cu  
lammps-stable\_290ct2020/lib/gpu/lal\_neighbor\_shared.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_neighbor\_shared.h  
lammps-stable\_290ct2020/lib/gpu/lal\_pppm.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_pppm.cu  
lammps-stable\_290ct2020/lib/gpu/lal\_pppm.h  
lammps-stable\_290ct2020/lib/gpu/lal\_pppm\_ext.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_precision.h  
lammps-stable\_290ct2020/lib/gpu/lal\_preprocessor.h  
lammps-stable\_290ct2020/lib/gpu/lal\_re\_squared.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_re\_squared.cu  
lammps-stable\_290ct2020/lib/gpu/lal\_re\_squared.h  
lammps-stable\_290ct2020/lib/gpu/lal\_re\_squared\_ext.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_re\_squared\_lj.cu  
lammps-stable\_290ct2020/lib/gpu/lal\_soft.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_soft.cu  
lammps-stable\_290ct2020/lib/gpu/lal\_soft.h  
lammps-stable\_290ct2020/lib/gpu/lal\_soft\_ext.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_sw.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_sw.cu  
lammps-stable\_290ct2020/lib/gpu/lal\_sw.h  
lammps-stable\_290ct2020/lib/gpu/lal\_sw\_ext.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_table.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_table.cu  
lammps-stable\_290ct2020/lib/gpu/lal\_table.h  
lammps-stable\_290ct2020/lib/gpu/lal\_table\_ext.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_tersoff.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_tersoff.cu  
lammps-stable\_290ct2020/lib/gpu/lal\_tersoff.h  
lammps-stable\_290ct2020/lib/gpu/lal\_tersoff\_ext.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_tersoff\_extra.h  
lammps-stable\_290ct2020/lib/gpu/lal\_tersoff\_mod.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_tersoff\_mod.cu  
lammps-stable\_290ct2020/lib/gpu/lal\_tersoff\_mod.h  
lammps-stable\_290ct2020/lib/gpu/lal\_tersoff\_mod\_ext.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_tersoff\_mod\_extra.h  
lammps-stable\_290ct2020/lib/gpu/lal\_tersoff\_zbl.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_tersoff\_zbl.cu  
lammps-stable\_290ct2020/lib/gpu/lal\_tersoff\_zbl.h  
lammps-stable\_290ct2020/lib/gpu/lal\_tersoff\_zbl\_ext.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_tersoff\_zbl\_extra.h  
lammps-stable\_290ct2020/lib/gpu/lal\_uvm.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_uvm.cu  
lammps-stable\_290ct2020/lib/gpu/lal\_uvm.h  
lammps-stable\_290ct2020/lib/gpu/lal\_uvm\_ext.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_vashishta.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_vashishta.cu  
lammps-stable\_290ct2020/lib/gpu/lal\_vashishta.h  
lammps-stable\_290ct2020/lib/gpu/lal\_vashishta\_ext.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_yukawa.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_yukawa.cu  
lammps-stable\_290ct2020/lib/gpu/lal\_yukawa.h  
lammps-stable\_290ct2020/lib/gpu/lal\_yukawa\_colloid.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_yukawa\_colloid.cu  
lammps-stable\_290ct2020/lib/gpu/lal\_yukawa\_colloid.h  
lammps-stable\_290ct2020/lib/gpu/lal\_yukawa\_colloid\_ext.cpp  
lammps-stable\_290ct2020/lib/gpu/lal\_yukawa\_ext.cpp

```
lammps-stable_290ct2020/lib/gpu/lal_zbl.cpp
lammps-stable_290ct2020/lib/gpu/lal_zbl.cu
lammps-stable_290ct2020/lib/gpu/lal_zbl.h
lammps-stable_290ct2020/lib/gpu/lal_zbl_ext.cpp
lammps-stable_290ct2020/lib/h5md/
lammps-stable_290ct2020/lib/h5md/Install.py
lammps-stable_290ct2020/lib/h5md/LICENSE
lammps-stable_290ct2020/lib/h5md/Makefile.h5cc
lammps-stable_290ct2020/lib/h5md/Makefile.lammps.empty
lammps-stable_290ct2020/lib/h5md/Makefile.mpi
lammps-stable_290ct2020/lib/h5md/Makefile.serial
lammps-stable_290ct2020/lib/h5md/README
lammps-stable_290ct2020/lib/h5md/include/
lammps-stable_290ct2020/lib/h5md/include/ch5md.h
lammps-stable_290ct2020/lib/h5md/src/
lammps-stable_290ct2020/lib/h5md/src/ch5md.c
lammps-stable_290ct2020/lib/install_helpers.py
lammps-stable_290ct2020/lib/kim/
lammps-stable_290ct2020/lib/kim/Install.py
lammps-stable_290ct2020/lib/kim/Makefile.lammps
lammps-stable_290ct2020/lib/kim/README
lammps-stable_290ct2020/lib/kokkos/
lammps-stable_290ct2020/lib/kokkos/BUILD.md
lammps-stable_290ct2020/lib/kokkos/CHANGELOG.md
lammps-stable_290ct2020/lib/kokkos/CMakeLists.txt
lammps-stable_290ct2020/lib/kokkos/CONTRIBUTING.md
lammps-stable_290ct2020/lib/kokkos/Copyright.txt
lammps-stable_290ct2020/lib/kokkos/HOW_TO_SNAPSHOT
lammps-stable_290ct2020/lib/kokkos/LICENSE
lammps-stable_290ct2020/lib/kokkos/Makefile.kokkos
lammps-stable_290ct2020/lib/kokkos/Makefile.targets
lammps-stable_290ct2020/lib/kokkos/README.md
lammps-stable_290ct2020/lib/kokkos/Spack.md
lammps-stable_290ct2020/lib/kokkos/algorithms/
lammps-stable_290ct2020/lib/kokkos/algorithms/CMakeLists.txt
lammps-stable_290ct2020/lib/kokkos/algorithms/cmake/
lammps-stable_290ct2020/lib/kokkos/algorithms/cmake/Dependencies.cmake
lammps-stable_290ct2020/lib/kokkos/algorithms/cmake/KokkosAlgorithms_config.
h.in
lammps-stable_290ct2020/lib/kokkos/algorithms/src/
lammps-stable_290ct2020/lib/kokkos/algorithms/src/CMakeLists.txt
lammps-stable_290ct2020/lib/kokkos/algorithms/src/KokkosAlgorithms_dummy.cpp
lammps-stable_290ct2020/lib/kokkos/algorithms/src/Kokkos_Random.hpp
lammps-stable_290ct2020/lib/kokkos/algorithms/src/Kokkos_Sort.hpp
lammps-stable_290ct2020/lib/kokkos/algorithms/unit_tests/
lammps-stable_290ct2020/lib/kokkos/algorithms/unit_tests/CMakeLists.txt
lammps-stable_290ct2020/lib/kokkos/algorithms/unit_tests/Makefile
lammps-stable_290ct2020/lib/kokkos/algorithms/unit_tests/TestCuda.cpp
lammps-stable_290ct2020/lib/kokkos/algorithms/unit_tests/TestHIP.cpp
lammps-stable_290ct2020/lib/kokkos/algorithms/unit_tests/TestHPX.cpp
lammps-stable_290ct2020/lib/kokkos/algorithms/unit_tests/TestOpenMP.cpp
lammps-stable_290ct2020/lib/kokkos/algorithms/unit_tests/TestOpenMP_Random.cp
p
lammps-stable_290ct2020/lib/kokkos/algorithms/unit_tests/TestOpenMP_Sort1D.cp
p
lammps-stable_290ct2020/lib/kokkos/algorithms/unit_tests/TestOpenMP_Sort3D.cp
p
lammps-stable_290ct2020/lib/kokkos/algorithms/unit_tests/TestOpenMP_SortDynam
icView.cpp
lammps-stable_290ct2020/lib/kokkos/algorithms/unit_tests/TestROCM.cpp
```

```
lammps-stable_290ct2020/lib/kokkos/algorithms/unit_tests/TestRandom.hpp
lammps-stable_290ct2020/lib/kokkos/algorithms/unit_tests/TestSerial.cpp
lammps-stable_290ct2020/lib/kokkos/algorithms/unit_tests/TestSort.hpp
lammps-stable_290ct2020/lib/kokkos/algorithms/unit_tests/TestThreads.cpp
lammps-stable_290ct2020/lib/kokkos/algorithms/unit_tests/UnitTestMain.cpp
lammps-stable_290ct2020/lib/kokkos/appveyor.yml
lammps-stable_290ct2020/lib/kokkos/benchmarks/
lammps-stable_290ct2020/lib/kokkos/benchmarks/atomic/
lammps-stable_290ct2020/lib/kokkos/benchmarks/atomic/Makefile
lammps-stable_290ct2020/lib/kokkos/benchmarks/atomic/main.cpp
lammps-stable_290ct2020/lib/kokkos/benchmarks/benchmark_suite/
lammps-stable_290ct2020/lib/kokkos/benchmarks/benchmark_suite/scripts/
lammps-stable_290ct2020/lib/kokkos/benchmarks/benchmark_suite/scripts/build_c
ode.bash
lammps-stable_290ct2020/lib/kokkos/benchmarks/benchmark_suite/scripts/checkou
t_repos.bash
lammps-stable_290ct2020/lib/kokkos/benchmarks/benchmark_suite/scripts/run_ben
chmark.bash
lammps-stable_290ct2020/lib/kokkos/benchmarks/benchmark_suite/scripts/run_tes
ts.bash
lammps-stable_290ct2020/lib/kokkos/benchmarks/bytes_and_flops/
lammps-stable_290ct2020/lib/kokkos/benchmarks/bytes_and_flops/Makefile
lammps-stable_290ct2020/lib/kokkos/benchmarks/bytes_and_flops/bench.hpp
lammps-stable_290ct2020/lib/kokkos/benchmarks/bytes_and_flops/bench_stride.hp
p
lammps-stable_290ct2020/lib/kokkos/benchmarks/bytes_and_flops/bench_unroll_st
ride.hpp
lammps-stable_290ct2020/lib/kokkos/benchmarks/bytes_and_flops/main.cpp
lammps-stable_290ct2020/lib/kokkos/benchmarks/gather/
lammps-stable_290ct2020/lib/kokkos/benchmarks/gather/Makefile
lammps-stable_290ct2020/lib/kokkos/benchmarks/gather/gather.hpp
lammps-stable_290ct2020/lib/kokkos/benchmarks/gather/gather_unroll.hpp
lammps-stable_290ct2020/lib/kokkos/benchmarks/gather/main.cpp
lammps-stable_290ct2020/lib/kokkos/benchmarks/gups/
lammps-stable_290ct2020/lib/kokkos/benchmarks/gups/Makefile
lammps-stable_290ct2020/lib/kokkos/benchmarks/gups/gups-kokkos.cc
lammps-stable_290ct2020/lib/kokkos/benchmarks/policy_performance/
lammps-stable_290ct2020/lib/kokkos/benchmarks/policy_performance/Makefile
lammps-stable_290ct2020/lib/kokkos/benchmarks/policy_performance/main.cpp
lammps-stable_290ct2020/lib/kokkos/benchmarks/policy_performance/policy_perf_
test.hpp
lammps-stable_290ct2020/lib/kokkos/benchmarks/policy_performance/script_basic_
_testing.sh
lammps-stable_290ct2020/lib/kokkos/benchmarks/policy_performance/script_sampl
e_usage.sh
lammps-stable_290ct2020/lib/kokkos/benchmarks/stream/
lammps-stable_290ct2020/lib/kokkos/benchmarks/stream/Makefile
lammps-stable_290ct2020/lib/kokkos/benchmarks/stream/stream-kokkos.cc
lammps-stable_290ct2020/lib/kokkos/bin/
lammps-stable_290ct2020/lib/kokkos/bin/hpcbind
lammps-stable_290ct2020/lib/kokkos/bin/nvcc_wrapper
lammps-stable_290ct2020/lib/kokkos/bin/runtest
lammps-stable_290ct2020/lib/kokkos/cmake/
lammps-stable_290ct2020/lib/kokkos/cmake/Dependencies.cmake
lammps-stable_290ct2020/lib/kokkos/cmake/KokkosConfig.cmake.in
lammps-stable_290ct2020/lib/kokkos/cmake/KokkosConfigCommon.cmake.in
lammps-stable_290ct2020/lib/kokkos/cmake/KokkosCore_config.h.in
lammps-stable_290ct2020/lib/kokkos/cmake/KokkosTrilinosConfig.cmake.in
lammps-stable_290ct2020/lib/kokkos/cmake/Modules/
lammps-stable_290ct2020/lib/kokkos/cmake/Modules/CudaToolkit.cmake
```

```
lammps-stable_290ct2020/lib/kokkos/cmake/Modules/FindTPLCUDA.cmake
lammps-stable_290ct2020/lib/kokkos/cmake/Modules/FindTPLHPX.cmake
lammps-stable_290ct2020/lib/kokkos/cmake/Modules/FindTPLHWLOC.cmake
lammps-stable_290ct2020/lib/kokkos/cmake/Modules/FindTPLLIBDL.cmake
lammps-stable_290ct2020/lib/kokkos/cmake/Modules/FindTPLLIBNUMA.cmake
lammps-stable_290ct2020/lib/kokkos/cmake/Modules/FindTPLLIBRT.cmake
lammps-stable_290ct2020/lib/kokkos/cmake/Modules/FindTPLMEMKIND.cmake
lammps-stable_290ct2020/lib/kokkos/cmake/Modules/FindTPLPTHREAD.cmake
lammps-stable_290ct2020/lib/kokkos/cmake/README.md
lammps-stable_290ct2020/lib/kokkos/cmake/compile_tests/
lammps-stable_290ct2020/lib/kokkos/cmake/compile_tests/clang_omp.cpp
lammps-stable_290ct2020/lib/kokkos/cmake/compile_tests/cuda_compute_capability.cc
lammps-stable_290ct2020/lib/kokkos/cmake/compile_tests/pthread.cpp
lammps-stable_290ct2020/lib/kokkos/cmake/cray.cmake
lammps-stable_290ct2020/lib/kokkos/cmake/deps/
lammps-stable_290ct2020/lib/kokkos/cmake/deps/CUDA.cmake
lammps-stable_290ct2020/lib/kokkos/cmake/deps/CUSPARSE.cmake
lammps-stable_290ct2020/lib/kokkos/cmake/deps/HWLOC.cmake
lammps-stable_290ct2020/lib/kokkos/cmake/deps/Pthread.cmake
lammps-stable_290ct2020/lib/kokkos/cmake/fake_tribits.cmake
lammps-stable_290ct2020/lib/kokkos/cmake/gnu.cmake
lammps-stable_290ct2020/lib/kokkos/cmake/intel.cmake
lammps-stable_290ct2020/lib/kokkos/cmake/kokkos_arch.cmake
lammps-stable_290ct2020/lib/kokkos/cmake/kokkos_check_env.cmake
lammps-stable_290ct2020/lib/kokkos/cmake/kokkos_compiler_id.cmake
lammps-stable_290ct2020/lib/kokkos/cmake/kokkos_corner_cases.cmake
lammps-stable_290ct2020/lib/kokkos/cmake/kokkos_enable_devices.cmake
lammps-stable_290ct2020/lib/kokkos/cmake/kokkos_enable_options.cmake
lammps-stable_290ct2020/lib/kokkos/cmake/kokkos_functions.cmake
lammps-stable_290ct2020/lib/kokkos/cmake/kokkos_install.cmake
lammps-stable_290ct2020/lib/kokkos/cmake/kokkos_pick_cxx_std.cmake
lammps-stable_290ct2020/lib/kokkos/cmake/kokkos_test_cxx_std.cmake
lammps-stable_290ct2020/lib/kokkos/cmake/kokkos_tpls.cmake
lammps-stable_290ct2020/lib/kokkos/cmake/kokkos_tribits.cmake
lammps-stable_290ct2020/lib/kokkos/cmake/msvc.cmake
lammps-stable_290ct2020/lib/kokkos/cmake/pgi.cmake
lammps-stable_290ct2020/lib/kokkos/cmake/tpls/
lammps-stable_290ct2020/lib/kokkos/cmake/tpls/FindTPLCUSPARSE.cmake
lammps-stable_290ct2020/lib/kokkos/cmake/tpls/FindTPLHWLOC.cmake
lammps-stable_290ct2020/lib/kokkos/cmake/tpls/FindTPLPthread.cmake
lammps-stable_290ct2020/lib/kokkos/config/
lammps-stable_290ct2020/lib/kokkos/config/test_all_sandia
lammps-stable_290ct2020/lib/kokkos/config/yaml/
lammps-stable_290ct2020/lib/kokkos/config/yaml/volta.yaml
lammps-stable_290ct2020/lib/kokkos/containers/
lammps-stable_290ct2020/lib/kokkos/containers/CMakeLists.txt
lammps-stable_290ct2020/lib/kokkos/containers/cmake/
lammps-stable_290ct2020/lib/kokkos/containers/cmake/Dependencies.cmake
lammps-stable_290ct2020/lib/kokkos/containers/cmake/KokkosContainers_config.h.in
lammps-stable_290ct2020/lib/kokkos/containers/performance_tests/
lammps-stable_290ct2020/lib/kokkos/containers/performance_tests/CMakeLists.txt
lammps-stable_290ct2020/lib/kokkos/containers/performance_tests/Makefile
lammps-stable_290ct2020/lib/kokkos/containers/performance_tests/TestCuda.cpp
lammps-stable_290ct2020/lib/kokkos/containers/performance_tests/TestDynRankView.hpp
lammps-stable_290ct2020/lib/kokkos/containers/performance_tests/TestGlobal2LocalIds.hpp
```

```
lammps-stable_290ct2020/lib/kokkos/containers/performance_tests/TestHPX.cpp
lammps-stable_290ct2020/lib/kokkos/containers/performance_tests/TestMain.cpp
lammps-stable_290ct2020/lib/kokkos/containers/performance_tests/TestOpenMP.cpp
lammps-stable_290ct2020/lib/kokkos/containers/performance_tests/TestROCM.cpp
lammps-stable_290ct2020/lib/kokkos/containers/performance_tests/TestScatterView.hpp
lammps-stable_290ct2020/lib/kokkos/containers/performance_tests/TestThreads.cpp
lammps-stable_290ct2020/lib/kokkos/containers/performance_tests/TestUnorderedMapPerformance.hpp
lammps-stable_290ct2020/lib/kokkos/containers/src/
lammps-stable_290ct2020/lib/kokkos/containers/src/CMakeLists.txt
lammps-stable_290ct2020/lib/kokkos/containers/src/Kokkos_Bitset.hpp
lammps-stable_290ct2020/lib/kokkos/containers/src/Kokkos_DualView.hpp
lammps-stable_290ct2020/lib/kokkos/containers/src/Kokkos_DynRankView.hpp
lammps-stable_290ct2020/lib/kokkos/containers/src/Kokkos_DynamicView.hpp
lammps-stable_290ct2020/lib/kokkos/containers/src/Kokkos_ErrorReporter.hpp
lammps-stable_290ct2020/lib/kokkos/containers/src/Kokkos_Functional.hpp
lammps-stable_290ct2020/lib/kokkos/containers/src/Kokkos_OffsetView.hpp
lammps-stable_290ct2020/lib/kokkos/containers/src/Kokkos_ScatterView.hpp
lammps-stable_290ct2020/lib/kokkos/containers/src/Kokkos_StaticCrsGraph.hpp
lammps-stable_290ct2020/lib/kokkos/containers/src/Kokkos_UnorderedMap.hpp
lammps-stable_290ct2020/lib/kokkos/containers/src/Kokkos_Vector.hpp
lammps-stable_290ct2020/lib/kokkos/containers/src/impl/
lammps-stable_290ct2020/lib/kokkos/containers/src/impl/Kokkos_Bitset_impl.hpp
lammps-stable_290ct2020/lib/kokkos/containers/src/impl/Kokkos_Functional_impl.hpp
lammps-stable_290ct2020/lib/kokkos/containers/src/impl/Kokkos_StaticCrsGraph_factory.hpp
lammps-stable_290ct2020/lib/kokkos/containers/src/impl/Kokkos_UnorderedMap_impl.cpp
lammps-stable_290ct2020/lib/kokkos/containers/src/impl/Kokkos_UnorderedMap_impl.hpp
lammps-stable_290ct2020/lib/kokkos/containers/unit_tests/
lammps-stable_290ct2020/lib/kokkos/containers/unit_tests/CMakeLists.txt
lammps-stable_290ct2020/lib/kokkos/containers/unit_tests/Makefile
lammps-stable_290ct2020/lib/kokkos/containers/unit_tests/TestBitset.hpp
lammps-stable_290ct2020/lib/kokkos/containers/unit_tests/TestCuda_Category.hpp
lammps-stable_290ct2020/lib/kokkos/containers/unit_tests/TestDualView.hpp
lammps-stable_290ct2020/lib/kokkos/containers/unit_tests/TestDynViewAPI.hpp
lammps-stable_290ct2020/lib/kokkos/containers/unit_tests/TestDynViewAPI_generic.hpp
lammps-stable_290ct2020/lib/kokkos/containers/unit_tests/TestDynViewAPI_rank12345.hpp
lammps-stable_290ct2020/lib/kokkos/containers/unit_tests/TestDynViewAPI_rank67.hpp
lammps-stable_290ct2020/lib/kokkos/containers/unit_tests/TestDynamicView.hpp
lammps-stable_290ct2020/lib/kokkos/containers/unit_tests/TestErrorReporter.hpp
lammps-stable_290ct2020/lib/kokkos/containers/unit_tests/TestHIP_Category.hpp
lammps-stable_290ct2020/lib/kokkos/containers/unit_tests/TestHPX_Category.hpp
lammps-stable_290ct2020/lib/kokkos/containers/unit_tests/TestOffsetView.hpp
lammps-stable_290ct2020/lib/kokkos/containers/unit_tests/TestOpenMP_Category.hpp
lammps-stable_290ct2020/lib/kokkos/containers/unit_tests/TestScatterView.hpp
lammps-stable_290ct2020/lib/kokkos/containers/unit_tests/TestSerial_Category.hpp
lammps-stable_290ct2020/lib/kokkos/containers/unit_tests/TestStaticCrsGraph.h
```



pp  
lammps-stable\_290ct2020/lib/kokkos/containers/unit\_tests/TestThreads\_Category.hpp  
lammps-stable\_290ct2020/lib/kokkos/containers/unit\_tests/TestUnorderedMap.hpp  
lammps-stable\_290ct2020/lib/kokkos/containers/unit\_tests/TestVector.hpp  
lammps-stable\_290ct2020/lib/kokkos/containers/unit\_tests/TestViewCtorPropEmbeddedDim.hpp  
lammps-stable\_290ct2020/lib/kokkos/containers/unit\_tests/UnitTestMain.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/  
lammps-stable\_290ct2020/lib/kokkos/core/CMakeLists.txt  
lammps-stable\_290ct2020/lib/kokkos/core/cmake/  
lammps-stable\_290ct2020/lib/kokkos/core/cmake/Dependencies.cmake  
lammps-stable\_290ct2020/lib/kokkos/core/cmake/KokkosCore\_config.h.in  
lammps-stable\_290ct2020/lib/kokkos/core/perf\_test/  
lammps-stable\_290ct2020/lib/kokkos/core/perf\_test/CMakeLists.txt  
lammps-stable\_290ct2020/lib/kokkos/core/perf\_test/Makefile  
lammps-stable\_290ct2020/lib/kokkos/core/perf\_test/PerfTestBlasKernels.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/perf\_test/PerfTestDriver.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/perf\_test/PerfTestGramSchmidt.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/perf\_test/PerfTestHexGrad.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/perf\_test/PerfTestMDRange.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/perf\_test/PerfTestMain.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/perf\_test/PerfTest\_Category.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/perf\_test/PerfTest\_CustomReduction.cpp  
p  
lammps-stable\_290ct2020/lib/kokkos/core/perf\_test/PerfTest\_ExecSpacePartitioning.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/perf\_test/PerfTest\_ViewAllocate.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/perf\_test/PerfTest\_ViewCopy.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/perf\_test/PerfTest\_ViewCopy\_a123.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/perf\_test/PerfTest\_ViewCopy\_a45.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/perf\_test/PerfTest\_ViewCopy\_a6.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/perf\_test/PerfTest\_ViewCopy\_a7.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/perf\_test/PerfTest\_ViewCopy\_a8.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/perf\_test/PerfTest\_ViewCopy\_b123.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/perf\_test/PerfTest\_ViewCopy\_b45.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/perf\_test/PerfTest\_ViewCopy\_b6.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/perf\_test/PerfTest\_ViewCopy\_b7.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/perf\_test/PerfTest\_ViewCopy\_b8.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/perf\_test/PerfTest\_ViewCopy\_c123.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/perf\_test/PerfTest\_ViewCopy\_c45.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/perf\_test/PerfTest\_ViewCopy\_c6.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/perf\_test/PerfTest\_ViewCopy\_c7.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/perf\_test/PerfTest\_ViewCopy\_c8.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/perf\_test/PerfTest\_ViewCopy\_d123.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/perf\_test/PerfTest\_ViewCopy\_d45.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/perf\_test/PerfTest\_ViewCopy\_d6.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/perf\_test/PerfTest\_ViewCopy\_d7.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/perf\_test/PerfTest\_ViewCopy\_d8.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/perf\_test/PerfTest\_ViewFill.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/perf\_test/PerfTest\_ViewFill\_123.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/perf\_test/PerfTest\_ViewFill\_45.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/perf\_test/PerfTest\_ViewFill\_6.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/perf\_test/PerfTest\_ViewFill\_7.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/perf\_test/PerfTest\_ViewFill\_8.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/perf\_test/PerfTest\_ViewResize.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/perf\_test/PerfTest\_ViewResize\_123.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/perf\_test/PerfTest\_ViewResize\_45.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/perf\_test/PerfTest\_ViewResize\_6.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/perf\_test/PerfTest\_ViewResize\_7.cpp

```
lammps-stable_290ct2020/lib/kokkos/core/perf_test/PerfTest_ViewResize_8.cpp
lammps-stable_290ct2020/lib/kokkos/core/perf_test/run_mempool.sh
lammps-stable_290ct2020/lib/kokkos/core/perf_test/run_mempool_fill.sh
lammps-stable_290ct2020/lib/kokkos/core/perf_test/run_taskdag.sh
lammps-stable_290ct2020/lib/kokkos/core/perf_test/test_atomic.cpp
lammps-stable_290ct2020/lib/kokkos/core/perf_test/test_mempool.cpp
lammps-stable_290ct2020/lib/kokkos/core/perf_test/test_taskdag.cpp
lammps-stable_290ct2020/lib/kokkos/core/src/
lammps-stable_290ct2020/lib/kokkos/core/src/CMakeLists.txt
lammps-stable_290ct2020/lib/kokkos/core/src/Cuda/
lammps-stable_290ct2020/lib/kokkos/core/src/Cuda/KokkosExp_Cuda_IterateTile.h
pp
lammps-stable_290ct2020/lib/kokkos/core/src/Cuda/KokkosExp_Cuda_IterateTile_R
efactor.hpp
lammps-stable_290ct2020/lib/kokkos/core/src/Cuda/Kokkos_CudaSpace.cpp
lammps-stable_290ct2020/lib/kokkos/core/src/Cuda/Kokkos_Cuda_Alloc.hpp
lammps-stable_290ct2020/lib/kokkos/core/src/Cuda/Kokkos_Cuda_Atomic_Intrinsic
s.hpp
lammps-stable_290ct2020/lib/kokkos/core/src/Cuda/Kokkos_Cuda_Atomic_Intrinsic
s_Restore_Builtins.hpp
lammps-stable_290ct2020/lib/kokkos/core/src/Cuda/Kokkos_Cuda_BlockSize_Deduct
ion.hpp
lammps-stable_290ct2020/lib/kokkos/core/src/Cuda/Kokkos_Cuda_Error.hpp
lammps-stable_290ct2020/lib/kokkos/core/src/Cuda/Kokkos_Cuda_Instance.cpp
lammps-stable_290ct2020/lib/kokkos/core/src/Cuda/Kokkos_Cuda_Instance.hpp
lammps-stable_290ct2020/lib/kokkos/core/src/Cuda/Kokkos_Cuda_KernelLaunch.hpp
lammps-stable_290ct2020/lib/kokkos/core/src/Cuda/Kokkos_Cuda_Locks.cpp
lammps-stable_290ct2020/lib/kokkos/core/src/Cuda/Kokkos_Cuda_Locks.hpp
lammps-stable_290ct2020/lib/kokkos/core/src/Cuda/Kokkos_Cuda_Parallel.hpp
lammps-stable_290ct2020/lib/kokkos/core/src/Cuda/Kokkos_Cuda_ReduceScan.hpp
lammps-stable_290ct2020/lib/kokkos/core/src/Cuda/Kokkos_Cuda_Task.cpp
lammps-stable_290ct2020/lib/kokkos/core/src/Cuda/Kokkos_Cuda_Task.hpp
lammps-stable_290ct2020/lib/kokkos/core/src/Cuda/Kokkos_Cuda_Team.hpp
lammps-stable_290ct2020/lib/kokkos/core/src/Cuda/Kokkos_Cuda_UniqueToken.hpp
lammps-stable_290ct2020/lib/kokkos/core/src/Cuda/Kokkos_Cuda_Vectorization.hp
p
lammps-stable_290ct2020/lib/kokkos/core/src/Cuda/Kokkos_Cuda_Version_9_8_Comp
atibility.hpp
lammps-stable_290ct2020/lib/kokkos/core/src/Cuda/Kokkos_Cuda_View.hpp
lammps-stable_290ct2020/lib/kokkos/core/src/Cuda/Kokkos_Cuda_WorkGraphPolicy.
hpp
lammps-stable_290ct2020/lib/kokkos/core/src/Cuda/Kokkos_Cuda_abort.hpp
lammps-stable_290ct2020/lib/kokkos/core/src/Cuda/Kokkos_Cuda_fwd.hpp
lammps-stable_290ct2020/lib/kokkos/core/src/HIP/
lammps-stable_290ct2020/lib/kokkos/core/src/HIP/KokkosExp_HIP_IterateTile.hpp
lammps-stable_290ct2020/lib/kokkos/core/src/HIP/Kokkos_HIP_Abort.hpp
lammps-stable_290ct2020/lib/kokkos/core/src/HIP/Kokkos_HIP_Atomic.hpp
lammps-stable_290ct2020/lib/kokkos/core/src/HIP/Kokkos_HIP_BlockSize_Deductio
n.hpp
lammps-stable_290ct2020/lib/kokkos/core/src/HIP/Kokkos_HIP_Error.hpp
lammps-stable_290ct2020/lib/kokkos/core/src/HIP/Kokkos_HIP_Instance.cpp
lammps-stable_290ct2020/lib/kokkos/core/src/HIP/Kokkos_HIP_Instance.hpp
lammps-stable_290ct2020/lib/kokkos/core/src/HIP/Kokkos_HIP_KernelLaunch.cpp
lammps-stable_290ct2020/lib/kokkos/core/src/HIP/Kokkos_HIP_KernelLaunch.hpp
lammps-stable_290ct2020/lib/kokkos/core/src/HIP/Kokkos_HIP_Locks.cpp
lammps-stable_290ct2020/lib/kokkos/core/src/HIP/Kokkos_HIP_Locks.hpp
lammps-stable_290ct2020/lib/kokkos/core/src/HIP/Kokkos_HIP_Parallel_MDRange.h
pp
lammps-stable_290ct2020/lib/kokkos/core/src/HIP/Kokkos_HIP_Parallel_Range.hpp
lammps-stable_290ct2020/lib/kokkos/core/src/HIP/Kokkos_HIP_Parallel_Team.hpp
```

lammps-stable\_290ct2020/lib/kokkos/core/src/HIP/Kokkos\_HIP\_ReduceScan.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/HIP/Kokkos\_HIP\_Shuffle\_Reduce.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/HIP/Kokkos\_HIP\_Space.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/HIP/Kokkos\_HIP\_Team.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/HIP/Kokkos\_HIP\_UniqueToken.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/HIP/Kokkos\_HIP\_Vectorization.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/HIP/Kokkos\_HIP\_WorkGraphPolicy.hpp  
p  
lammps-stable\_290ct2020/lib/kokkos/core/src/HPX/  
lammps-stable\_290ct2020/lib/kokkos/core/src/HPX/Kokkos\_HPX.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/HPX/Kokkos\_HPX\_ChunkedRoundRobinExecutor.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/HPX/Kokkos\_HPX\_Task.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/HPX/Kokkos\_HPX\_Task.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/HPX/Kokkos\_HPX\_WorkGraphPolicy.hpp  
p  
lammps-stable\_290ct2020/lib/kokkos/core/src/KokkosExp\_MDRangePolicy.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/Kokkos\_AcquireUniqueTokenImpl.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/Kokkos\_AnonymousSpace.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/Kokkos\_Array.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/Kokkos\_Atomic.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/Kokkos\_Complex.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/Kokkos\_Concepts.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/Kokkos\_CopyViews.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/Kokkos\_Core.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/Kokkos\_Core\_fwd.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/Kokkos\_Crs.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/Kokkos\_Cuda.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/Kokkos\_CudaSpace.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/Kokkos\_ExecPolicy.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/Kokkos\_Extents.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/Kokkos\_Future.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/Kokkos\_HBWSpace.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/Kokkos\_HIP.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/Kokkos\_HIP\_Space.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/Kokkos\_HPX.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/Kokkos\_HostSpace.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/Kokkos\_Layout.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/Kokkos\_Macros.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/Kokkos\_MasterLock.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/Kokkos\_MemoryPool.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/Kokkos\_MemoryTraits.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/Kokkos\_NumericTraits.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/Kokkos\_OpenMP.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/Kokkos\_OpenMPTarget.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/Kokkos\_OpenMPTargetSpace.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/Kokkos\_Pair.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/Kokkos\_Parallel.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/Kokkos\_Parallel\_Reduce.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/Kokkos\_PointerOwnership.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/Kokkos\_Profiling\_ProfileSection.hpp  
pp  
lammps-stable\_290ct2020/lib/kokkos/core/src/Kokkos\_ROCm.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/Kokkos\_ROCmSpace.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/Kokkos\_ScratchSpace.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/Kokkos\_Serial.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/Kokkos\_TaskPolicy.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/Kokkos\_TaskScheduler.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/Kokkos\_TaskScheduler\_fwd.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/Kokkos\_Threads.hpp

```
lammps-stable_290ct2020/lib/kokkos/core/src/Kokkos_Timer.hpp
lammps-stable_290ct2020/lib/kokkos/core/src/Kokkos_UniqueToken.hpp
lammps-stable_290ct2020/lib/kokkos/core/src/Kokkos_Vectorization.hpp
lammps-stable_290ct2020/lib/kokkos/core/src/Kokkos_View.hpp
lammps-stable_290ct2020/lib/kokkos/core/src/Kokkos_WorkGraphPolicy.hpp
lammps-stable_290ct2020/lib/kokkos/core/src/Kokkos_hwloc.hpp
lammps-stable_290ct2020/lib/kokkos/core/src/OpenMP/
lammps-stable_290ct2020/lib/kokkos/core/src/OpenMP/Kokkos_OpenMP_Exec.cpp
lammps-stable_290ct2020/lib/kokkos/core/src/OpenMP/Kokkos_OpenMP_Exec.hpp
lammps-stable_290ct2020/lib/kokkos/core/src/OpenMP/Kokkos_OpenMP_Parallel.hpp
lammps-stable_290ct2020/lib/kokkos/core/src/OpenMP/Kokkos_OpenMP_Task.cpp
lammps-stable_290ct2020/lib/kokkos/core/src/OpenMP/Kokkos_OpenMP_Task.hpp
lammps-stable_290ct2020/lib/kokkos/core/src/OpenMP/Kokkos_OpenMP_Team.hpp
lammps-stable_290ct2020/lib/kokkos/core/src/OpenMP/Kokkos_OpenMP_WorkGraphPolicy.hpp
lammps-stable_290ct2020/lib/kokkos/core/src/OpenMPTarget/
lammps-stable_290ct2020/lib/kokkos/core/src/OpenMPTarget/Kokkos_OpenMPTargetSpace.cpp
lammps-stable_290ct2020/lib/kokkos/core/src/OpenMPTarget/Kokkos_OpenMPTarget_Exec.cpp
lammps-stable_290ct2020/lib/kokkos/core/src/OpenMPTarget/Kokkos_OpenMPTarget_Exec.hpp
lammps-stable_290ct2020/lib/kokkos/core/src/OpenMPTarget/Kokkos_OpenMPTarget_Instance.cpp
lammps-stable_290ct2020/lib/kokkos/core/src/OpenMPTarget/Kokkos_OpenMPTarget_Instance.hpp
lammps-stable_290ct2020/lib/kokkos/core/src/OpenMPTarget/Kokkos_OpenMPTarget_Parallel.hpp
lammps-stable_290ct2020/lib/kokkos/core/src/OpenMPTarget/Kokkos_OpenMPTarget_Parallel_MDRange.hpp
lammps-stable_290ct2020/lib/kokkos/core/src/OpenMPTarget/Kokkos_OpenMPTarget_Task.cpp
lammps-stable_290ct2020/lib/kokkos/core/src/OpenMPTarget/Kokkos_OpenMPTarget_Task.hpp
lammps-stable_290ct2020/lib/kokkos/core/src/ROCM/
lammps-stable_290ct2020/lib/kokkos/core/src/ROCM/KokkosExp_ROCM_IterateTile_Refactor.hpp
lammps-stable_290ct2020/lib/kokkos/core/src/ROCM/Kokkos_ROCM_Atomic.hpp
lammps-stable_290ct2020/lib/kokkos/core/src/ROCM/Kokkos_ROCM_Config.hpp
lammps-stable_290ct2020/lib/kokkos/core/src/ROCM/Kokkos_ROCM_Exec.cpp
lammps-stable_290ct2020/lib/kokkos/core/src/ROCM/Kokkos_ROCM_Exec.hpp
lammps-stable_290ct2020/lib/kokkos/core/src/ROCM/Kokkos_ROCM_Impl.cpp
lammps-stable_290ct2020/lib/kokkos/core/src/ROCM/Kokkos_ROCM_Invoke.hpp
lammps-stable_290ct2020/lib/kokkos/core/src/ROCM/Kokkos_ROCM_Join.hpp
lammps-stable_290ct2020/lib/kokkos/core/src/ROCM/Kokkos_ROCM_Parallel.hpp
lammps-stable_290ct2020/lib/kokkos/core/src/ROCM/Kokkos_ROCM_Reduce.hpp
lammps-stable_290ct2020/lib/kokkos/core/src/ROCM/Kokkos_ROCM_ReduceScan.hpp
lammps-stable_290ct2020/lib/kokkos/core/src/ROCM/Kokkos_ROCM_Scan.hpp
lammps-stable_290ct2020/lib/kokkos/core/src/ROCM/Kokkos_ROCM_Space.cpp
lammps-stable_290ct2020/lib/kokkos/core/src/ROCM/Kokkos_ROCM_Task.cpp
lammps-stable_290ct2020/lib/kokkos/core/src/ROCM/Kokkos_ROCM_Task.hpp
lammps-stable_290ct2020/lib/kokkos/core/src/ROCM/Kokkos_ROCM_Tile.hpp
lammps-stable_290ct2020/lib/kokkos/core/src/ROCM/Kokkos_ROCM_Vectorization.hpp
lammps-stable_290ct2020/lib/kokkos/core/src/ROCM/hc_math_std.hpp
lammps-stable_290ct2020/lib/kokkos/core/src/Threads/
lammps-stable_290ct2020/lib/kokkos/core/src/Threads/Kokkos_ThreadsExec.cpp
lammps-stable_290ct2020/lib/kokkos/core/src/Threads/Kokkos_ThreadsExec.hpp
lammps-stable_290ct2020/lib/kokkos/core/src/Threads/Kokkos_ThreadsExec_base.cpp
pp
```

lammps-stable\_290ct2020/lib/kokkos/core/src/Threads/Kokkos\_ThreadsTeam.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/Threads/Kokkos\_Threads\_Parallel.h  
pp  
lammps-stable\_290ct2020/lib/kokkos/core/src/Threads/Kokkos\_Threads\_WorkGraphPolicy.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/dummy.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/CMakeLists.txt  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/KokkosExp\_Host\_IterateTile.h  
pp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/KokkosExp\_ViewMapping.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_AnalyzePolicy.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_Atomic\_Assembly.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_Atomic\_Compare\_Exchange\_Strong.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_Atomic\_Compare\_Exchange\_Weak.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_Atomic\_Decrement.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_Atomic\_Exchange.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_Atomic\_Fetch\_Add.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_Atomic\_Fetch\_And.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_Atomic\_Fetch\_Or.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_Atomic\_Fetch\_Sub.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_Atomic\_Generic.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_Atomic\_Generic\_Secondary.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_Atomic\_Increment.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_Atomic\_Load.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_Atomic\_Memory\_Order.h  
pp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_Atomic\_MinMax.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_Atomic\_Store.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_Atomic\_View.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_Atomic\_Windows.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_BitOps.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_CPUDiscovery.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_CPUDiscovery.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_ChaseLev.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_ClockTic.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_Combined\_Reducer.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_ConcurrentBitset.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_Core.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_EBO.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_Error.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_Error.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_ExecPolicy.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_FixedBufferMemoryPool.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_FunctorAdapter.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_FunctorAnalysis.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_HBWSpace.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_HostBarrier.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_HostBarrier.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_HostSpace.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_HostSpace\_deepcopy.cpp  
p  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_HostSpace\_deepcopy.hpp  
p  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_HostThreadTeam.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_HostThreadTeam.hpp

lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_LIFO.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_LinkedListNode.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_MemoryPool.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_MemoryPoolAllocator.h  
pp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_MemorySpace.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_MemorySpace.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_Memory\_Fence.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_MultipleTaskQueue.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_OptionalRef.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_PhysicalLayout.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_Profiling.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_Profiling.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_Profiling\_C\_Interface.h  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_Profiling\_DeviceInfo.  
hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_Profiling\_Interface.h  
pp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_Serial.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_Serial\_Task.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_Serial\_Task.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_Serial\_WorkGraphPolic  
y.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_SharedAlloc.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_SharedAlloc.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_SimpleTaskScheduler.h  
pp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_SingleTaskQueue.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_Spinwait.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_Spinwait.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_Stacktrace.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_Stacktrace.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_Tags.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_TaskBase.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_TaskNode.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_TaskPolicyData.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_TaskQueue.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_TaskQueueCommon.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_TaskQueueMemoryManage  
r.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_TaskQueueMultiple.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_TaskQueueMultiple\_imp  
l.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_TaskQueue\_impl.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_TaskResult.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_TaskTeamMember.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_Timer.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_Tools.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_Traits.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_Uutilities.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_VLAEmulation.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_ViewArray.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_ViewCtor.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_ViewLayoutTiled.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_ViewMapping.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_ViewTracker.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_ViewUniformType.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_Volatile\_Load.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/src/impl/Kokkos\_hwloc.cpp

```
lammps-stable_290ct2020/lib/kokkos/core/unit_test/  
lammps-stable_290ct2020/lib/kokkos/core/unit_test/CMakeLists.txt  
lammps-stable_290ct2020/lib/kokkos/core/unit_test/IncrementalTest.cpp.in  
lammps-stable_290ct2020/lib/kokkos/core/unit_test/Makefile  
lammps-stable_290ct2020/lib/kokkos/core/unit_test/TestAggregate.hpp  
lammps-stable_290ct2020/lib/kokkos/core/unit_test/TestAtomic.hpp  
lammps-stable_290ct2020/lib/kokkos/core/unit_test/TestAtomicOperations.hpp  
lammps-stable_290ct2020/lib/kokkos/core/unit_test/TestAtomicOperations_comple  
xdouble.hpp  
lammps-stable_290ct2020/lib/kokkos/core/unit_test/TestAtomicOperations_comple  
xfloat.hpp  
lammps-stable_290ct2020/lib/kokkos/core/unit_test/TestAtomicOperations_doubl  
e.hpp  
lammps-stable_290ct2020/lib/kokkos/core/unit_test/TestAtomicOperations_float.  
hpp  
lammps-stable_290ct2020/lib/kokkos/core/unit_test/TestAtomicOperations_int.hp  
p  
lammps-stable_290ct2020/lib/kokkos/core/unit_test/TestAtomicOperations_longin  
t.hpp  
lammps-stable_290ct2020/lib/kokkos/core/unit_test/TestAtomicOperations_longlo  
ngint.hpp  
lammps-stable_290ct2020/lib/kokkos/core/unit_test/TestAtomicOperations_unsign  
edint.hpp  
lammps-stable_290ct2020/lib/kokkos/core/unit_test/TestAtomicOperations_unsign  
edlongint.hpp  
lammps-stable_290ct2020/lib/kokkos/core/unit_test/TestAtomicViews.hpp  
lammps-stable_290ct2020/lib/kokkos/core/unit_test/TestCTestDevice.cpp  
lammps-stable_290ct2020/lib/kokkos/core/unit_test/TestCXX11.hpp  
lammps-stable_290ct2020/lib/kokkos/core/unit_test/TestCXX11Deduction.hpp  
lammps-stable_290ct2020/lib/kokkos/core/unit_test/TestCompilerMacros.hpp  
lammps-stable_290ct2020/lib/kokkos/core/unit_test/TestComplex.hpp  
lammps-stable_290ct2020/lib/kokkos/core/unit_test/TestConcepts.hpp  
lammps-stable_290ct2020/lib/kokkos/core/unit_test/TestConcurrentBitset.hpp  
lammps-stable_290ct2020/lib/kokkos/core/unit_test/TestCrs.hpp  
lammps-stable_290ct2020/lib/kokkos/core/unit_test/TestDeepCopy.hpp  
lammps-stable_290ct2020/lib/kokkos/core/unit_test/TestDefaultDeviceTypeInit.h  
pp  
lammps-stable_290ct2020/lib/kokkos/core/unit_test/TestFunctorAnalysis.hpp  
lammps-stable_290ct2020/lib/kokkos/core/unit_test/TestHWLOC.cpp  
lammps-stable_290ct2020/lib/kokkos/core/unit_test/TestHostBarrier.cpp  
lammps-stable_290ct2020/lib/kokkos/core/unit_test/TestInit.hpp  
lammps-stable_290ct2020/lib/kokkos/core/unit_test/TestIrregularLayout.hpp  
lammps-stable_290ct2020/lib/kokkos/core/unit_test/TestLocalDeepCopy.hpp  
lammps-stable_290ct2020/lib/kokkos/core/unit_test/TestMDRange.hpp  
lammps-stable_290ct2020/lib/kokkos/core/unit_test/TestMDRange_a.hpp  
lammps-stable_290ct2020/lib/kokkos/core/unit_test/TestMDRange_b.hpp  
lammps-stable_290ct2020/lib/kokkos/core/unit_test/TestMDRange_c.hpp  
lammps-stable_290ct2020/lib/kokkos/core/unit_test/TestMDRange_d.hpp  
lammps-stable_290ct2020/lib/kokkos/core/unit_test/TestMDRange_e.hpp  
lammps-stable_290ct2020/lib/kokkos/core/unit_test/TestMemoryPool.hpp  
lammps-stable_290ct2020/lib/kokkos/core/unit_test/TestNonTrivialScalarTypes.h  
pp  
lammps-stable_290ct2020/lib/kokkos/core/unit_test/TestPolicyConstruction.hpp  
lammps-stable_290ct2020/lib/kokkos/core/unit_test/TestRange.hpp  
lammps-stable_290ct2020/lib/kokkos/core/unit_test/TestRangeRequire.hpp  
lammps-stable_290ct2020/lib/kokkos/core/unit_test/TestReduce.hpp  
lammps-stable_290ct2020/lib/kokkos/core/unit_test/TestReduceCombinatorial.hp  
p  
lammps-stable_290ct2020/lib/kokkos/core/unit_test/TestReduceDeviceView.hpp  
lammps-stable_290ct2020/lib/kokkos/core/unit_test/TestReducers.hpp
```

lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/TestReducers\_a.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/TestReducers\_b.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/TestReducers\_c.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/TestReducers\_d.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/TestResize.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/TestScan.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/TestSharedAlloc.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/TestStackTrace.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/TestStackTrace.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/TestStackTrace\_f0.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/TestStackTrace\_f1.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/TestStackTrace\_f2.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/TestStackTrace\_f3.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/TestStackTrace\_f4.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/TestTaskScheduler.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/TestTaskScheduler\_single.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/TestTeam.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/TestTeamTeamSize.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/TestTeamVector.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/TestTeamVectorRange.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/TestTemplateMetaFunctions.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/TestUniqueToken.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/TestUtilities.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/TextViewAPI.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/TextViewAPI\_a.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/TextViewAPI\_b.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/TextViewAPI\_c.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/TextViewAPI\_d.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/TextViewAPI\_e.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/TextViewCopy.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/TextViewCtorPropEmbeddedDim.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/TextViewIsAssignable.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/TextViewLayoutStrideAssignment.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/TextViewLayoutTiled.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/TextViewMapping\_a.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/TextViewMapping\_b.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/TextViewMapping\_subview.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/TextViewOfClass.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/TextViewResize.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/TextViewSpaceAssign.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/TextViewSubview.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/TextView\_64bit.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/TestWorkGraph.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/Test\_InterOp\_Streams.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/UnitTestMain.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/UnitTestMainInit.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/UnitTest\_PushFinalizeHook.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/UnitTest\_PushFinalizeHook\_terminate.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/configuration/  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/configuration/test-code/  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/configuration/test-code/CMakeLists.txt  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/configuration/test-code/Makefile



```
lammps-stable_290ct2020/lib/kokkos/core/unit_test/configuration/test-code/main.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/configuration/test-code/test_config.bash
lammps-stable_290ct2020/lib/kokkos/core/unit_test/configuration/test-code/test_config_arch_list.bash
lammps-stable_290ct2020/lib/kokkos/core/unit_test/configuration/test-code/test_config_device_list.bash
lammps-stable_290ct2020/lib/kokkos/core/unit_test/configuration/test-code/test_config_options_list.bash
lammps-stable_290ct2020/lib/kokkos/core/unit_test/configuration/test-code/test_config_run.bash
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCudaHostPinned_Category.hpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCudaHostPinned_SharedAlloc.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCudaHostPinned_ViewAPI_a.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCudaHostPinned_ViewAPI_b.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCudaHostPinned_ViewAPI_c.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCudaHostPinned_ViewAPI_d.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCudaHostPinned_ViewAPI_e.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCudaHostPinned_ViewCopy.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCudaHostPinned_ViewMapping_a.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCudaHostPinned_ViewMapping_b.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCudaHostPinned_ViewMapping_subview.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCudaUVM_Category.hpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCudaUVM_SharedAlloc.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCudaUVM_ViewAPI_a.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCudaUVM_ViewAPI_b.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCudaUVM_ViewAPI_c.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCudaUVM_ViewAPI_d.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCudaUVM_ViewAPI_e.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCudaUVM_ViewCopy.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCudaUVM_ViewMapping_a.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCudaUVM_ViewMapping_b.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCudaUVM_ViewMapping_subview.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_AtomicOperations_complexdouble.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_AtomicOperations
```

```
ons_complexfloat.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_AtomicOperations_double.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_AtomicOperations_float.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_AtomicOperations_int.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_AtomicOperations_longint.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_AtomicOperations_longlongint.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_AtomicOperations_unsignedint.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_AtomicOperations_unsignedlongint.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_AtomicViews.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_Atomics.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_Category.hpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_Complex.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_Concepts.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_Crs.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_DebugPinUVMSpace.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_DebugSerialExecution.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_DeepCopyAlignment.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_FunctorAnalysis.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_Init.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_InterOp_Init.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_InterOp_Streams.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_LocalDeepCopy.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_MDRange_a.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_MDRange_b.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_MDRange_c.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_MDRange_d.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_MDRange_e.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_Other.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_RangePolicy.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_RangePolicyRequire.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_Reducers_a.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_Reducers_b.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_Reducers_c.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_Reducers_d.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_Reductions.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_Reductions_DeviceView.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_Scan.cpp
```

```
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_SharedAlloc.c
pp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_Spaces.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_SubView_a.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_SubView_b.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_SubView_c01.c
pp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_SubView_c02.c
pp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_SubView_c03.c
pp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_SubView_c04.c
pp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_SubView_c05.c
pp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_SubView_c06.c
pp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_SubView_c07.c
pp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_SubView_c08.c
pp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_SubView_c09.c
pp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_SubView_c10.c
pp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_SubView_c11.c
pp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_SubView_c12.c
pp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_SubView_c13.c
pp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_SubView_c_all.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_Task.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_Team.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_TeamReduction
Scan.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_TeamScratch.c
pp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_TeamTeamSize.
cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_TeamVectorRan
ge.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_UniqueToken.c
pp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_ViewAPI_a.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_ViewAPI_b.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_ViewAPI_c.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_ViewAPI_d.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_ViewAPI_e.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_ViewLayoutStr
ideAssignment.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_ViewMapping_
a.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_ViewMapping_
b.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_ViewMapping_s
ubview.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/cuda/TestCuda_ViewOfClass.c
pp
```

lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/cuda/TestCuda\_ViewResize.cp  
p  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/cuda/TestCuda\_View\_64bit.cp  
p  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/cuda/TestCuda\_WorkGraph.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/default/  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/default/TestDefaultDeviceDe  
velop.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/default/TestDefaultDeviceTy  
pe.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/default/TestDefaultDeviceTy  
peInit\_1.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/default/TestDefaultDeviceTy  
peInit\_10.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/default/TestDefaultDeviceTy  
peInit\_11.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/default/TestDefaultDeviceTy  
peInit\_12.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/default/TestDefaultDeviceTy  
peInit\_13.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/default/TestDefaultDeviceTy  
peInit\_14.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/default/TestDefaultDeviceTy  
peInit\_15.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/default/TestDefaultDeviceTy  
peInit\_16.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/default/TestDefaultDeviceTy  
peInit\_2.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/default/TestDefaultDeviceTy  
peInit\_3.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/default/TestDefaultDeviceTy  
peInit\_4.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/default/TestDefaultDeviceTy  
peInit\_5.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/default/TestDefaultDeviceTy  
peInit\_6.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/default/TestDefaultDeviceTy  
peInit\_7.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/default/TestDefaultDeviceTy  
peInit\_8.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/default/TestDefaultDeviceTy  
peInit\_9.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/default/TestDefaultDeviceTy  
peResize.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/default/TestDefaultDeviceTy  
pe\_Category.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/default/TestDefaultDeviceTy  
pe\_a1.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/default/TestDefaultDeviceTy  
pe\_a2.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/default/TestDefaultDeviceTy  
pe\_a3.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/default/TestDefaultDeviceTy  
pe\_b1.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/default/TestDefaultDeviceTy  
pe\_b2.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/default/TestDefaultDeviceTy  
pe\_b3.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/default/TestDefaultDeviceTy  
pe\_c1.cpp

lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/default/TestDefaultDeviceTy  
pe\_c2.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/default/TestDefaultDeviceTy  
pe\_c3.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/default/TestDefaultDeviceTy  
pe\_d.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/diffconfig.sh  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/headers\_self\_contained/  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/headers\_self\_contained/CMak  
eLists.txt  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/headers\_self\_contained/tstH  
eader.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hip/  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hip/TestHIPHostPinned\_Categ  
ory.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hip/TestHIPHostPinned\_Share  
dAlloc.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hip/TestHIPHostPinned\_ViewA  
PI\_a.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hip/TestHIPHostPinned\_ViewA  
PI\_b.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hip/TestHIPHostPinned\_ViewA  
PI\_c.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hip/TestHIPHostPinned\_ViewA  
PI\_d.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hip/TestHIPHostPinned\_ViewA  
PI\_e.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hip/TestHIPHostPinned\_ViewC  
opy.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hip/TestHIPHostPinned\_ViewM  
apping\_a.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hip/TestHIPHostPinned\_ViewM  
apping\_b.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hip/TestHIPHostPinned\_ViewM  
apping\_subview.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hip/TestHIP\_AtomicOperation  
s\_complexdouble.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hip/TestHIP\_AtomicOperation  
s\_complexfloat.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hip/TestHIP\_AtomicOperation  
s\_double.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hip/TestHIP\_AtomicOperation  
s\_float.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hip/TestHIP\_AtomicOperation  
s\_int.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hip/TestHIP\_AtomicOperation  
s\_longint.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hip/TestHIP\_AtomicOperation  
s\_longlongint.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hip/TestHIP\_AtomicOperation  
s\_unsignedint.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hip/TestHIP\_AtomicOperation  
s\_unsignedlongint.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hip/TestHIP\_AtomicViews.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hip/TestHIP\_Atomics.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hip/TestHIP\_Category.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hip/TestHIP\_Complex.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hip/TestHIP\_Concepts.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hip/TestHIP\_Crs.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hip/TestHIP\_DeepCopyAlignme

```
nt.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hip/TestHIP_FunctorAnalysis.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hip/TestHIP_Init.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hip/TestHIP_InterOp_Init.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hip/TestHIP_InterOp_Stream.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hip/TestHIP_LocalDeepCopy.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hip/TestHIP_MDRange_a.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hip/TestHIP_MDRange_b.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hip/TestHIP_MDRange_c.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hip/TestHIP_MDRange_d.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hip/TestHIP_MDRange_e.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hip/TestHIP_Other.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hip/TestHIP_RangePolicy.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hip/TestHIP_RangePolicyRequire.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hip/TestHIP_Reducers_a.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hip/TestHIP_Reducers_b.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hip/TestHIP_Reducers_c.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hip/TestHIP_Reducers_d.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hip/TestHIP_Reductions.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hip/TestHIP_Reductions_DeviceView.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hip/TestHIP_Scan.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hip/TestHIP_ScanUnit.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hip/TestHIP_SharedAlloc.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hip/TestHIP_Spaces.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hip/TestHIP_SubView_a.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hip/TestHIP_SubView_b.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hip/TestHIP_SubView_c01.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hip/TestHIP_SubView_c02.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hip/TestHIP_SubView_c03.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hip/TestHIP_SubView_c04.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hip/TestHIP_SubView_c05.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hip/TestHIP_SubView_c06.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hip/TestHIP_SubView_c07.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hip/TestHIP_SubView_c08.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hip/TestHIP_SubView_c09.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hip/TestHIP_SubView_c10.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hip/TestHIP_SubView_c11.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hip/TestHIP_SubView_c12.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hip/TestHIP_SubView_c13.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hip/TestHIP_Team.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hip/TestHIP_TeamReductionScan.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hip/TestHIP_TeamScratch.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hip/TestHIP_UniqueToken.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hip/TestHIP_ViewAPI_a.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hip/TestHIP_ViewAPI_b.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hip/TestHIP_ViewAPI_c.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hip/TestHIP_ViewAPI_d.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hip/TestHIP_ViewAPI_e.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hip/TestHIP_ViewLayoutStrideAssignment.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hip/TestHIP_ViewMapping_a.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hip/TestHIP_ViewMapping_b.cpp
```

```
pp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hip/TestHIP_ViewMapping_sub
view.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hip/TestHIP_ViewOfClass.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hip/TestHIP_ViewResize.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hip/TestHIP_View_64bit.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hip/TestHIP_WorkGraph.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hpx/
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hpx/TestHPX_AtomicOperation
s_complexdouble.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hpx/TestHPX_AtomicOperation
s_complexfloat.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hpx/TestHPX_AtomicOperation
s_double.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hpx/TestHPX_AtomicOperation
s_float.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hpx/TestHPX_AtomicOperation
s_int.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hpx/TestHPX_AtomicOperation
s_longint.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hpx/TestHPX_AtomicOperation
s_longlongint.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hpx/TestHPX_AtomicOperation
s_unsignedint.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hpx/TestHPX_AtomicOperation
s_unsignedlongint.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hpx/TestHPX_AtomicViews.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hpx/TestHPX_Atomics.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hpx/TestHPX_Category.hpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hpx/TestHPX_Complex.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hpx/TestHPX_Concepts.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hpx/TestHPX_Crs.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hpx/TestHPX_DeepCopyAlignme
nt.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hpx/TestHPX_FunctorAnalysi
s.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hpx/TestHPX_IndependentInst
ances.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hpx/TestHPX_IndependentInst
ancesDelayedExecution.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hpx/TestHPX_IndependentInst
ancesInstanceId.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hpx/TestHPX_IndependentInst
ancesRefCounting.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hpx/TestHPX_Init.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hpx/TestHPX_InterOp.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hpx/TestHPX_LocalDeepCopy.c
pp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hpx/TestHPX_MDRange_a.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hpx/TestHPX_MDRange_b.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hpx/TestHPX_MDRange_c.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hpx/TestHPX_MDRange_d.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hpx/TestHPX_MDRange_e.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hpx/TestHPX_Other.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hpx/TestHPX_RangePolicy.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hpx/TestHPX_RangePolicyRequ
ire.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hpx/TestHPX_Reducers_a.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hpx/TestHPX_Reducers_b.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/hpx/TestHPX_Reducers_c.cpp
```

lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hpx/TestHPX\_Reducers\_d.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hpx/TestHPX\_Reductions.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hpx/TestHPX\_Reductions\_DeviceView.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hpx/TestHPX\_Scan.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hpx/TestHPX\_SharedAlloc.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hpx/TestHPX\_SubView\_a.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hpx/TestHPX\_SubView\_b.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hpx/TestHPX\_SubView\_c01.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hpx/TestHPX\_SubView\_c02.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hpx/TestHPX\_SubView\_c03.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hpx/TestHPX\_SubView\_c04.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hpx/TestHPX\_SubView\_c05.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hpx/TestHPX\_SubView\_c06.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hpx/TestHPX\_SubView\_c07.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hpx/TestHPX\_SubView\_c08.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hpx/TestHPX\_SubView\_c09.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hpx/TestHPX\_SubView\_c10.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hpx/TestHPX\_SubView\_c11.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hpx/TestHPX\_SubView\_c12.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hpx/TestHPX\_SubView\_c13.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hpx/TestHPX\_SubView\_c\_all.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hpx/TestHPX\_Task.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hpx/TestHPX\_Team.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hpx/TestHPX\_TeamReductionScan.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hpx/TestHPX\_TeamScratch.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hpx/TestHPX\_TeamTeamSize.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hpx/TestHPX\_TeamVectorRange.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hpx/TestHPX\_UniqueToken.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hpx/TestHPX\_ViewAPI\_a.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hpx/TestHPX\_ViewAPI\_b.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hpx/TestHPX\_ViewAPI\_c.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hpx/TestHPX\_ViewAPI\_d.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hpx/TestHPX\_ViewAPI\_e.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hpx/TestHPX\_ViewLayoutStrideAssignment.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hpx/TestHPX\_ViewMapping\_a.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hpx/TestHPX\_ViewMapping\_b.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hpx/TestHPX\_ViewMapping\_subview.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hpx/TestHPX\_ViewOfClass.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hpx/TestHPX\_ViewResize.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hpx/TestHPX\_View\_64bit.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/hpx/TestHPX\_WorkGraph.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/incremental/  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/incremental/Test01\_execspace.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/incremental/Test02\_atomic\_host.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/incremental/Test03a\_MemorySpace\_malloc.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/incremental/Test03b\_MemorySpace\_free.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/incremental/Test04\_Parallel



For\_RangePolicy.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/incremental/Test05\_ParallelReduce\_RangePolicy.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/incremental/Test06\_ParallelFor\_MDRangePolicy.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/incremental/Test08\_deep\_copy.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/incremental/Test10\_HierarchicalBasics.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/incremental/Test11a\_ParallelFor\_TeamThreadRange.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/incremental/Test11b\_ParallelFor\_TeamVectorRange.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/incremental/Test11c\_ParallelFor\_ThreadVectorRange.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/incremental/Test12a\_ThreadScratch.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/incremental/Test12b\_TeamScratch.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/incremental/Test13a\_ParallelRed\_TeamThreadRange.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/incremental/Test13b\_ParallelRed\_TeamVectorRange.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/incremental/Test13c\_ParallelRed\_ThreadVectorRange.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/incremental/Test14\_MDRangeReduce.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/incremental/Test16\_ParallelScan.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/incremental/Test17\_CompleteAtomic.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmp/  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmp/TestOpenMP.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmp/TestOpenMP\_AtomicOperations\_complexdouble.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmp/TestOpenMP\_AtomicOperations\_complexfloat.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmp/TestOpenMP\_AtomicOperations\_double.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmp/TestOpenMP\_AtomicOperations\_float.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmp/TestOpenMP\_AtomicOperations\_int.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmp/TestOpenMP\_AtomicOperations\_longint.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmp/TestOpenMP\_AtomicOperations\_longlongint.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmp/TestOpenMP\_AtomicOperations\_unsignedint.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmp/TestOpenMP\_AtomicOperations\_unsignedlongint.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmp/TestOpenMP\_AtomicViews.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmp/TestOpenMP\_Atomics.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmp/TestOpenMP\_Category.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmp/TestOpenMP\_Complex.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmp/TestOpenMP\_Concepts.

```
cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/openmp/TestOpenMP_Crs.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/openmp/TestOpenMP_DeepCopyA
lignment.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/openmp/TestOpenMP_FunctorAn
alysis.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/openmp/TestOpenMP_Init.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/openmp/TestOpenMP_InterOp.c
pp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/openmp/TestOpenMP_LocalDeep
Copy.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/openmp/TestOpenMP_MDRange_
a.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/openmp/TestOpenMP_MDRange_
b.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/openmp/TestOpenMP_MDRange_
c.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/openmp/TestOpenMP_MDRange_
d.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/openmp/TestOpenMP_MDRange_
e.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/openmp/TestOpenMP_Other.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/openmp/TestOpenMP_RangePoli
cy.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/openmp/TestOpenMP_RangePoli
cyRequire.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/openmp/TestOpenMP_Reducers_
a.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/openmp/TestOpenMP_Reducers_
b.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/openmp/TestOpenMP_Reducers_
c.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/openmp/TestOpenMP_Reducers_
d.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/openmp/TestOpenMP_Reduction
s.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/openmp/TestOpenMP_Reduction
s_DeviceView.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/openmp/TestOpenMP_Scan.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/openmp/TestOpenMP_SharedAll
oc.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/openmp/TestOpenMP_SubView_
a.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/openmp/TestOpenMP_SubView_
b.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/openmp/TestOpenMP_SubView_c
01.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/openmp/TestOpenMP_SubView_c
02.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/openmp/TestOpenMP_SubView_c
03.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/openmp/TestOpenMP_SubView_c
04.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/openmp/TestOpenMP_SubView_c
05.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/openmp/TestOpenMP_SubView_c
06.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/openmp/TestOpenMP_SubView_c
07.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/openmp/TestOpenMP_SubView_c
```

08.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmp/TestOpenMP\_SubView\_c  
09.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmp/TestOpenMP\_SubView\_c  
10.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmp/TestOpenMP\_SubView\_c  
11.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmp/TestOpenMP\_SubView\_c  
12.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmp/TestOpenMP\_SubView\_c  
13.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmp/TestOpenMP\_SubView\_c  
\_all.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmp/TestOpenMP\_Task.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmp/TestOpenMP\_Team.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmp/TestOpenMP\_TeamReduc  
tionScan.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmp/TestOpenMP\_TeamScrat  
ch.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmp/TestOpenMP\_TeamTeamS  
ize.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmp/TestOpenMP\_TeamVecto  
rRange.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmp/TestOpenMP\_UniqueTok  
en.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmp/TestOpenMP\_ViewAPI\_  
a.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmp/TestOpenMP\_ViewAPI\_  
b.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmp/TestOpenMP\_ViewAPI\_  
c.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmp/TestOpenMP\_ViewAPI\_  
d.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmp/TestOpenMP\_ViewAPI\_  
e.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmp/TestOpenMP\_ViewLayou  
tStrideAssignment.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmp/TestOpenMP\_ViewMappi  
ng\_a.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmp/TestOpenMP\_ViewMappi  
ng\_b.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmp/TestOpenMP\_ViewMappi  
ng\_subview.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmp/TestOpenMP\_ViewOfCla  
ss.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmp/TestOpenMP\_ViewResiz  
e.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmp/TestOpenMP\_View\_64bi  
t.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmp/TestOpenMP\_WorkGrap  
h.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarg  
et.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarg  
et\_AtomicOperations\_complexdouble.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarg  
et\_AtomicOperations\_complexfloat.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarg  
et\_AtomicOperations\_double.cpp

lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_AtomicOperations\_float.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_AtomicOperations\_int.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_AtomicOperations\_longint.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_AtomicOperations\_longlongint.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_AtomicOperations\_unsignedint.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_AtomicOperations\_unsignedlongint.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_AtomicViews.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_Atomics.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_Category.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_Complex.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_Concepts.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_Crs.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_DeepCopyAlignment.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_FunctorAnalysis.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_Init.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_LocalDeepCopy.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_MDRange\_a.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_MDRange\_b.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_MDRange\_c.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_MDRange\_d.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_MDRange\_e.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_Other.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_RangePolicy.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_RangePolicyRequire.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_Reducers\_a.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_Reducers\_b.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_Reducers\_c.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_Reducers\_d.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_Reductions.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_Reductions\_DeviceView.cpp

lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_Scan.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_SharedAlloc.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_SubView\_a.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_SubView\_b.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_SubView\_c01.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_SubView\_c02.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_SubView\_c03.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_SubView\_c04.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_SubView\_c05.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_SubView\_c06.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_SubView\_c07.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_SubView\_c08.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_SubView\_c09.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_SubView\_c10.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_SubView\_c11.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_SubView\_c12.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_SubView\_c13.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_Team.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_TeamReductionScan.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_TeamScratch.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_TeamTeamSize.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_TeamVectorRange.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_UniqueToken.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_ViewAPI\_a.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_ViewAPI\_b.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_ViewAPI\_c.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_ViewAPI\_d.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_ViewAPI\_e.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_ViewLayoutStrideAssignment.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_ViewMapping\_a.cpp

lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_ViewMapping\_b.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_ViewMapping\_subview.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_ViewOfClass.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_ViewResize.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_View\_64bit.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/openmptarget/TestOpenMPTarget\_WorkGraph.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/rocm/  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/rocm/TestROCMHostPinned\_Category.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/rocm/TestROCMHostPinned\_SharedAlloc.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/rocm/TestROCMHostPinned\_ViewAPI\_a.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/rocm/TestROCMHostPinned\_ViewAPI\_b.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/rocm/TestROCMHostPinned\_ViewAPI\_c.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/rocm/TestROCMHostPinned\_ViewAPI\_d.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/rocm/TestROCMHostPinned\_ViewAPI\_e.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/rocm/TestROCMHostPinned\_ViewCopy.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/rocm/TestROCMHostPinned\_ViewMapping\_a.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/rocm/TestROCMHostPinned\_ViewMapping\_b.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/rocm/TestROCMHostPinned\_ViewMapping\_subview.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/rocm/TestROCMHostPinned\_View\_64bit.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/rocm/TestROCM\_All.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/rocm/TestROCM\_AtomicOperations\_double.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/rocm/TestROCM\_AtomicOperations\_float.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/rocm/TestROCM\_AtomicOperations\_int.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/rocm/TestROCM\_AtomicOperations\_longint.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/rocm/TestROCM\_AtomicOperations\_longlongint.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/rocm/TestROCM\_AtomicOperations\_unsignedint.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/rocm/TestROCM\_AtomicOperations\_unsignedlongint.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/rocm/TestROCM\_AtomicViews.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/rocm/TestROCM\_Atomics.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/rocm/TestROCM\_Category.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/rocm/TestROCM\_Complex.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/rocm/TestROCM\_Crs.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/rocm/TestROCM\_DeepCopyAlignment.cpp

```
lammps-stable_290ct2020/lib/kokkos/core/unit_test/rocm/TestROcm_Init.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/rocm/TestROcm_MDRangeReduce
_a.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/rocm/TestROcm_MDRangeReduce
_b.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/rocm/TestROcm_MDRangeReduce
_c.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/rocm/TestROcm_MDRangeReduce
_d.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/rocm/TestROcm_MDRangeReduce
_e.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/rocm/TestROcm_MDRange_a.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/rocm/TestROcm_MDRange_b.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/rocm/TestROcm_MDRange_c.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/rocm/TestROcm_MDRange_d.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/rocm/TestROcm_MDRange_e.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/rocm/TestROcm_Other.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/rocm/TestROcm_RangePolicy.c
pp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/rocm/TestROcm_Reducers_a.cp
p
lammps-stable_290ct2020/lib/kokkos/core/unit_test/rocm/TestROcm_Reducers_b.cp
p
lammps-stable_290ct2020/lib/kokkos/core/unit_test/rocm/TestROcm_Reducers_c.cp
p
lammps-stable_290ct2020/lib/kokkos/core/unit_test/rocm/TestROcm_Reducers_d.cp
p
lammps-stable_290ct2020/lib/kokkos/core/unit_test/rocm/TestROcm_Reductions.cp
p
lammps-stable_290ct2020/lib/kokkos/core/unit_test/rocm/TestROcm_Scan.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/rocm/TestROcm_SharedAlloc.c
pp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/rocm/TestROcm_Spaces.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/rocm/TestROcm_SubView_a.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/rocm/TestROcm_SubView_b.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/rocm/TestROcm_SubView_c01.c
pp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/rocm/TestROcm_SubView_c02.c
pp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/rocm/TestROcm_SubView_c03.c
pp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/rocm/TestROcm_SubView_c04.c
pp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/rocm/TestROcm_SubView_c05.c
pp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/rocm/TestROcm_SubView_c06.c
pp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/rocm/TestROcm_SubView_c07.c
pp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/rocm/TestROcm_SubView_c08.c
pp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/rocm/TestROcm_SubView_c09.c
pp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/rocm/TestROcm_SubView_c10.c
pp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/rocm/TestROcm_SubView_c11.c
pp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/rocm/TestROcm_SubView_c12.c
pp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/rocm/TestROcm_SubView_c13.c
```

```
pp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/rocm/TestROCM_Team.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/rocm/TestROCM_TeamReduction
Scan.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/rocm/TestROCM_TeamScratch.c
pp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/rocm/TestROCM_TeamTeamSize.
cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/rocm/TestROCM_ViewAPI_a.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/rocm/TestROCM_ViewAPI_b.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/rocm/TestROCM_ViewAPI_c.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/rocm/TestROCM_ViewAPI_d.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/rocm/TestROCM_ViewAPI_e.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/rocm/TestROCM_ViewMapping_
a.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/rocm/TestROCM_ViewMapping_
b.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/rocm/TestROCM_ViewMapping_s
ubview.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/rocm/TestROCM_ViewOfClass.c
pp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/serial/
lammps-stable_290ct2020/lib/kokkos/core/unit_test/serial/TestSerial_AtomicOpe
rations_complexdouble.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/serial/TestSerial_AtomicOpe
rations_complexfloat.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/serial/TestSerial_AtomicOpe
rations_double.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/serial/TestSerial_AtomicOpe
rations_float.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/serial/TestSerial_AtomicOpe
rations_int.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/serial/TestSerial_AtomicOpe
rations_longint.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/serial/TestSerial_AtomicOpe
rations_longlongint.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/serial/TestSerial_AtomicOpe
rations_unsignedint.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/serial/TestSerial_AtomicOpe
rations_unsignedlongint.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/serial/TestSerial_AtomicVie
ws.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/serial/TestSerial_Atomics.c
pp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/serial/TestSerial_Category.
hpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/serial/TestSerial_Complex.c
pp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/serial/TestSerial_Concepts.
cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/serial/TestSerial_Crs.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/serial/TestSerial_DeepCopyA
lignment.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/serial/TestSerial_FunctorAn
alysis.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/serial/TestSerial_Init.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/serial/TestSerial_LocalDeep
Copy.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/serial/TestSerial_MDRange_
a.cpp
```



lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/serial/TestSerial\_MDRange\_ b.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/serial/TestSerial\_MDRange\_ c.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/serial/TestSerial\_MDRange\_ d.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/serial/TestSerial\_MDRange\_ e.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/serial/TestSerial\_Other.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/serial/TestSerial\_RangePoli cy.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/serial/TestSerial\_RangePoli cyRequire.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/serial/TestSerial\_Reducers\_ a.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/serial/TestSerial\_Reducers\_ b.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/serial/TestSerial\_Reducers\_ c.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/serial/TestSerial\_Reducers\_ d.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/serial/TestSerial\_Reduction s.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/serial/TestSerial\_Reduction s\_DeviceView.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/serial/TestSerial\_Scan.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/serial/TestSerial\_SharedAll oc.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/serial/TestSerial\_SubView\_ a.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/serial/TestSerial\_SubView\_ b.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/serial/TestSerial\_SubView\_c 01.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/serial/TestSerial\_SubView\_c 02.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/serial/TestSerial\_SubView\_c 03.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/serial/TestSerial\_SubView\_c 04.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/serial/TestSerial\_SubView\_c 05.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/serial/TestSerial\_SubView\_c 06.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/serial/TestSerial\_SubView\_c 07.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/serial/TestSerial\_SubView\_c 08.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/serial/TestSerial\_SubView\_c 09.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/serial/TestSerial\_SubView\_c 10.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/serial/TestSerial\_SubView\_c 11.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/serial/TestSerial\_SubView\_c 12.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/serial/TestSerial\_SubView\_c 13.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/serial/TestSerial\_SubView\_c \_all.cpp

```
lammps-stable_290ct2020/lib/kokkos/core/unit_test/serial/TestSerial_Task.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/serial/TestSerial_Team.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/serial/TestSerial_TeamReductionScan.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/serial/TestSerial_TeamScratch.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/serial/TestSerial_TeamTeamSize.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/serial/TestSerial_TeamVectorRange.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/serial/TestSerial_UniqueToken.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/serial/TestSerial_ViewAPI_a.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/serial/TestSerial_ViewAPI_b.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/serial/TestSerial_ViewAPI_c.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/serial/TestSerial_ViewAPI_d.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/serial/TestSerial_ViewAPI_e.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/serial/TestSerial_ViewLayoutStrideAssignment.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/serial/TestSerial_ViewMapping_a.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/serial/TestSerial_ViewMapping_b.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/serial/TestSerial_ViewMapping_subview.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/serial/TestSerial_ViewOfClass.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/serial/TestSerial_ViewResize.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/serial/TestSerial_View_64bit.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/serial/TestSerial_WorkGraph.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/standalone/
lammps-stable_290ct2020/lib/kokkos/core/unit_test/standalone/Makefile
lammps-stable_290ct2020/lib/kokkos/core/unit_test/standalone/UnitTestMainInit.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/testmake.sh
lammps-stable_290ct2020/lib/kokkos/core/unit_test/threads/
lammps-stable_290ct2020/lib/kokkos/core/unit_test/threads/TestThreads_AtomicOperations_complexdouble.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/threads/TestThreads_AtomicOperations_complexfloat.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/threads/TestThreads_AtomicOperations_double.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/threads/TestThreads_AtomicOperations_float.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/threads/TestThreads_AtomicOperations_int.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/threads/TestThreads_AtomicOperations_longint.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/threads/TestThreads_AtomicOperations_longlongint.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/threads/TestThreads_AtomicOperations_unsignedint.cpp
```

lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_AtomicOperations\_unsignedlongint.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_AtomicViews.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_Atomics.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_Category.hpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_Complex.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_Concepts.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_Crs.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_DeepCopyAlignment.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_FunctorAnalysis.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_Init.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_LocalDeepCopy.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_MDRange\_a.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_MDRange\_b.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_MDRange\_c.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_MDRange\_d.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_MDRange\_e.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_Other.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_RangePolicy.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_RangePolicyRequire.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_Reducers\_a.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_Reducers\_b.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_Reducers\_c.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_Reducers\_d.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_Reductions.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_Reductions\_DeviceView.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_Scan.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_SharedAlloc.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_SubView\_a.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_SubView\_b.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_SubView\_c01.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_SubView

\_c02.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_SubView  
\_c03.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_SubView  
\_c04.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_SubView  
\_c05.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_SubView  
\_c06.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_SubView  
\_c07.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_SubView  
\_c08.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_SubView  
\_c09.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_SubView  
\_c10.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_SubView  
\_c11.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_SubView  
\_c12.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_SubView  
\_c13.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_Team.cp  
p  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_TeamRed  
uctionScan.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_TeamScr  
atch.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_TeamTea  
mSize.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_TeamVec  
torRange.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_UniqueT  
oken.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_ViewAPI  
\_a.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_ViewAPI  
\_b.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_ViewAPI  
\_c.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_ViewAPI  
\_d.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_ViewAPI  
\_e.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_ViewLay  
outStrideAssignment.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_ViewMap  
ping\_a.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_ViewMap  
ping\_b.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_ViewMap  
ping\_subview.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_ViewOfC  
lass.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_ViewRes  
ize.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_View\_64  
bit.cpp  
lammps-stable\_290ct2020/lib/kokkos/core/unit\_test/threads/TestThreads\_WorkGra

```
ph.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/tools/
lammps-stable_290ct2020/lib/kokkos/core/unit_test/tools/TestAllCalls.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/tools/TestCInterface.c
lammps-stable_290ct2020/lib/kokkos/core/unit_test/tools/TestTuning.cpp
lammps-stable_290ct2020/lib/kokkos/core/unit_test/tools/printing-tool.cpp
lammps-stable_290ct2020/lib/kokkos/example/
lammps-stable_290ct2020/lib/kokkos/example/CMakeLists.txt
lammps-stable_290ct2020/lib/kokkos/example/README
lammps-stable_290ct2020/lib/kokkos/example/build_cmake_in_tree/
lammps-stable_290ct2020/lib/kokkos/example/build_cmake_in_tree/CMakeLists.txt
lammps-stable_290ct2020/lib/kokkos/example/build_cmake_in_tree/cmake_example.
cpp
lammps-stable_290ct2020/lib/kokkos/example/build_cmake_installed/
lammps-stable_290ct2020/lib/kokkos/example/build_cmake_installed/CMakeLists.t
xt
lammps-stable_290ct2020/lib/kokkos/example/build_cmake_installed/cmake_exampl
e.cpp
lammps-stable_290ct2020/lib/kokkos/example/build_cmake_installed/foo.f
lammps-stable_290ct2020/lib/kokkos/example/make_buildlink/
lammps-stable_290ct2020/lib/kokkos/example/make_buildlink/Makefile
lammps-stable_290ct2020/lib/kokkos/example/make_buildlink/README
lammps-stable_290ct2020/lib/kokkos/example/make_buildlink/main.cpp
lammps-stable_290ct2020/lib/kokkos/example/query_device/
lammps-stable_290ct2020/lib/kokkos/example/query_device/CMakeLists.txt
lammps-stable_290ct2020/lib/kokkos/example/query_device/Makefile
lammps-stable_290ct2020/lib/kokkos/example/query_device/query_device.cpp
lammps-stable_290ct2020/lib/kokkos/example/tutorial/
lammps-stable_290ct2020/lib/kokkos/example/tutorial/01_hello_world/
lammps-stable_290ct2020/lib/kokkos/example/tutorial/01_hello_world/CMakeList
s.txt
lammps-stable_290ct2020/lib/kokkos/example/tutorial/01_hello_world/Makefile
lammps-stable_290ct2020/lib/kokkos/example/tutorial/01_hello_world/hello_worl
d.cpp
lammps-stable_290ct2020/lib/kokkos/example/tutorial/01_hello_world_lambda/
lammps-stable_290ct2020/lib/kokkos/example/tutorial/01_hello_world_lambda/CMA
keLists.txt
lammps-stable_290ct2020/lib/kokkos/example/tutorial/01_hello_world_lambda/Mak
efile
lammps-stable_290ct2020/lib/kokkos/example/tutorial/01_hello_world_lambda/hel
lo_world_lambda.cpp
lammps-stable_290ct2020/lib/kokkos/example/tutorial/02_simple_reduce/
lammps-stable_290ct2020/lib/kokkos/example/tutorial/02_simple_reduce/CMakeLis
ts.txt
lammps-stable_290ct2020/lib/kokkos/example/tutorial/02_simple_reduce/Makefile
lammps-stable_290ct2020/lib/kokkos/example/tutorial/02_simple_reduce/simple_r
educer.cpp
lammps-stable_290ct2020/lib/kokkos/example/tutorial/02_simple_reduce_lambda/
lammps-stable_290ct2020/lib/kokkos/example/tutorial/02_simple_reduce_lambda/C
MakeLists.txt
lammps-stable_290ct2020/lib/kokkos/example/tutorial/02_simple_reduce_lambda/M
akefile
lammps-stable_290ct2020/lib/kokkos/example/tutorial/02_simple_reduce_lambda/s
imple_reduce_lambda.cpp
lammps-stable_290ct2020/lib/kokkos/example/tutorial/03_simple_view/
lammps-stable_290ct2020/lib/kokkos/example/tutorial/03_simple_view/CMakeList
s.txt
lammps-stable_290ct2020/lib/kokkos/example/tutorial/03_simple_view/Makefile
lammps-stable_290ct2020/lib/kokkos/example/tutorial/03_simple_view/simple_vie
w.cpp
```

```
lammps-stable_290ct2020/lib/kokkos/example/tutorial/03_simple_view_lambda/  
lammps-stable_290ct2020/lib/kokkos/example/tutorial/03_simple_view_lambda/CMakeLists.txt  
lammps-stable_290ct2020/lib/kokkos/example/tutorial/03_simple_view_lambda/Makefile  
lammps-stable_290ct2020/lib/kokkos/example/tutorial/03_simple_view_lambda/simple_view_lambda.cpp  
lammps-stable_290ct2020/lib/kokkos/example/tutorial/04_simple_memoryspaces/  
lammps-stable_290ct2020/lib/kokkos/example/tutorial/04_simple_memoryspaces/CMakeLists.txt  
lammps-stable_290ct2020/lib/kokkos/example/tutorial/04_simple_memoryspaces/Makefile  
lammps-stable_290ct2020/lib/kokkos/example/tutorial/04_simple_memoryspaces/simple_memoryspaces.cpp  
lammps-stable_290ct2020/lib/kokkos/example/tutorial/05_simple_atomics/  
lammps-stable_290ct2020/lib/kokkos/example/tutorial/05_simple_atomics/CMakeLists.txt  
lammps-stable_290ct2020/lib/kokkos/example/tutorial/05_simple_atomics/Makefile  
lammps-stable_290ct2020/lib/kokkos/example/tutorial/05_simple_atomics/simple_atomics.cpp  
lammps-stable_290ct2020/lib/kokkos/example/tutorial/06_simple_mdrangepolicy/  
lammps-stable_290ct2020/lib/kokkos/example/tutorial/06_simple_mdrangepolicy/CMakeLists.txt  
lammps-stable_290ct2020/lib/kokkos/example/tutorial/06_simple_mdrangepolicy/Makefile  
lammps-stable_290ct2020/lib/kokkos/example/tutorial/06_simple_mdrangepolicy/simple_mdrangepolicy.cpp  
lammps-stable_290ct2020/lib/kokkos/example/tutorial/Advanced_Views/  
lammps-stable_290ct2020/lib/kokkos/example/tutorial/Advanced_Views/01_data_layouts/  
lammps-stable_290ct2020/lib/kokkos/example/tutorial/Advanced_Views/01_data_layouts/CMakeLists.txt  
lammps-stable_290ct2020/lib/kokkos/example/tutorial/Advanced_Views/01_data_layouts/Makefile  
lammps-stable_290ct2020/lib/kokkos/example/tutorial/Advanced_Views/01_data_layouts/data_layouts.cpp  
lammps-stable_290ct2020/lib/kokkos/example/tutorial/Advanced_Views/02_memory_traits/  
lammps-stable_290ct2020/lib/kokkos/example/tutorial/Advanced_Views/02_memory_traits/CMakeLists.txt  
lammps-stable_290ct2020/lib/kokkos/example/tutorial/Advanced_Views/02_memory_traits/Makefile  
lammps-stable_290ct2020/lib/kokkos/example/tutorial/Advanced_Views/02_memory_traits/memory_traits.cpp  
lammps-stable_290ct2020/lib/kokkos/example/tutorial/Advanced_Views/03_subviews/  
lammps-stable_290ct2020/lib/kokkos/example/tutorial/Advanced_Views/03_subviews/CMakeLists.txt  
lammps-stable_290ct2020/lib/kokkos/example/tutorial/Advanced_Views/03_subviews/Makefile  
lammps-stable_290ct2020/lib/kokkos/example/tutorial/Advanced_Views/03_subviews/subviews.cpp  
lammps-stable_290ct2020/lib/kokkos/example/tutorial/Advanced_Views/04_dualviews/  
lammps-stable_290ct2020/lib/kokkos/example/tutorial/Advanced_Views/04_dualviews/CMakeLists.txt  
lammps-stable_290ct2020/lib/kokkos/example/tutorial/Advanced_Views/04_dualviews/Makefile  
lammps-stable_290ct2020/lib/kokkos/example/tutorial/Advanced_Views/04_dualviews
```

```
ws/dual_view.cpp
lammps-stable_290ct2020/lib/kokkos/example/tutorial/Advanced_Views/05_NVIDIA_UVM/
lammps-stable_290ct2020/lib/kokkos/example/tutorial/Advanced_Views/05_NVIDIA_UVM/CMakeLists.txt
lammps-stable_290ct2020/lib/kokkos/example/tutorial/Advanced_Views/05_NVIDIA_UVM/Makefile
lammps-stable_290ct2020/lib/kokkos/example/tutorial/Advanced_Views/05_NVIDIA_UVM/uvn_example.cpp
lammps-stable_290ct2020/lib/kokkos/example/tutorial/Advanced_Views/06_AtomicViews/
lammps-stable_290ct2020/lib/kokkos/example/tutorial/Advanced_Views/06_AtomicViews/Makefile
lammps-stable_290ct2020/lib/kokkos/example/tutorial/Advanced_Views/07_Overlapping_DeepCopy/
lammps-stable_290ct2020/lib/kokkos/example/tutorial/Advanced_Views/07_Overlapping_DeepCopy/Makefile
lammps-stable_290ct2020/lib/kokkos/example/tutorial/Advanced_Views/07_Overlapping_DeepCopy/overlapping_deepcopy.cpp
lammps-stable_290ct2020/lib/kokkos/example/tutorial/Advanced_Views/CMakeLists.txt
lammps-stable_290ct2020/lib/kokkos/example/tutorial/Advanced_Views/Makefile
lammps-stable_290ct2020/lib/kokkos/example/tutorial/Algorithms/
lammps-stable_290ct2020/lib/kokkos/example/tutorial/Algorithms/01_random_numbers/
lammps-stable_290ct2020/lib/kokkos/example/tutorial/Algorithms/01_random_numbers/Makefile
lammps-stable_290ct2020/lib/kokkos/example/tutorial/Algorithms/01_random_numbers/random_numbers.cpp
lammps-stable_290ct2020/lib/kokkos/example/tutorial/Algorithms/Makefile
lammps-stable_290ct2020/lib/kokkos/example/tutorial/CMakeLists.txt
lammps-stable_290ct2020/lib/kokkos/example/tutorial/Hierarchical_Parallelism/
lammps-stable_290ct2020/lib/kokkos/example/tutorial/Hierarchical_Parallelism/01_thread_teams/
lammps-stable_290ct2020/lib/kokkos/example/tutorial/Hierarchical_Parallelism/01_thread_teams/CMakeLists.txt
lammps-stable_290ct2020/lib/kokkos/example/tutorial/Hierarchical_Parallelism/01_thread_teams/Makefile
lammps-stable_290ct2020/lib/kokkos/example/tutorial/Hierarchical_Parallelism/01_thread_teams/thread_teams.cpp
lammps-stable_290ct2020/lib/kokkos/example/tutorial/Hierarchical_Parallelism/01_thread_teams_lambda/
lammps-stable_290ct2020/lib/kokkos/example/tutorial/Hierarchical_Parallelism/01_thread_teams_lambda/CMakeLists.txt
lammps-stable_290ct2020/lib/kokkos/example/tutorial/Hierarchical_Parallelism/01_thread_teams_lambda/Makefile
lammps-stable_290ct2020/lib/kokkos/example/tutorial/Hierarchical_Parallelism/01_thread_teams_lambda/thread_teams_lambda.cpp
lammps-stable_290ct2020/lib/kokkos/example/tutorial/Hierarchical_Parallelism/02_nested_parallel_for/
lammps-stable_290ct2020/lib/kokkos/example/tutorial/Hierarchical_Parallelism/02_nested_parallel_for/CMakeLists.txt
lammps-stable_290ct2020/lib/kokkos/example/tutorial/Hierarchical_Parallelism/02_nested_parallel_for/Makefile
lammps-stable_290ct2020/lib/kokkos/example/tutorial/Hierarchical_Parallelism/02_nested_parallel_for/nested_parallel_for.cpp
lammps-stable_290ct2020/lib/kokkos/example/tutorial/Hierarchical_Parallelism/03_vectorization/
lammps-stable_290ct2020/lib/kokkos/example/tutorial/Hierarchical_Parallelism/03_vectorization/CMakeLists.txt
```

```
lammps-stable_290ct2020/lib/kokkos/example/tutorial/Hierarchical_Parallelism/
03_vectorization/Makefile
lammps-stable_290ct2020/lib/kokkos/example/tutorial/Hierarchical_Parallelism/
03_vectorization/vectorization.cpp
lammps-stable_290ct2020/lib/kokkos/example/tutorial/Hierarchical_Parallelism/
04_team_scan/
lammps-stable_290ct2020/lib/kokkos/example/tutorial/Hierarchical_Parallelism/
04_team_scan/CMakeLists.txt
lammps-stable_290ct2020/lib/kokkos/example/tutorial/Hierarchical_Parallelism/
04_team_scan/Makefile
lammps-stable_290ct2020/lib/kokkos/example/tutorial/Hierarchical_Parallelism/
04_team_scan/team_scan.cpp
lammps-stable_290ct2020/lib/kokkos/example/tutorial/Hierarchical_Parallelism/
CMakeLists.txt
lammps-stable_290ct2020/lib/kokkos/example/tutorial/Hierarchical_Parallelism/
Makefile
lammps-stable_290ct2020/lib/kokkos/example/tutorial/Makefile
lammps-stable_290ct2020/lib/kokkos/example/tutorial/README
lammps-stable_290ct2020/lib/kokkos/example/tutorial/launch_bounds/
lammps-stable_290ct2020/lib/kokkos/example/tutorial/launch_bounds/CMakeLists.
txt
lammps-stable_290ct2020/lib/kokkos/example/tutorial/launch_bounds/Makefile
lammps-stable_290ct2020/lib/kokkos/example/tutorial/launch_bounds/launch_boun
ds_reduce.cpp
lammps-stable_290ct2020/lib/kokkos/example/virtual_functions/
lammps-stable_290ct2020/lib/kokkos/example/virtual_functions/Makefile
lammps-stable_290ct2020/lib/kokkos/example/virtual_functions/classes.cpp
lammps-stable_290ct2020/lib/kokkos/example/virtual_functions/classes.hpp
lammps-stable_290ct2020/lib/kokkos/example/virtual_functions/main.cpp
lammps-stable_290ct2020/lib/kokkos/generate_makefile.bash
lammps-stable_290ct2020/lib/kokkos/gnu_generate_makefile.bash
lammps-stable_290ct2020/lib/kokkos/master_history.txt
lammps-stable_290ct2020/lib/latte/
lammps-stable_290ct2020/lib/latte/Install.py
lammps-stable_290ct2020/lib/latte/Makefile.lammps.gfortran
lammps-stable_290ct2020/lib/latte/Makefile.lammps.ifort
lammps-stable_290ct2020/lib/latte/Makefile.lammps.linalg
lammps-stable_290ct2020/lib/latte/Makefile.lammps.mpi
lammps-stable_290ct2020/lib/latte/Makefile.lammps.serial
lammps-stable_290ct2020/lib/latte/README
lammps-stable_290ct2020/lib/linalg/
lammps-stable_290ct2020/lib/linalg/Install.py
lammps-stable_290ct2020/lib/linalg/Makefile.gfortran
lammps-stable_290ct2020/lib/linalg/Makefile.mpi
lammps-stable_290ct2020/lib/linalg/Makefile.serial
lammps-stable_290ct2020/lib/linalg/README
lammps-stable_290ct2020/lib/linalg/dasum.f
lammps-stable_290ct2020/lib/linalg/daxpy.f
lammps-stable_290ct2020/lib/linalg/dbdsqr.f
lammps-stable_290ct2020/lib/linalg/dcabs1.f
lammps-stable_290ct2020/lib/linalg/dcopy.f
lammps-stable_290ct2020/lib/linalg/ddot.f
lammps-stable_290ct2020/lib/linalg/dgebd2.f
lammps-stable_290ct2020/lib/linalg/dgebrd.f
lammps-stable_290ct2020/lib/linalg/dgecon.f
lammps-stable_290ct2020/lib/linalg/dgelq2.f
lammps-stable_290ct2020/lib/linalg/dgelqf.f
lammps-stable_290ct2020/lib/linalg/dgelsd.f
lammps-stable_290ct2020/lib/linalg/dgelss.f
lammps-stable_290ct2020/lib/linalg/dgemm.f
```



lammps-stable\_290ct2020/lib/linalg/dgemv.f  
lammps-stable\_290ct2020/lib/linalg/dgeqr2.f  
lammps-stable\_290ct2020/lib/linalg/dgeqrf.f  
lammps-stable\_290ct2020/lib/linalg/dger.f  
lammps-stable\_290ct2020/lib/linalg/dgesv.f  
lammps-stable\_290ct2020/lib/linalg/dgesvd.f  
lammps-stable\_290ct2020/lib/linalg/dgetf2.f  
lammps-stable\_290ct2020/lib/linalg/dgetrf.f  
lammps-stable\_290ct2020/lib/linalg/dgetrf2.f  
lammps-stable\_290ct2020/lib/linalg/dgetri.f  
lammps-stable\_290ct2020/lib/linalg/dgetrs.f  
lammps-stable\_290ct2020/lib/linalg/disnan.f  
lammps-stable\_290ct2020/lib/linalg/dlabad.f  
lammps-stable\_290ct2020/lib/linalg/dlabrd.f  
lammps-stable\_290ct2020/lib/linalg/dlacn2.f  
lammps-stable\_290ct2020/lib/linalg/dlacpy.f  
lammps-stable\_290ct2020/lib/linalg/dladiv.f  
lammps-stable\_290ct2020/lib/linalg/dlae2.f  
lammps-stable\_290ct2020/lib/linalg/dlaed0.f  
lammps-stable\_290ct2020/lib/linalg/dlaed1.f  
lammps-stable\_290ct2020/lib/linalg/dlaed2.f  
lammps-stable\_290ct2020/lib/linalg/dlaed3.f  
lammps-stable\_290ct2020/lib/linalg/dlaed4.f  
lammps-stable\_290ct2020/lib/linalg/dlaed5.f  
lammps-stable\_290ct2020/lib/linalg/dlaed6.f  
lammps-stable\_290ct2020/lib/linalg/dlaed7.f  
lammps-stable\_290ct2020/lib/linalg/dlaed8.f  
lammps-stable\_290ct2020/lib/linalg/dlaed9.f  
lammps-stable\_290ct2020/lib/linalg/dlaeda.f  
lammps-stable\_290ct2020/lib/linalg/dlaev2.f  
lammps-stable\_290ct2020/lib/linalg/dlaisnan.f  
lammps-stable\_290ct2020/lib/linalg/dlals0.f  
lammps-stable\_290ct2020/lib/linalg/dlalsa.f  
lammps-stable\_290ct2020/lib/linalg/dlalsd.f  
lammps-stable\_290ct2020/lib/linalg/dlamch.f  
lammps-stable\_290ct2020/lib/linalg/dlamrg.f  
lammps-stable\_290ct2020/lib/linalg/dlange.f  
lammps-stable\_290ct2020/lib/linalg/dlanst.f  
lammps-stable\_290ct2020/lib/linalg/dlansy.f  
lammps-stable\_290ct2020/lib/linalg/dlapy2.f  
lammps-stable\_290ct2020/lib/linalg/dlapy3.f  
lammps-stable\_290ct2020/lib/linalg/dlarf.f  
lammps-stable\_290ct2020/lib/linalg/dlarfb.f  
lammps-stable\_290ct2020/lib/linalg/dlarfg.f  
lammps-stable\_290ct2020/lib/linalg/dlarft.f  
lammps-stable\_290ct2020/lib/linalg/dlartg.f  
lammps-stable\_290ct2020/lib/linalg/dlas2.f  
lammps-stable\_290ct2020/lib/linalg/dlascl.f  
lammps-stable\_290ct2020/lib/linalg/dlasd4.f  
lammps-stable\_290ct2020/lib/linalg/dlasd5.f  
lammps-stable\_290ct2020/lib/linalg/dlasd6.f  
lammps-stable\_290ct2020/lib/linalg/dlasd7.f  
lammps-stable\_290ct2020/lib/linalg/dlasd8.f  
lammps-stable\_290ct2020/lib/linalg/dlasda.f  
lammps-stable\_290ct2020/lib/linalg/dlasdq.f  
lammps-stable\_290ct2020/lib/linalg/dlasdt.f  
lammps-stable\_290ct2020/lib/linalg/dlaset.f  
lammps-stable\_290ct2020/lib/linalg/dlasq1.f  
lammps-stable\_290ct2020/lib/linalg/dlasq2.f  
lammps-stable\_290ct2020/lib/linalg/dlasq3.f

lammps-stable\_290ct2020/lib/linalg/dlasq4.f  
lammps-stable\_290ct2020/lib/linalg/dlasq5.f  
lammps-stable\_290ct2020/lib/linalg/dlasq6.f  
lammps-stable\_290ct2020/lib/linalg/dlasr.f  
lammps-stable\_290ct2020/lib/linalg/dlasrt.f  
lammps-stable\_290ct2020/lib/linalg/dlassq.f  
lammps-stable\_290ct2020/lib/linalg/dlasv2.f  
lammps-stable\_290ct2020/lib/linalg/dlaswp.f  
lammps-stable\_290ct2020/lib/linalg/dlatrd.f  
lammps-stable\_290ct2020/lib/linalg/dlatrs.f  
lammps-stable\_290ct2020/lib/linalg/dnrm2.f  
lammps-stable\_290ct2020/lib/linalg/dorg2l.f  
lammps-stable\_290ct2020/lib/linalg/dorg2r.f  
lammps-stable\_290ct2020/lib/linalg/dorgbr.f  
lammps-stable\_290ct2020/lib/linalg/dorgl2.f  
lammps-stable\_290ct2020/lib/linalg/dorglq.f  
lammps-stable\_290ct2020/lib/linalg/dorgql.f  
lammps-stable\_290ct2020/lib/linalg/dorgqr.f  
lammps-stable\_290ct2020/lib/linalg/dorgtr.f  
lammps-stable\_290ct2020/lib/linalg/dorm2l.f  
lammps-stable\_290ct2020/lib/linalg/dorm2r.f  
lammps-stable\_290ct2020/lib/linalg/dormbr.f  
lammps-stable\_290ct2020/lib/linalg/dorml2.f  
lammps-stable\_290ct2020/lib/linalg/dormlq.f  
lammps-stable\_290ct2020/lib/linalg/dormql.f  
lammps-stable\_290ct2020/lib/linalg/dormqr.f  
lammps-stable\_290ct2020/lib/linalg/dormtr.f  
lammps-stable\_290ct2020/lib/linalg/dpotf2.f  
lammps-stable\_290ct2020/lib/linalg/dpotrf.f  
lammps-stable\_290ct2020/lib/linalg/dpotrf2.f  
lammps-stable\_290ct2020/lib/linalg/drot.f  
lammps-stable\_290ct2020/lib/linalg/drscL.f  
lammps-stable\_290ct2020/lib/linalg/dscal.f  
lammps-stable\_290ct2020/lib/linalg/dstedc.f  
lammps-stable\_290ct2020/lib/linalg/dsteqr.f  
lammps-stable\_290ct2020/lib/linalg/dsterf.f  
lammps-stable\_290ct2020/lib/linalg/dswap.f  
lammps-stable\_290ct2020/lib/linalg/dsyev.f  
lammps-stable\_290ct2020/lib/linalg/dsyevd.f  
lammps-stable\_290ct2020/lib/linalg/dsygs2.f  
lammps-stable\_290ct2020/lib/linalg/dsygst.f  
lammps-stable\_290ct2020/lib/linalg/dsygv.f  
lammps-stable\_290ct2020/lib/linalg/dsygvd.f  
lammps-stable\_290ct2020/lib/linalg/dsymm.f  
lammps-stable\_290ct2020/lib/linalg/dsymv.f  
lammps-stable\_290ct2020/lib/linalg/dsyr2.f  
lammps-stable\_290ct2020/lib/linalg/dsyr2k.f  
lammps-stable\_290ct2020/lib/linalg/dsyrk.f  
lammps-stable\_290ct2020/lib/linalg/dsytd2.f  
lammps-stable\_290ct2020/lib/linalg/dsytrd.f  
lammps-stable\_290ct2020/lib/linalg/dtrmm.f  
lammps-stable\_290ct2020/lib/linalg/dtrmv.f  
lammps-stable\_290ct2020/lib/linalg/dtrsm.f  
lammps-stable\_290ct2020/lib/linalg/dtrsv.f  
lammps-stable\_290ct2020/lib/linalg/dtrti2.f  
lammps-stable\_290ct2020/lib/linalg/dtrtri.f  
lammps-stable\_290ct2020/lib/linalg/dznrm2.f  
lammps-stable\_290ct2020/lib/linalg/idamax.f  
lammps-stable\_290ct2020/lib/linalg/ieeeck.f  
lammps-stable\_290ct2020/lib/linalg/iladlc.f

```
lammps-stable_290ct2020/lib/linalg/iladlr.f
lammps-stable_290ct2020/lib/linalg/ilaenv.f
lammps-stable_290ct2020/lib/linalg/ilazlc.f
lammps-stable_290ct2020/lib/linalg/ilazlr.f
lammps-stable_290ct2020/lib/linalg/iparam2stage.F
lammps-stable_290ct2020/lib/linalg/iparmq.f
lammps-stable_290ct2020/lib/linalg/lsame.f
lammps-stable_290ct2020/lib/linalg/xerbla.f
lammps-stable_290ct2020/lib/linalg/zaxpy.f
lammps-stable_290ct2020/lib/linalg/zcopy.f
lammps-stable_290ct2020/lib/linalg/zdotc.f
lammps-stable_290ct2020/lib/linalg/zdscal.f
lammps-stable_290ct2020/lib/linalg/zgemm.f
lammps-stable_290ct2020/lib/linalg/zgemv.f
lammps-stable_290ct2020/lib/linalg/zgerc.f
lammps-stable_290ct2020/lib/linalg/zheev.f
lammps-stable_290ct2020/lib/linalg/zhemv.f
lammps-stable_290ct2020/lib/linalg/zher2.f
lammps-stable_290ct2020/lib/linalg/zher2k.f
lammps-stable_290ct2020/lib/linalg/zhetd2.f
lammps-stable_290ct2020/lib/linalg/zhetrd.f
lammps-stable_290ct2020/lib/linalg/zhpr.f
lammps-stable_290ct2020/lib/linalg/zlacgv.f
lammps-stable_290ct2020/lib/linalg/zladiv.f
lammps-stable_290ct2020/lib/linalg/zlanhe.f
lammps-stable_290ct2020/lib/linalg/zlarf.f
lammps-stable_290ct2020/lib/linalg/zlarfb.f
lammps-stable_290ct2020/lib/linalg/zlarfg.f
lammps-stable_290ct2020/lib/linalg/zlarft.f
lammps-stable_290ct2020/lib/linalg/zlascl.f
lammps-stable_290ct2020/lib/linalg/zlaset.f
lammps-stable_290ct2020/lib/linalg/zlasr.f
lammps-stable_290ct2020/lib/linalg/zlassq.f
lammps-stable_290ct2020/lib/linalg/zlatrd.f
lammps-stable_290ct2020/lib/linalg/zpptrf.f
lammps-stable_290ct2020/lib/linalg/zpptri.f
lammps-stable_290ct2020/lib/linalg/zscal.f
lammps-stable_290ct2020/lib/linalg/zsteqr.f
lammps-stable_290ct2020/lib/linalg/zswap.f
lammps-stable_290ct2020/lib/linalg/ztpmv.f
lammps-stable_290ct2020/lib/linalg/ztpsv.f
lammps-stable_290ct2020/lib/linalg/ztptri.f
lammps-stable_290ct2020/lib/linalg/ztrmm.f
lammps-stable_290ct2020/lib/linalg/ztrmv.f
lammps-stable_290ct2020/lib/linalg/zung2l.f
lammps-stable_290ct2020/lib/linalg/zung2r.f
lammps-stable_290ct2020/lib/linalg/zungl2.f
lammps-stable_290ct2020/lib/linalg/zungql.f
lammps-stable_290ct2020/lib/linalg/zungqr.f
lammps-stable_290ct2020/lib/linalg/zungtr.f
lammps-stable_290ct2020/lib/mesont/
lammps-stable_290ct2020/lib/mesont/.depend
lammps-stable_290ct2020/lib/mesont/CNTPot.f90
lammps-stable_290ct2020/lib/mesont/ExportCNT.f90
lammps-stable_290ct2020/lib/mesont/Install.py
lammps-stable_290ct2020/lib/mesont/LinFun2.f90
lammps-stable_290ct2020/lib/mesont/Makefile.gfortran
lammps-stable_290ct2020/lib/mesont/Makefile.ifort
lammps-stable_290ct2020/lib/mesont/Makefile.lammps.gfortran
lammps-stable_290ct2020/lib/mesont/Makefile.lammps.ifort
```

```
lammps-stable_290ct2020/lib/mesont/Makefile.serial
lammps-stable_290ct2020/lib/mesont/README
lammps-stable_290ct2020/lib/mesont/Spline1.f90
lammps-stable_290ct2020/lib/mesont/Spline2.f90
lammps-stable_290ct2020/lib/mesont/TPMForceField.f90
lammps-stable_290ct2020/lib/mesont/TPMGeom.f90
lammps-stable_290ct2020/lib/mesont/TPMLib.f90
lammps-stable_290ct2020/lib/mesont/TPMM0.f90
lammps-stable_290ct2020/lib/mesont/TPMM1.f90
lammps-stable_290ct2020/lib/mesont/TubePotBase.f90
lammps-stable_290ct2020/lib/mesont/TubePotMono.f90
lammps-stable_290ct2020/lib/mesont/TubePotTrue.f90
lammps-stable_290ct2020/lib/message/
lammps-stable_290ct2020/lib/message/Install.py
lammps-stable_290ct2020/lib/message/Makefile.lammps.nozmq
lammps-stable_290ct2020/lib/message/Makefile.lammps.zmq
lammps-stable_290ct2020/lib/message/README
lammps-stable_290ct2020/lib/message/cslib/
lammps-stable_290ct2020/lib/message/cslib/LICENSE
lammps-stable_290ct2020/lib/message/cslib/README
lammps-stable_290ct2020/lib/message/cslib/src/
lammps-stable_290ct2020/lib/message/cslib/src/Makefile
lammps-stable_290ct2020/lib/message/cslib/src/STUBS_MPI/
lammps-stable_290ct2020/lib/message/cslib/src/STUBS_MPI/mpi_dummy.h
lammps-stable_290ct2020/lib/message/cslib/src/STUBS_ZMQ/
lammps-stable_290ct2020/lib/message/cslib/src/STUBS_ZMQ/zmq.h
lammps-stable_290ct2020/lib/message/cslib/src/cslib.cpp
lammps-stable_290ct2020/lib/message/cslib/src/cslib.h
lammps-stable_290ct2020/lib/message/cslib/src/cslib.py
lammps-stable_290ct2020/lib/message/cslib/src/cslib_wrap.cpp
lammps-stable_290ct2020/lib/message/cslib/src/cslib_wrap.f90
lammps-stable_290ct2020/lib/message/cslib/src/cslib_wrap.h
lammps-stable_290ct2020/lib/message/cslib/src/msg.cpp
lammps-stable_290ct2020/lib/message/cslib/src/msg.h
lammps-stable_290ct2020/lib/message/cslib/src/msg_file.cpp
lammps-stable_290ct2020/lib/message/cslib/src/msg_file.h
lammps-stable_290ct2020/lib/message/cslib/src/msg_mpi_one.cpp
lammps-stable_290ct2020/lib/message/cslib/src/msg_mpi_one.h
lammps-stable_290ct2020/lib/message/cslib/src/msg_mpi_two.cpp
lammps-stable_290ct2020/lib/message/cslib/src/msg_mpi_two.h
lammps-stable_290ct2020/lib/message/cslib/src/msg_zmq.cpp
lammps-stable_290ct2020/lib/message/cslib/src/msg_zmq.h
lammps-stable_290ct2020/lib/molfile/
lammps-stable_290ct2020/lib/molfile/Makefile.lammps
lammps-stable_290ct2020/lib/molfile/README
lammps-stable_290ct2020/lib/molfile/molfile_plugin.h
lammps-stable_290ct2020/lib/molfile/vmdplugin.h
lammps-stable_290ct2020/lib/mscg/
lammps-stable_290ct2020/lib/mscg/Install.py
lammps-stable_290ct2020/lib/mscg/Makefile.lammps.default
lammps-stable_290ct2020/lib/mscg/Makefile.lammps.g++_simple
lammps-stable_290ct2020/lib/mscg/Makefile.lammps.mpi
lammps-stable_290ct2020/lib/mscg/Makefile.lammps.serial
lammps-stable_290ct2020/lib/mscg/Makefile.mpi
lammps-stable_290ct2020/lib/mscg/Makefile.serial
lammps-stable_290ct2020/lib/mscg/README
lammps-stable_290ct2020/lib/netcdf/
lammps-stable_290ct2020/lib/netcdf/Makefile.lammps
lammps-stable_290ct2020/lib/netcdf/README
lammps-stable_290ct2020/lib/plumed/
```

```
lammps-stable_290ct2020/lib/plumed/Install.py
lammps-stable_290ct2020/lib/plumed/Makefile.lammps.runtime
lammps-stable_290ct2020/lib/plumed/Makefile.lammps.runtime.macosx
lammps-stable_290ct2020/lib/plumed/Makefile.lammps.shared
lammps-stable_290ct2020/lib/plumed/Makefile.lammps.static
lammps-stable_290ct2020/lib/plumed/README
lammps-stable_290ct2020/lib/poems/
lammps-stable_290ct2020/lib/poems/.depend
lammps-stable_290ct2020/lib/poems/Authors_List.txt
lammps-stable_290ct2020/lib/poems/Copyright_Notice
lammps-stable_290ct2020/lib/poems/Grants_List.txt
lammps-stable_290ct2020/lib/poems/Install.py
lammps-stable_290ct2020/lib/poems/Makefile.g++
lammps-stable_290ct2020/lib/poems/Makefile.icc
lammps-stable_290ct2020/lib/poems/Makefile.lammps.empty
lammps-stable_290ct2020/lib/poems/Makefile.mpi
lammps-stable_290ct2020/lib/poems/Makefile.serial
lammps-stable_290ct2020/lib/poems/POEMSCchain.h
lammps-stable_290ct2020/lib/poems/POEMS_License.txt
lammps-stable_290ct2020/lib/poems/README
lammps-stable_290ct2020/lib/poems/SystemProcessor.h
lammps-stable_290ct2020/lib/poems/bodies.h
lammps-stable_290ct2020/lib/poems/body.cpp
lammps-stable_290ct2020/lib/poems/body.h
lammps-stable_290ct2020/lib/poems/body23joint.cpp
lammps-stable_290ct2020/lib/poems/body23joint.h
lammps-stable_290ct2020/lib/poems/colmatmap.cpp
lammps-stable_290ct2020/lib/poems/colmatmap.h
lammps-stable_290ct2020/lib/poems/colmatrix.cpp
lammps-stable_290ct2020/lib/poems/colmatrix.h
lammps-stable_290ct2020/lib/poems/defines.h
lammps-stable_290ct2020/lib/poems/eulerparameters.cpp
lammps-stable_290ct2020/lib/poems/eulerparameters.h
lammps-stable_290ct2020/lib/poems/fastmatrixops.cpp
lammps-stable_290ct2020/lib/poems/fastmatrixops.h
lammps-stable_290ct2020/lib/poems/fixedpoint.cpp
lammps-stable_290ct2020/lib/poems/fixedpoint.h
lammps-stable_290ct2020/lib/poems/freebodyjoint.cpp
lammps-stable_290ct2020/lib/poems/freebodyjoint.h
lammps-stable_290ct2020/lib/poems/inertialframe.cpp
lammps-stable_290ct2020/lib/poems/inertialframe.h
lammps-stable_290ct2020/lib/poems/joint.cpp
lammps-stable_290ct2020/lib/poems/joint.h
lammps-stable_290ct2020/lib/poems/joints.h
lammps-stable_290ct2020/lib/poems/mat3x3.cpp
lammps-stable_290ct2020/lib/poems/mat3x3.h
lammps-stable_290ct2020/lib/poems/mat4x4.cpp
lammps-stable_290ct2020/lib/poems/mat4x4.h
lammps-stable_290ct2020/lib/poems/mat6x6.cpp
lammps-stable_290ct2020/lib/poems/mat6x6.h
lammps-stable_290ct2020/lib/poems/matrices.h
lammps-stable_290ct2020/lib/poems/matrix.cpp
lammps-stable_290ct2020/lib/poems/matrix.h
lammps-stable_290ct2020/lib/poems/matrixfun.cpp
lammps-stable_290ct2020/lib/poems/matrixfun.h
lammps-stable_290ct2020/lib/poems/mixedjoint.cpp
lammps-stable_290ct2020/lib/poems/mixedjoint.h
lammps-stable_290ct2020/lib/poems/norm.cpp
lammps-stable_290ct2020/lib/poems/norm.h
lammps-stable_290ct2020/lib/poems/onbody.cpp
```

```
lammps-stable_290ct2020/lib/poems/onbody.h
lammps-stable_290ct2020/lib/poems/onfunctions.cpp
lammps-stable_290ct2020/lib/poems/onfunctions.h
lammps-stable_290ct2020/lib/poems/onsolver.cpp
lammps-stable_290ct2020/lib/poems/onsolver.h
lammps-stable_290ct2020/lib/poems/particle.cpp
lammps-stable_290ct2020/lib/poems/particle.h
lammps-stable_290ct2020/lib/poems/poemslist.h
lammps-stable_290ct2020/lib/poems/poemsnode.h
lammps-stable_290ct2020/lib/poems/poemsobject.cpp
lammps-stable_290ct2020/lib/poems/poemsobject.h
lammps-stable_290ct2020/lib/poems/poemstree.h
lammps-stable_290ct2020/lib/poems/poemstreenode.cpp
lammps-stable_290ct2020/lib/poems/poemstreenode.h
lammps-stable_290ct2020/lib/poems/point.cpp
lammps-stable_290ct2020/lib/poems/point.h
lammps-stable_290ct2020/lib/poems/points.h
lammps-stable_290ct2020/lib/poems/prismaticjoint.cpp
lammps-stable_290ct2020/lib/poems/prismaticjoint.h
lammps-stable_290ct2020/lib/poems/revolutejoint.cpp
lammps-stable_290ct2020/lib/poems/revolutejoint.h
lammps-stable_290ct2020/lib/poems/rigidbody.cpp
lammps-stable_290ct2020/lib/poems/rigidbody.h
lammps-stable_290ct2020/lib/poems/rowmatrix.cpp
lammps-stable_290ct2020/lib/poems/rowmatrix.h
lammps-stable_290ct2020/lib/poems/solver.cpp
lammps-stable_290ct2020/lib/poems/solver.h
lammps-stable_290ct2020/lib/poems/sphericaljoint.cpp
lammps-stable_290ct2020/lib/poems/sphericaljoint.h
lammps-stable_290ct2020/lib/poems/system.cpp
lammps-stable_290ct2020/lib/poems/system.h
lammps-stable_290ct2020/lib/poems/vect3.cpp
lammps-stable_290ct2020/lib/poems/vect3.h
lammps-stable_290ct2020/lib/poems/vect4.cpp
lammps-stable_290ct2020/lib/poems/vect4.h
lammps-stable_290ct2020/lib/poems/vect6.cpp
lammps-stable_290ct2020/lib/poems/vect6.h
lammps-stable_290ct2020/lib/poems/virtualcolmatrix.cpp
lammps-stable_290ct2020/lib/poems/virtualcolmatrix.h
lammps-stable_290ct2020/lib/poems/virtualmatrix.cpp
lammps-stable_290ct2020/lib/poems/virtualmatrix.h
lammps-stable_290ct2020/lib/poems/virtualrowmatrix.cpp
lammps-stable_290ct2020/lib/poems/virtualrowmatrix.h
lammps-stable_290ct2020/lib/poems/workspace.cpp
lammps-stable_290ct2020/lib/poems/workspace.h
lammps-stable_290ct2020/lib/pylint.rc
lammps-stable_290ct2020/lib/python/
lammps-stable_290ct2020/lib/python/Makefile.lammps
lammps-stable_290ct2020/lib/python/Makefile.lammps.python2
lammps-stable_290ct2020/lib/python/Makefile.lammps.python2.7
lammps-stable_290ct2020/lib/python/Makefile.lammps.python3
lammps-stable_290ct2020/lib/python/README
lammps-stable_290ct2020/lib/qmmm/
lammps-stable_290ct2020/lib/qmmm/Install.py
lammps-stable_290ct2020/lib/qmmm/Makefile.gfortran
lammps-stable_290ct2020/lib/qmmm/Makefile.gfortran-cmake
lammps-stable_290ct2020/lib/qmmm/Makefile.ifort
lammps-stable_290ct2020/lib/qmmm/Makefile.lammps.empty
lammps-stable_290ct2020/lib/qmmm/Makefile.mpi
lammps-stable_290ct2020/lib/qmmm/Makefile.serial
```

```
lammps-stable_290ct2020/lib/qmmm/README
lammps-stable_290ct2020/lib/qmmm/example-ec/
lammps-stable_290ct2020/lib/qmmm/example-ec/README
lammps-stable_290ct2020/lib/qmmm/example-ec/mm-master/
lammps-stable_290ct2020/lib/qmmm/example-ec/mm-master/data.water
lammps-stable_290ct2020/lib/qmmm/example-ec/mm-master/water.in
lammps-stable_290ct2020/lib/qmmm/example-ec/mm-slave/
lammps-stable_290ct2020/lib/qmmm/example-ec/mm-slave/data.single_water
lammps-stable_290ct2020/lib/qmmm/example-ec/mm-slave/water_single.in
lammps-stable_290ct2020/lib/qmmm/example-ec/qm-pw/
lammps-stable_290ct2020/lib/qmmm/example-ec/qm-pw/pseudo/
lammps-stable_290ct2020/lib/qmmm/example-ec/qm-pw/pseudo/H.blyp-vbc.UPF
lammps-stable_290ct2020/lib/qmmm/example-ec/qm-pw/pseudo/H.pbe-van_ak.UPF
lammps-stable_290ct2020/lib/qmmm/example-ec/qm-pw/pseudo/O.blyp-mt.UPF
lammps-stable_290ct2020/lib/qmmm/example-ec/qm-pw/pseudo/O.pbe-van_bm.UPF
lammps-stable_290ct2020/lib/qmmm/example-ec/qm-pw/water.in
lammps-stable_290ct2020/lib/qmmm/example-ec/qmmm.inp
lammps-stable_290ct2020/lib/qmmm/example-mc/
lammps-stable_290ct2020/lib/qmmm/example-mc/README
lammps-stable_290ct2020/lib/qmmm/example-mc/mm-master/
lammps-stable_290ct2020/lib/qmmm/example-mc/mm-master/data.water
lammps-stable_290ct2020/lib/qmmm/example-mc/mm-master/water.in
lammps-stable_290ct2020/lib/qmmm/example-mc/mm-slave/
lammps-stable_290ct2020/lib/qmmm/example-mc/mm-slave/data.single_water
lammps-stable_290ct2020/lib/qmmm/example-mc/mm-slave/water_single.in
lammps-stable_290ct2020/lib/qmmm/example-mc/qm-pw/
lammps-stable_290ct2020/lib/qmmm/example-mc/qm-pw/pseudo/
lammps-stable_290ct2020/lib/qmmm/example-mc/qm-pw/pseudo/H.pbe-van_ak.UPF
lammps-stable_290ct2020/lib/qmmm/example-mc/qm-pw/pseudo/O.pbe-van_bm.UPF
lammps-stable_290ct2020/lib/qmmm/example-mc/qm-pw/water.in
lammps-stable_290ct2020/lib/qmmm/example-mc/qmmm.inp
lammps-stable_290ct2020/lib/qmmm/libqmmm.c
lammps-stable_290ct2020/lib/qmmm/libqmmm.h
lammps-stable_290ct2020/lib/qmmm/pwqmmm.c
lammps-stable_290ct2020/lib/quip/
lammps-stable_290ct2020/lib/quip/Makefile.lammps
lammps-stable_290ct2020/lib/quip/README
lammps-stable_290ct2020/lib/scafacos/
lammps-stable_290ct2020/lib/scafacos/Install.py
lammps-stable_290ct2020/lib/scafacos/README
lammps-stable_290ct2020/lib/smd/
lammps-stable_290ct2020/lib/smd/Install.py
lammps-stable_290ct2020/lib/smd/Makefile.lammps
lammps-stable_290ct2020/lib/smd/README
lammps-stable_290ct2020/lib/voronoi/
lammps-stable_290ct2020/lib/voronoi/Install.py
lammps-stable_290ct2020/lib/voronoi/Makefile.lammps
lammps-stable_290ct2020/lib/voronoi/README
lammps-stable_290ct2020/lib/voronoi/voro-make.patch
lammps-stable_290ct2020/lib/vtk/
lammps-stable_290ct2020/lib/vtk/Makefile.lammps
lammps-stable_290ct2020/lib/vtk/Makefile.lammps.arch_vtk6
lammps-stable_290ct2020/lib/vtk/Makefile.lammps.centos6_vtk5
lammps-stable_290ct2020/lib/vtk/Makefile.lammps.centos7_vtk6
lammps-stable_290ct2020/lib/vtk/Makefile.lammps.fedora28_vtk7
lammps-stable_290ct2020/lib/vtk/Makefile.lammps.ubuntu14.04_vtk5
lammps-stable_290ct2020/lib/vtk/Makefile.lammps.ubuntu14.04_vtk6
lammps-stable_290ct2020/lib/vtk/Makefile.lammps.ubuntu18.04_vtk7
lammps-stable_290ct2020/lib/vtk/README
lammps-stable_290ct2020/potentials/
```

lammps-stable\_290ct2020/potentials/Ag\_u3.eam  
lammps-stable\_290ct2020/potentials/AlCu.adp  
lammps-stable\_290ct2020/potentials/AlCu.bop.table  
lammps-stable\_290ct2020/potentials/AlCu.eam.alloy  
lammps-stable\_290ct2020/potentials/AlCuH.bop.table  
lammps-stable\_290ct2020/potentials/AlFe\_mm.eam.fs  
lammps-stable\_290ct2020/potentials/AlO.eam.alloy  
lammps-stable\_290ct2020/potentials/AlO.streitz  
lammps-stable\_290ct2020/potentials/AlSiMgCuFe.meam  
lammps-stable\_290ct2020/potentials/Al\_jnp.eam  
lammps-stable\_290ct2020/potentials/Al\_jpc.agni  
lammps-stable\_290ct2020/potentials/Al\_mm.eam.fs  
lammps-stable\_290ct2020/potentials/Al\_prb.agni  
lammps-stable\_290ct2020/potentials/Al\_zhou.eam.alloy  
lammps-stable\_290ct2020/potentials/Au\_u3.eam  
lammps-stable\_290ct2020/potentials/BN.extep  
lammps-stable\_290ct2020/potentials/BNC.tersoff  
lammps-stable\_290ct2020/potentials/BNCH-old.ILP  
lammps-stable\_290ct2020/potentials/BNCH.ILP  
lammps-stable\_290ct2020/potentials/BNC\_MBD\_bulk.ILP  
lammps-stable\_290ct2020/potentials/BNC\_TS\_bulk.ILP  
lammps-stable\_290ct2020/potentials/C.drip  
lammps-stable\_290ct2020/potentials/C.lcbop  
lammps-stable\_290ct2020/potentials/CC.KC  
lammps-stable\_290ct2020/potentials/CC.KC-full  
lammps-stable\_290ct2020/potentials/CC.Lebedeva  
lammps-stable\_290ct2020/potentials/CCu\_v2.bop.table  
lammps-stable\_290ct2020/potentials/CH.KC  
lammps-stable\_290ct2020/potentials/CH.airebo  
lammps-stable\_290ct2020/potentials/CH.airebo-m  
lammps-stable\_290ct2020/potentials/CH.rebo  
lammps-stable\_290ct2020/potentials/CH\_taper.KC  
lammps-stable\_290ct2020/potentials/CdTe.bop.table  
lammps-stable\_290ct2020/potentials/CdTe.sw  
lammps-stable\_290ct2020/potentials/CdTeSe.bop.table  
lammps-stable\_290ct2020/potentials/CdTeZnSeHgS0.sw  
lammps-stable\_290ct2020/potentials/CdZnTe\_v1.bop.table  
lammps-stable\_290ct2020/potentials/CdZnTe\_v2.bop.table  
lammps-stable\_290ct2020/potentials/CoAl.eam.alloy  
lammps-stable\_290ct2020/potentials/Cu.meam  
lammps-stable\_290ct2020/potentials/CuH.bop.table  
lammps-stable\_290ct2020/potentials/CuNi.eam.alloy  
lammps-stable\_290ct2020/potentials/CuTa.eam.alloy  
lammps-stable\_290ct2020/potentials/CuTa\_eam.poly  
lammps-stable\_290ct2020/potentials/CuZr\_mm.eam.fs  
lammps-stable\_290ct2020/potentials/Cu\_Zuo\_JPCA2020.quadratic.snap  
lammps-stable\_290ct2020/potentials/Cu\_Zuo\_JPCA2020.quadratic.snapcoeff  
lammps-stable\_290ct2020/potentials/Cu\_Zuo\_JPCA2020.quadratic.snapparam  
lammps-stable\_290ct2020/potentials/Cu\_Zuo\_JPCA2020.snap  
lammps-stable\_290ct2020/potentials/Cu\_Zuo\_JPCA2020.snapcoeff  
lammps-stable\_290ct2020/potentials/Cu\_Zuo\_JPCA2020.snapparam  
lammps-stable\_290ct2020/potentials/Cu\_mishin1.eam.alloy  
lammps-stable\_290ct2020/potentials/Cu\_smf7.eam  
lammps-stable\_290ct2020/potentials/Cu\_u3.eam  
lammps-stable\_290ct2020/potentials/Cu\_u6.eam  
lammps-stable\_290ct2020/potentials/Cu\_zhou.eam.alloy  
lammps-stable\_290ct2020/potentials/FeCH\_BOP\_I.poly  
lammps-stable\_290ct2020/potentials/FeCH\_BOP\_II.poly  
lammps-stable\_290ct2020/potentials/FeCr.cdeam  
lammps-stable\_290ct2020/potentials/FeP\_mm.eam.fs



lammps-stable\_290ct2020/potentials/Fe\_mm.eam.fs  
lammps-stable\_290ct2020/potentials/GaAs.bop.table  
lammps-stable\_290ct2020/potentials/GaN.sw  
lammps-stable\_290ct2020/potentials/GaN.tersoff  
lammps-stable\_290ct2020/potentials/GaN\_sw.poly  
lammps-stable\_290ct2020/potentials/GaN\_tersoff.poly  
lammps-stable\_290ct2020/potentials/Ge.tersoff  
lammps-stable\_290ct2020/potentials/Ge\_Zuo\_JPCA2020.quadratic.snap  
lammps-stable\_290ct2020/potentials/Ge\_Zuo\_JPCA2020.quadratic.snapcoeff  
lammps-stable\_290ct2020/potentials/Ge\_Zuo\_JPCA2020.quadratic.snapparam  
lammps-stable\_290ct2020/potentials/Ge\_Zuo\_JPCA2020.snap  
lammps-stable\_290ct2020/potentials/Ge\_Zuo\_JPCA2020.snapcoeff  
lammps-stable\_290ct2020/potentials/Ge\_Zuo\_JPCA2020.snapparam  
lammps-stable\_290ct2020/potentials/He\_He\_JW2013.table  
lammps-stable\_290ct2020/potentials/InP.vashishta  
lammps-stable\_290ct2020/potentials/InP\_JCPA2020.mliap  
lammps-stable\_290ct2020/potentials/InP\_JCPA2020.mliap.descriptor  
lammps-stable\_290ct2020/potentials/InP\_JCPA2020.mliap.model  
lammps-stable\_290ct2020/potentials/InP\_JCPA2020.snap  
lammps-stable\_290ct2020/potentials/InP\_JCPA2020.snapcoeff  
lammps-stable\_290ct2020/potentials/InP\_JCPA2020.snapparam  
lammps-stable\_290ct2020/potentials/Li\_Zuo\_JPCA2020.quadratic.snap  
lammps-stable\_290ct2020/potentials/Li\_Zuo\_JPCA2020.quadratic.snapcoeff  
lammps-stable\_290ct2020/potentials/Li\_Zuo\_JPCA2020.quadratic.snapparam  
lammps-stable\_290ct2020/potentials/Li\_Zuo\_JPCA2020.snap  
lammps-stable\_290ct2020/potentials/Li\_Zuo\_JPCA2020.snapcoeff  
lammps-stable\_290ct2020/potentials/Li\_Zuo\_JPCA2020.snapparam  
lammps-stable\_290ct2020/potentials/MOH.nb3b.harmonic  
lammps-stable\_290ct2020/potentials/Mg\_mm.eam.fs  
lammps-stable\_290ct2020/potentials/Mo5.2.mgpt.README  
lammps-stable\_290ct2020/potentials/Mo5.2.mgpt.parmin  
lammps-stable\_290ct2020/potentials/Mo5.2.mgpt.potin  
lammps-stable\_290ct2020/potentials/Mo\_Chen\_PRM2017.snap  
lammps-stable\_290ct2020/potentials/Mo\_Chen\_PRM2017.snapcoeff  
lammps-stable\_290ct2020/potentials/Mo\_Chen\_PRM2017.snapparam  
lammps-stable\_290ct2020/potentials/Mo\_Zuo\_JPCA2020.quadratic.snap  
lammps-stable\_290ct2020/potentials/Mo\_Zuo\_JPCA2020.quadratic.snapcoeff  
lammps-stable\_290ct2020/potentials/Mo\_Zuo\_JPCA2020.quadratic.snapparam  
lammps-stable\_290ct2020/potentials/Mo\_Zuo\_JPCA2020.snap  
lammps-stable\_290ct2020/potentials/Mo\_Zuo\_JPCA2020.snapcoeff  
lammps-stable\_290ct2020/potentials/Mo\_Zuo\_JPCA2020.snapparam  
lammps-stable\_290ct2020/potentials/Ni.adp  
lammps-stable\_290ct2020/potentials/Ni.meam  
lammps-stable\_290ct2020/potentials/NiAlH\_jea.eam.alloy  
lammps-stable\_290ct2020/potentials/NiAlH\_jea.eam.fs  
lammps-stable\_290ct2020/potentials/Ni\_Zuo\_JPCA2020.quadratic.snap  
lammps-stable\_290ct2020/potentials/Ni\_Zuo\_JPCA2020.quadratic.snapcoeff  
lammps-stable\_290ct2020/potentials/Ni\_Zuo\_JPCA2020.quadratic.snapparam  
lammps-stable\_290ct2020/potentials/Ni\_Zuo\_JPCA2020.snap  
lammps-stable\_290ct2020/potentials/Ni\_Zuo\_JPCA2020.snapcoeff  
lammps-stable\_290ct2020/potentials/Ni\_Zuo\_JPCA2020.snapparam  
lammps-stable\_290ct2020/potentials/Ni\_smf7.eam  
lammps-stable\_290ct2020/potentials/Ni\_u3.eam  
lammps-stable\_290ct2020/potentials/Pd\_u3.eam  
lammps-stable\_290ct2020/potentials/Pt\_u3.eam  
lammps-stable\_290ct2020/potentials/README  
lammps-stable\_290ct2020/potentials/README.reax  
lammps-stable\_290ct2020/potentials/Si.b.meam.sw.spline  
lammps-stable\_290ct2020/potentials/Si.edip  
lammps-stable\_290ct2020/potentials/Si.sw

lammps-stable\_290ct2020/potentials/Si.tersoff  
lammps-stable\_290ct2020/potentials/Si.tersoff.mod  
lammps-stable\_290ct2020/potentials/Si.tersoff.modc  
lammps-stable\_290ct2020/potentials/SiC.edip  
lammps-stable\_290ct2020/potentials/SiC.gw  
lammps-stable\_290ct2020/potentials/SiC.gw.zbl  
lammps-stable\_290ct2020/potentials/SiC.meam  
lammps-stable\_290ct2020/potentials/SiC.tersoff  
lammps-stable\_290ct2020/potentials/SiC.tersoff.zbl  
lammps-stable\_290ct2020/potentials/SiC.vashishta  
lammps-stable\_290ct2020/potentials/SiCGe.tersoff  
lammps-stable\_290ct2020/potentials/SiC\_1989.tersoff  
lammps-stable\_290ct2020/potentials/SiC\_1990.tersoff  
lammps-stable\_290ct2020/potentials/SiC\_1994.tersoff  
lammps-stable\_290ct2020/potentials/SiC\_Erhart-Albe.tersoff  
lammps-stable\_290ct2020/potentials/Si0.1990.vashishta  
lammps-stable\_290ct2020/potentials/Si0.1994.vashishta  
lammps-stable\_290ct2020/potentials/Si0.1997.vashishta  
lammps-stable\_290ct2020/potentials/Si0.tersoff  
lammps-stable\_290ct2020/potentials/Si\_1.meam.spline  
lammps-stable\_290ct2020/potentials/Si\_2.meam.spline  
lammps-stable\_290ct2020/potentials/Si\_Zuo\_JPCA2020.quadratic.snap  
lammps-stable\_290ct2020/potentials/Si\_Zuo\_JPCA2020.quadratic.snapcoeff  
lammps-stable\_290ct2020/potentials/Si\_Zuo\_JPCA2020.quadratic.snapparam  
lammps-stable\_290ct2020/potentials/Si\_Zuo\_JPCA2020.snap  
lammps-stable\_290ct2020/potentials/Si\_Zuo\_JPCA2020.snapcoeff  
lammps-stable\_290ct2020/potentials/Si\_Zuo\_JPCA2020.snapparam  
lammps-stable\_290ct2020/potentials/TABTP\_10\_10.mesont  
lammps-stable\_290ct2020/potentials/Ta06A.mliap  
lammps-stable\_290ct2020/potentials/Ta06A.mliap.descriptor  
lammps-stable\_290ct2020/potentials/Ta06A.mliap.model  
lammps-stable\_290ct2020/potentials/Ta06A.snap  
lammps-stable\_290ct2020/potentials/Ta06A.snapcoeff  
lammps-stable\_290ct2020/potentials/Ta06A.snapparam  
lammps-stable\_290ct2020/potentials/Ta4.mgpt.README  
lammps-stable\_290ct2020/potentials/Ta4.mgpt.parmin  
lammps-stable\_290ct2020/potentials/Ta4.mgpt.potin  
lammps-stable\_290ct2020/potentials/Ta6.8x.mgpt.README  
lammps-stable\_290ct2020/potentials/Ta6.8x.mgpt.parmin  
lammps-stable\_290ct2020/potentials/Ta6.8x.mgpt.potin  
lammps-stable\_290ct2020/potentials/Ti.meam.spline  
lammps-stable\_290ct2020/potentials/Ti.meam.sw.spline  
lammps-stable\_290ct2020/potentials/Ti0.meam.spline  
lammps-stable\_290ct2020/potentials/TlBr\_msw.poly  
lammps-stable\_290ct2020/potentials/V6.1.mgpt.README  
lammps-stable\_290ct2020/potentials/V6.1.mgpt.parmin  
lammps-stable\_290ct2020/potentials/V6.1.mgpt.potin  
lammps-stable\_290ct2020/potentials/VFe\_mm.eam.fs  
lammps-stable\_290ct2020/potentials/W.quadratic.mliap  
lammps-stable\_290ct2020/potentials/W.quadratic.mliap.descriptor  
lammps-stable\_290ct2020/potentials/W.quadratic.mliap.model  
lammps-stable\_290ct2020/potentials/WBe\_Wood\_PRB2019.mliap  
lammps-stable\_290ct2020/potentials/WBe\_Wood\_PRB2019.mliap.descriptor  
lammps-stable\_290ct2020/potentials/WBe\_Wood\_PRB2019.mliap.model  
lammps-stable\_290ct2020/potentials/WBe\_Wood\_PRB2019.snap  
lammps-stable\_290ct2020/potentials/WBe\_Wood\_PRB2019.snapcoeff  
lammps-stable\_290ct2020/potentials/WBe\_Wood\_PRB2019.snapparam  
lammps-stable\_290ct2020/potentials/WL.meam  
lammps-stable\_290ct2020/potentials/W\_2940\_2017\_2.snap  
lammps-stable\_290ct2020/potentials/W\_2940\_2017\_2.snapcoeff

lammps-stable\_290ct2020/potentials/W\_2940\_2017\_2.snapparam  
lammps-stable\_290ct2020/potentials/W\_2940\_2017\_2\_He\_JW2013.snap  
lammps-stable\_290ct2020/potentials/W\_He\_JW2013.table  
lammps-stable\_290ct2020/potentials/W\_zhou.eam.alloy  
lammps-stable\_290ct2020/potentials/Zr\_mm.eam.fs  
lammps-stable\_290ct2020/potentials/charmm22.cmap  
lammps-stable\_290ct2020/potentials/charmm36.cmap  
lammps-stable\_290ct2020/potentials/ci-reaxFF\_ZBL.dat  
lammps-stable\_290ct2020/potentials/ffield.ci-reax.CH  
lammps-stable\_290ct2020/potentials/ffield.comb  
lammps-stable\_290ct2020/potentials/ffield.comb3  
lammps-stable\_290ct2020/potentials/ffield.eim  
lammps-stable\_290ct2020/potentials/ffield.reax.AB  
lammps-stable\_290ct2020/potentials/ffield.reax.Au0  
lammps-stable\_290ct2020/potentials/ffield.reax.FC  
lammps-stable\_290ct2020/potentials/ffield.reax.Fe\_0\_C\_H  
lammps-stable\_290ct2020/potentials/ffield.reax.V\_0\_C\_H  
lammps-stable\_290ct2020/potentials/ffield.reax.ZnOH  
lammps-stable\_290ct2020/potentials/ffield.reax.budzien  
lammps-stable\_290ct2020/potentials/ffield.reax.cho  
lammps-stable\_290ct2020/potentials/ffield.reax.lg  
lammps-stable\_290ct2020/potentials/ffield.reax.mattsson  
lammps-stable\_290ct2020/potentials/ffield.reax.rdx  
lammps-stable\_290ct2020/potentials/ffield.smtbq.Al  
lammps-stable\_290ct2020/potentials/ffield.smtbq.Al2O3  
lammps-stable\_290ct2020/potentials/ffield.smtbq.TiO2  
lammps-stable\_290ct2020/potentials/lib.comb3  
lammps-stable\_290ct2020/potentials/library.meam  
lammps-stable\_290ct2020/python/  
lammps-stable\_290ct2020/python/README  
lammps-stable\_290ct2020/python/examples/  
lammps-stable\_290ct2020/python/examples/demo.py  
lammps-stable\_290ct2020/python/examples/gui.py  
lammps-stable\_290ct2020/python/examples/in.demo  
lammps-stable\_290ct2020/python/examples/in.gui  
lammps-stable\_290ct2020/python/examples/in.mc  
lammps-stable\_290ct2020/python/examples/in.plot  
lammps-stable\_290ct2020/python/examples/in.simple  
lammps-stable\_290ct2020/python/examples/in.trivial  
lammps-stable\_290ct2020/python/examples/in.viz  
lammps-stable\_290ct2020/python/examples/matplotlib\_plot.py  
lammps-stable\_290ct2020/python/examples/mc.py  
lammps-stable\_290ct2020/python/examples/pizza/  
lammps-stable\_290ct2020/python/examples/pizza/dump.py  
lammps-stable\_290ct2020/python/examples/pizza/gl.py  
lammps-stable\_290ct2020/python/examples/pizza/gnu.py  
lammps-stable\_290ct2020/python/examples/pizza/pdbfile.py  
lammps-stable\_290ct2020/python/examples/pizza/vizinfo.py  
lammps-stable\_290ct2020/python/examples/pizza/vmd.py  
lammps-stable\_290ct2020/python/examples/plot.py  
lammps-stable\_290ct2020/python/examples/pylammps/  
lammps-stable\_290ct2020/python/examples/pylammps/README  
lammps-stable\_290ct2020/python/examples/pylammps/dihedrals/  
lammps-stable\_290ct2020/python/examples/pylammps/dihedrals/data.dihedral  
lammps-stable\_290ct2020/python/examples/pylammps/dihedrals/dihedral.ipynb  
lammps-stable\_290ct2020/python/examples/pylammps/interface\_usage.ipynb  
lammps-stable\_290ct2020/python/examples/pylammps/interface\_usage\_bonds.ipynb  
lammps-stable\_290ct2020/python/examples/pylammps/montecarlo/  
lammps-stable\_290ct2020/python/examples/pylammps/montecarlo/mc.ipynb  
lammps-stable\_290ct2020/python/examples/pylammps/mpi4py/

```
lammps-stable_290ct2020/python/examples/pylammps/mpi4py/hello.py
lammps-stable_290ct2020/python/examples/pylammps/mpi4py/in.melt
lammps-stable_290ct2020/python/examples/pylammps/mpi4py/melt.py
lammps-stable_290ct2020/python/examples/pylammps/simple.ipynb
lammps-stable_290ct2020/python/examples/simple.py
lammps-stable_290ct2020/python/examples/split.py
lammps-stable_290ct2020/python/examples/trivial.py
lammps-stable_290ct2020/python/examples/viz_atomeye.py
lammps-stable_290ct2020/python/examples/viz_gl.py
lammps-stable_290ct2020/python/examples/viz_pymol.py
lammps-stable_290ct2020/python/examples/viz_vmd.py
lammps-stable_290ct2020/python/examples/vizplotgui_atomeye.py
lammps-stable_290ct2020/python/examples/vizplotgui_gl.py
lammps-stable_290ct2020/python/examples/vizplotgui_pymol.py
lammps-stable_290ct2020/python/examples/vizplotgui_vmd.py
lammps-stable_290ct2020/python/install.py
lammps-stable_290ct2020/python/lammps.py
lammps-stable_290ct2020/src/
lammps-stable_290ct2020/src/ASPHERE/
lammps-stable_290ct2020/src/ASPHERE/compute_erotate_asphere.cpp
lammps-stable_290ct2020/src/ASPHERE/compute_erotate_asphere.h
lammps-stable_290ct2020/src/ASPHERE/compute_temp_asphere.cpp
lammps-stable_290ct2020/src/ASPHERE/compute_temp_asphere.h
lammps-stable_290ct2020/src/ASPHERE/fix_nh_asphere.cpp
lammps-stable_290ct2020/src/ASPHERE/fix_nh_asphere.h
lammps-stable_290ct2020/src/ASPHERE/fix_nph_asphere.cpp
lammps-stable_290ct2020/src/ASPHERE/fix_nph_asphere.h
lammps-stable_290ct2020/src/ASPHERE/fix_npt_asphere.cpp
lammps-stable_290ct2020/src/ASPHERE/fix_npt_asphere.h
lammps-stable_290ct2020/src/ASPHERE/fix_nve_asphere.cpp
lammps-stable_290ct2020/src/ASPHERE/fix_nve_asphere.h
lammps-stable_290ct2020/src/ASPHERE/fix_nve_asphere_noforce.cpp
lammps-stable_290ct2020/src/ASPHERE/fix_nve_asphere_noforce.h
lammps-stable_290ct2020/src/ASPHERE/fix_nve_line.cpp
lammps-stable_290ct2020/src/ASPHERE/fix_nve_line.h
lammps-stable_290ct2020/src/ASPHERE/fix_nve_tri.cpp
lammps-stable_290ct2020/src/ASPHERE/fix_nve_tri.h
lammps-stable_290ct2020/src/ASPHERE/fix_nvt_asphere.cpp
lammps-stable_290ct2020/src/ASPHERE/fix_nvt_asphere.h
lammps-stable_290ct2020/src/ASPHERE/pair_gayberne.cpp
lammps-stable_290ct2020/src/ASPHERE/pair_gayberne.h
lammps-stable_290ct2020/src/ASPHERE/pair_line_lj.cpp
lammps-stable_290ct2020/src/ASPHERE/pair_line_lj.h
lammps-stable_290ct2020/src/ASPHERE/pair_resquared.cpp
lammps-stable_290ct2020/src/ASPHERE/pair_resquared.h
lammps-stable_290ct2020/src/ASPHERE/pair_tri_lj.cpp
lammps-stable_290ct2020/src/ASPHERE/pair_tri_lj.h
lammps-stable_290ct2020/src/BODY/
lammps-stable_290ct2020/src/BODY/body_nparticle.cpp
lammps-stable_290ct2020/src/BODY/body_nparticle.h
lammps-stable_290ct2020/src/BODY/body_rounded_polygon.cpp
lammps-stable_290ct2020/src/BODY/body_rounded_polygon.h
lammps-stable_290ct2020/src/BODY/body_rounded_polyhedron.cpp
lammps-stable_290ct2020/src/BODY/body_rounded_polyhedron.h
lammps-stable_290ct2020/src/BODY/compute_body_local.cpp
lammps-stable_290ct2020/src/BODY/compute_body_local.h
lammps-stable_290ct2020/src/BODY/compute_temp_body.cpp
lammps-stable_290ct2020/src/BODY/compute_temp_body.h
lammps-stable_290ct2020/src/BODY/fix_nh_body.cpp
lammps-stable_290ct2020/src/BODY/fix_nh_body.h
```

```
lammps-stable_290ct2020/src/BODY/fix_nph_body.cpp
lammps-stable_290ct2020/src/BODY/fix_nph_body.h
lammps-stable_290ct2020/src/BODY/fix_npt_body.cpp
lammps-stable_290ct2020/src/BODY/fix_npt_body.h
lammps-stable_290ct2020/src/BODY/fix_nve_body.cpp
lammps-stable_290ct2020/src/BODY/fix_nve_body.h
lammps-stable_290ct2020/src/BODY/fix_nvt_body.cpp
lammps-stable_290ct2020/src/BODY/fix_nvt_body.h
lammps-stable_290ct2020/src/BODY/fix_wall_body_polygon.cpp
lammps-stable_290ct2020/src/BODY/fix_wall_body_polygon.h
lammps-stable_290ct2020/src/BODY/fix_wall_body_polyhedron.cpp
lammps-stable_290ct2020/src/BODY/fix_wall_body_polyhedron.h
lammps-stable_290ct2020/src/BODY/pair_body_nparticle.cpp
lammps-stable_290ct2020/src/BODY/pair_body_nparticle.h
lammps-stable_290ct2020/src/BODY/pair_body_rounded_polygon.cpp
lammps-stable_290ct2020/src/BODY/pair_body_rounded_polygon.h
lammps-stable_290ct2020/src/BODY/pair_body_rounded_polyhedron.cpp
lammps-stable_290ct2020/src/BODY/pair_body_rounded_polyhedron.h
lammps-stable_290ct2020/src/CLASS2/
lammps-stable_290ct2020/src/CLASS2/angle_class2.cpp
lammps-stable_290ct2020/src/CLASS2/angle_class2.h
lammps-stable_290ct2020/src/CLASS2/bond_class2.cpp
lammps-stable_290ct2020/src/CLASS2/bond_class2.h
lammps-stable_290ct2020/src/CLASS2/dihedral_class2.cpp
lammps-stable_290ct2020/src/CLASS2/dihedral_class2.h
lammps-stable_290ct2020/src/CLASS2/improper_class2.cpp
lammps-stable_290ct2020/src/CLASS2/improper_class2.h
lammps-stable_290ct2020/src/CLASS2/pair_lj_class2.cpp
lammps-stable_290ct2020/src/CLASS2/pair_lj_class2.h
lammps-stable_290ct2020/src/CLASS2/pair_lj_class2_coul_cut.cpp
lammps-stable_290ct2020/src/CLASS2/pair_lj_class2_coul_cut.h
lammps-stable_290ct2020/src/CLASS2/pair_lj_class2_coul_long.cpp
lammps-stable_290ct2020/src/CLASS2/pair_lj_class2_coul_long.h
lammps-stable_290ct2020/src/COLL0ID/
lammps-stable_290ct2020/src/COLL0ID/fix_wall_colloid.cpp
lammps-stable_290ct2020/src/COLL0ID/fix_wall_colloid.h
lammps-stable_290ct2020/src/COLL0ID/pair_brownian.cpp
lammps-stable_290ct2020/src/COLL0ID/pair_brownian.h
lammps-stable_290ct2020/src/COLL0ID/pair_brownian_poly.cpp
lammps-stable_290ct2020/src/COLL0ID/pair_brownian_poly.h
lammps-stable_290ct2020/src/COLL0ID/pair_colloid.cpp
lammps-stable_290ct2020/src/COLL0ID/pair_colloid.h
lammps-stable_290ct2020/src/COLL0ID/pair_lubricate.cpp
lammps-stable_290ct2020/src/COLL0ID/pair_lubricate.h
lammps-stable_290ct2020/src/COLL0ID/pair_lubricateU.cpp
lammps-stable_290ct2020/src/COLL0ID/pair_lubricateU.h
lammps-stable_290ct2020/src/COLL0ID/pair_lubricateU_poly.cpp
lammps-stable_290ct2020/src/COLL0ID/pair_lubricateU_poly.h
lammps-stable_290ct2020/src/COLL0ID/pair_lubricate_poly.cpp
lammps-stable_290ct2020/src/COLL0ID/pair_lubricate_poly.h
lammps-stable_290ct2020/src/COLL0ID/pair_yukawa_colloid.cpp
lammps-stable_290ct2020/src/COLL0ID/pair_yukawa_colloid.h
lammps-stable_290ct2020/src/COMPRESS/
lammps-stable_290ct2020/src/COMPRESS/Install.sh
lammps-stable_290ct2020/src/COMPRESS/README
lammps-stable_290ct2020/src/COMPRESS/dump_atom_gz.cpp
lammps-stable_290ct2020/src/COMPRESS/dump_atom_gz.h
lammps-stable_290ct2020/src/COMPRESS/dump_atom_zstd.cpp
lammps-stable_290ct2020/src/COMPRESS/dump_atom_zstd.h
lammps-stable_290ct2020/src/COMPRESS/dump_cfg_gz.cpp
```

```
lammps-stable_290ct2020/src/COMPRESS/dump_cfg_gz.h
lammps-stable_290ct2020/src/COMPRESS/dump_cfg_zstd.cpp
lammps-stable_290ct2020/src/COMPRESS/dump_cfg_zstd.h
lammps-stable_290ct2020/src/COMPRESS/dump_custom_gz.cpp
lammps-stable_290ct2020/src/COMPRESS/dump_custom_gz.h
lammps-stable_290ct2020/src/COMPRESS/dump_custom_zstd.cpp
lammps-stable_290ct2020/src/COMPRESS/dump_custom_zstd.h
lammps-stable_290ct2020/src/COMPRESS/dump_local_gz.cpp
lammps-stable_290ct2020/src/COMPRESS/dump_local_gz.h
lammps-stable_290ct2020/src/COMPRESS/dump_local_zstd.cpp
lammps-stable_290ct2020/src/COMPRESS/dump_local_zstd.h
lammps-stable_290ct2020/src/COMPRESS/dump_xyz_gz.cpp
lammps-stable_290ct2020/src/COMPRESS/dump_xyz_gz.h
lammps-stable_290ct2020/src/COMPRESS/dump_xyz_zstd.cpp
lammps-stable_290ct2020/src/COMPRESS/dump_xyz_zstd.h
lammps-stable_290ct2020/src/COMPRESS/zstd_file_writer.cpp
lammps-stable_290ct2020/src/COMPRESS/zstd_file_writer.h
lammps-stable_290ct2020/src/CORESHELL/
lammps-stable_290ct2020/src/CORESHELL/Install.sh
lammps-stable_290ct2020/src/CORESHELL/compute_temp_cs.cpp
lammps-stable_290ct2020/src/CORESHELL/compute_temp_cs.h
lammps-stable_290ct2020/src/CORESHELL/pair_born_coul_dsf_cs.cpp
lammps-stable_290ct2020/src/CORESHELL/pair_born_coul_dsf_cs.h
lammps-stable_290ct2020/src/CORESHELL/pair_born_coul_long_cs.cpp
lammps-stable_290ct2020/src/CORESHELL/pair_born_coul_long_cs.h
lammps-stable_290ct2020/src/CORESHELL/pair_born_coul_wolf_cs.cpp
lammps-stable_290ct2020/src/CORESHELL/pair_born_coul_wolf_cs.h
lammps-stable_290ct2020/src/CORESHELL/pair_buck_coul_long_cs.cpp
lammps-stable_290ct2020/src/CORESHELL/pair_buck_coul_long_cs.h
lammps-stable_290ct2020/src/CORESHELL/pair_coul_long_cs.cpp
lammps-stable_290ct2020/src/CORESHELL/pair_coul_long_cs.h
lammps-stable_290ct2020/src/CORESHELL/pair_coul_wolf_cs.cpp
lammps-stable_290ct2020/src/CORESHELL/pair_coul_wolf_cs.h
lammps-stable_290ct2020/src/CORESHELL/pair_lj_class2_coul_long_cs.cpp
lammps-stable_290ct2020/src/CORESHELL/pair_lj_class2_coul_long_cs.h
lammps-stable_290ct2020/src/CORESHELL/pair_lj_cut_coul_long_cs.cpp
lammps-stable_290ct2020/src/CORESHELL/pair_lj_cut_coul_long_cs.h
lammps-stable_290ct2020/src/DEPEND/
lammps-stable_290ct2020/src/DEPEND/fastdep.c
lammps-stable_290ct2020/src/DIPOLE/
lammps-stable_290ct2020/src/DIPOLE/atom_vec_dipole.cpp
lammps-stable_290ct2020/src/DIPOLE/atom_vec_dipole.h
lammps-stable_290ct2020/src/DIPOLE/pair_lj_cut_dipole_cut.cpp
lammps-stable_290ct2020/src/DIPOLE/pair_lj_cut_dipole_cut.h
lammps-stable_290ct2020/src/DIPOLE/pair_lj_cut_dipole_long.cpp
lammps-stable_290ct2020/src/DIPOLE/pair_lj_cut_dipole_long.h
lammps-stable_290ct2020/src/DIPOLE/pair_lj_long_dipole_long.cpp
lammps-stable_290ct2020/src/DIPOLE/pair_lj_long_dipole_long.h
lammps-stable_290ct2020/src/Depend.sh
lammps-stable_290ct2020/src/Fetch.sh
lammps-stable_290ct2020/src/GPU/
lammps-stable_290ct2020/src/GPU/Install.sh
lammps-stable_290ct2020/src/GPU/README
lammps-stable_290ct2020/src/GPU/fix_gpu.cpp
lammps-stable_290ct2020/src/GPU/fix_gpu.h
lammps-stable_290ct2020/src/GPU/gpu_extra.h
lammps-stable_290ct2020/src/GPU/pair_beck_gpu.cpp
lammps-stable_290ct2020/src/GPU/pair_beck_gpu.h
lammps-stable_290ct2020/src/GPU/pair_born_coul_long_cs_gpu.cpp
lammps-stable_290ct2020/src/GPU/pair_born_coul_long_cs_gpu.h
```

lammps-stable\_290ct2020/src/GPU/pair\_born\_coul\_long\_gpu.cpp  
lammps-stable\_290ct2020/src/GPU/pair\_born\_coul\_long\_gpu.h  
lammps-stable\_290ct2020/src/GPU/pair\_born\_coul\_wolf\_cs\_gpu.cpp  
lammps-stable\_290ct2020/src/GPU/pair\_born\_coul\_wolf\_cs\_gpu.h  
lammps-stable\_290ct2020/src/GPU/pair\_born\_coul\_wolf\_gpu.cpp  
lammps-stable\_290ct2020/src/GPU/pair\_born\_coul\_wolf\_gpu.h  
lammps-stable\_290ct2020/src/GPU/pair\_born\_gpu.cpp  
lammps-stable\_290ct2020/src/GPU/pair\_born\_gpu.h  
lammps-stable\_290ct2020/src/GPU/pair\_buck\_coul\_cut\_gpu.cpp  
lammps-stable\_290ct2020/src/GPU/pair\_buck\_coul\_cut\_gpu.h  
lammps-stable\_290ct2020/src/GPU/pair\_buck\_coul\_long\_gpu.cpp  
lammps-stable\_290ct2020/src/GPU/pair\_buck\_coul\_long\_gpu.h  
lammps-stable\_290ct2020/src/GPU/pair\_buck\_gpu.cpp  
lammps-stable\_290ct2020/src/GPU/pair\_buck\_gpu.h  
lammps-stable\_290ct2020/src/GPU/pair\_colloid\_gpu.cpp  
lammps-stable\_290ct2020/src/GPU/pair\_colloid\_gpu.h  
lammps-stable\_290ct2020/src/GPU/pair\_coul\_cut\_gpu.cpp  
lammps-stable\_290ct2020/src/GPU/pair\_coul\_cut\_gpu.h  
lammps-stable\_290ct2020/src/GPU/pair\_coul\_debye\_gpu.cpp  
lammps-stable\_290ct2020/src/GPU/pair\_coul\_debye\_gpu.h  
lammps-stable\_290ct2020/src/GPU/pair\_coul\_dsf\_gpu.cpp  
lammps-stable\_290ct2020/src/GPU/pair\_coul\_dsf\_gpu.h  
lammps-stable\_290ct2020/src/GPU/pair\_coul\_long\_cs\_gpu.cpp  
lammps-stable\_290ct2020/src/GPU/pair\_coul\_long\_cs\_gpu.h  
lammps-stable\_290ct2020/src/GPU/pair\_coul\_long\_gpu.cpp  
lammps-stable\_290ct2020/src/GPU/pair\_coul\_long\_gpu.h  
lammps-stable\_290ct2020/src/GPU/pair\_dpd\_gpu.cpp  
lammps-stable\_290ct2020/src/GPU/pair\_dpd\_gpu.h  
lammps-stable\_290ct2020/src/GPU/pair\_dpd\_tstat\_gpu.cpp  
lammps-stable\_290ct2020/src/GPU/pair\_dpd\_tstat\_gpu.h  
lammps-stable\_290ct2020/src/GPU/pair\_eam\_alloy\_gpu.cpp  
lammps-stable\_290ct2020/src/GPU/pair\_eam\_alloy\_gpu.h  
lammps-stable\_290ct2020/src/GPU/pair\_eam\_fs\_gpu.cpp  
lammps-stable\_290ct2020/src/GPU/pair\_eam\_fs\_gpu.h  
lammps-stable\_290ct2020/src/GPU/pair\_eam\_gpu.cpp  
lammps-stable\_290ct2020/src/GPU/pair\_eam\_gpu.h  
lammps-stable\_290ct2020/src/GPU/pair\_gauss\_gpu.cpp  
lammps-stable\_290ct2020/src/GPU/pair\_gauss\_gpu.h  
lammps-stable\_290ct2020/src/GPU/pair\_gayberne\_gpu.cpp  
lammps-stable\_290ct2020/src/GPU/pair\_gayberne\_gpu.h  
lammps-stable\_290ct2020/src/GPU/pair\_lj96\_cut\_gpu.cpp  
lammps-stable\_290ct2020/src/GPU/pair\_lj96\_cut\_gpu.h  
lammps-stable\_290ct2020/src/GPU/pair\_lj\_charmm\_coul\_long\_gpu.cpp  
lammps-stable\_290ct2020/src/GPU/pair\_lj\_charmm\_coul\_long\_gpu.h  
lammps-stable\_290ct2020/src/GPU/pair\_lj\_class2\_coul\_long\_gpu.cpp  
lammps-stable\_290ct2020/src/GPU/pair\_lj\_class2\_coul\_long\_gpu.h  
lammps-stable\_290ct2020/src/GPU/pair\_lj\_class2\_gpu.cpp  
lammps-stable\_290ct2020/src/GPU/pair\_lj\_class2\_gpu.h  
lammps-stable\_290ct2020/src/GPU/pair\_lj\_cubic\_gpu.cpp  
lammps-stable\_290ct2020/src/GPU/pair\_lj\_cubic\_gpu.h  
lammps-stable\_290ct2020/src/GPU/pair\_lj\_cut\_coul\_cut\_gpu.cpp  
lammps-stable\_290ct2020/src/GPU/pair\_lj\_cut\_coul\_cut\_gpu.h  
lammps-stable\_290ct2020/src/GPU/pair\_lj\_cut\_coul\_debye\_gpu.cpp  
lammps-stable\_290ct2020/src/GPU/pair\_lj\_cut\_coul\_debye\_gpu.h  
lammps-stable\_290ct2020/src/GPU/pair\_lj\_cut\_coul\_dsf\_gpu.cpp  
lammps-stable\_290ct2020/src/GPU/pair\_lj\_cut\_coul\_dsf\_gpu.h  
lammps-stable\_290ct2020/src/GPU/pair\_lj\_cut\_coul\_long\_gpu.cpp  
lammps-stable\_290ct2020/src/GPU/pair\_lj\_cut\_coul\_long\_gpu.h  
lammps-stable\_290ct2020/src/GPU/pair\_lj\_cut\_coul\_msm\_gpu.cpp  
lammps-stable\_290ct2020/src/GPU/pair\_lj\_cut\_coul\_msm\_gpu.h

lammps-stable\_290ct2020/src/GPU/pair\_lj\_cut\_dipole\_cut\_gpu.cpp  
lammps-stable\_290ct2020/src/GPU/pair\_lj\_cut\_dipole\_cut\_gpu.h  
lammps-stable\_290ct2020/src/GPU/pair\_lj\_cut\_dipole\_long\_gpu.cpp  
lammps-stable\_290ct2020/src/GPU/pair\_lj\_cut\_dipole\_long\_gpu.h  
lammps-stable\_290ct2020/src/GPU/pair\_lj\_cut\_gpu.cpp  
lammps-stable\_290ct2020/src/GPU/pair\_lj\_cut\_gpu.h  
lammps-stable\_290ct2020/src/GPU/pair\_lj\_cut\_tip4p\_long\_gpu.cpp  
lammps-stable\_290ct2020/src/GPU/pair\_lj\_cut\_tip4p\_long\_gpu.h  
lammps-stable\_290ct2020/src/GPU/pair\_lj\_expand\_coul\_long\_gpu.cpp  
lammps-stable\_290ct2020/src/GPU/pair\_lj\_expand\_coul\_long\_gpu.h  
lammps-stable\_290ct2020/src/GPU/pair\_lj\_expand\_gpu.cpp  
lammps-stable\_290ct2020/src/GPU/pair\_lj\_expand\_gpu.h  
lammps-stable\_290ct2020/src/GPU/pair\_lj\_gromacs\_gpu.cpp  
lammps-stable\_290ct2020/src/GPU/pair\_lj\_gromacs\_gpu.h  
lammps-stable\_290ct2020/src/GPU/pair\_lj\_sdk\_coul\_long\_gpu.cpp  
lammps-stable\_290ct2020/src/GPU/pair\_lj\_sdk\_coul\_long\_gpu.h  
lammps-stable\_290ct2020/src/GPU/pair\_lj\_sdk\_gpu.cpp  
lammps-stable\_290ct2020/src/GPU/pair\_lj\_sdk\_gpu.h  
lammps-stable\_290ct2020/src/GPU/pair\_lj\_sf\_dipole\_sf\_gpu.cpp  
lammps-stable\_290ct2020/src/GPU/pair\_lj\_sf\_dipole\_sf\_gpu.h  
lammps-stable\_290ct2020/src/GPU/pair\_mie\_cut\_gpu.cpp  
lammps-stable\_290ct2020/src/GPU/pair\_mie\_cut\_gpu.h  
lammps-stable\_290ct2020/src/GPU/pair\_morse\_gpu.cpp  
lammps-stable\_290ct2020/src/GPU/pair\_morse\_gpu.h  
lammps-stable\_290ct2020/src/GPU/pair\_resquared\_gpu.cpp  
lammps-stable\_290ct2020/src/GPU/pair\_resquared\_gpu.h  
lammps-stable\_290ct2020/src/GPU/pair\_soft\_gpu.cpp  
lammps-stable\_290ct2020/src/GPU/pair\_soft\_gpu.h  
lammps-stable\_290ct2020/src/GPU/pair\_sw\_gpu.cpp  
lammps-stable\_290ct2020/src/GPU/pair\_sw\_gpu.h  
lammps-stable\_290ct2020/src/GPU/pair\_table\_gpu.cpp  
lammps-stable\_290ct2020/src/GPU/pair\_table\_gpu.h  
lammps-stable\_290ct2020/src/GPU/pair\_tersoff\_gpu.cpp  
lammps-stable\_290ct2020/src/GPU/pair\_tersoff\_gpu.h  
lammps-stable\_290ct2020/src/GPU/pair\_tersoff\_mod\_gpu.cpp  
lammps-stable\_290ct2020/src/GPU/pair\_tersoff\_mod\_gpu.h  
lammps-stable\_290ct2020/src/GPU/pair\_tersoff\_zbl\_gpu.cpp  
lammps-stable\_290ct2020/src/GPU/pair\_tersoff\_zbl\_gpu.h  
lammps-stable\_290ct2020/src/GPU/pair\_uvm\_gpu.cpp  
lammps-stable\_290ct2020/src/GPU/pair\_uvm\_gpu.h  
lammps-stable\_290ct2020/src/GPU/pair\_vashishta\_gpu.cpp  
lammps-stable\_290ct2020/src/GPU/pair\_vashishta\_gpu.h  
lammps-stable\_290ct2020/src/GPU/pair\_yukawa\_colloid\_gpu.cpp  
lammps-stable\_290ct2020/src/GPU/pair\_yukawa\_colloid\_gpu.h  
lammps-stable\_290ct2020/src/GPU/pair\_yukawa\_gpu.cpp  
lammps-stable\_290ct2020/src/GPU/pair\_yukawa\_gpu.h  
lammps-stable\_290ct2020/src/GPU/pair\_zbl\_gpu.cpp  
lammps-stable\_290ct2020/src/GPU/pair\_zbl\_gpu.h  
lammps-stable\_290ct2020/src/GPU/pppm\_gpu.cpp  
lammps-stable\_290ct2020/src/GPU/pppm\_gpu.h  
lammps-stable\_290ct2020/src/GRANULAR/  
lammps-stable\_290ct2020/src/GRANULAR/fix\_freeze.cpp  
lammps-stable\_290ct2020/src/GRANULAR/fix\_freeze.h  
lammps-stable\_290ct2020/src/GRANULAR/fix\_pour.cpp  
lammps-stable\_290ct2020/src/GRANULAR/fix\_pour.h  
lammps-stable\_290ct2020/src/GRANULAR/fix\_wall\_gran.cpp  
lammps-stable\_290ct2020/src/GRANULAR/fix\_wall\_gran.h  
lammps-stable\_290ct2020/src/GRANULAR/fix\_wall\_gran\_region.cpp  
lammps-stable\_290ct2020/src/GRANULAR/fix\_wall\_gran\_region.h  
lammps-stable\_290ct2020/src/GRANULAR/pair\_gran\_hertz\_history.cpp



```
lammps-stable_290ct2020/src/GRANULAR/pair_gran_hertz_history.h
lammps-stable_290ct2020/src/GRANULAR/pair_gran_hooke.cpp
lammps-stable_290ct2020/src/GRANULAR/pair_gran_hooke.h
lammps-stable_290ct2020/src/GRANULAR/pair_gran_hooke_history.cpp
lammps-stable_290ct2020/src/GRANULAR/pair_gran_hooke_history.h
lammps-stable_290ct2020/src/GRANULAR/pair_granular.cpp
lammps-stable_290ct2020/src/GRANULAR/pair_granular.h
lammps-stable_290ct2020/src/Install.sh
lammps-stable_290ct2020/src/KIM/
lammps-stable_290ct2020/src/KIM/Install.sh
lammps-stable_290ct2020/src/KIM/README
lammps-stable_290ct2020/src/KIM/fix_store_kim.cpp
lammps-stable_290ct2020/src/KIM/fix_store_kim.h
lammps-stable_290ct2020/src/KIM/kim_init.cpp
lammps-stable_290ct2020/src/KIM/kim_init.h
lammps-stable_290ct2020/src/KIM/kim_interactions.cpp
lammps-stable_290ct2020/src/KIM/kim_interactions.h
lammps-stable_290ct2020/src/KIM/kim_param.cpp
lammps-stable_290ct2020/src/KIM/kim_param.h
lammps-stable_290ct2020/src/KIM/kim_property.cpp
lammps-stable_290ct2020/src/KIM/kim_property.h
lammps-stable_290ct2020/src/KIM/kim_query.cpp
lammps-stable_290ct2020/src/KIM/kim_query.h
lammps-stable_290ct2020/src/KIM/kim_units.cpp
lammps-stable_290ct2020/src/KIM/kim_units.h
lammps-stable_290ct2020/src/KIM/pair_kim.cpp
lammps-stable_290ct2020/src/KIM/pair_kim.h
lammps-stable_290ct2020/src/KOKKOS/
lammps-stable_290ct2020/src/KOKKOS/Install.sh
lammps-stable_290ct2020/src/KOKKOS/README
lammps-stable_290ct2020/src/KOKKOS/angle_charmm_kokkos.cpp
lammps-stable_290ct2020/src/KOKKOS/angle_charmm_kokkos.h
lammps-stable_290ct2020/src/KOKKOS/angle_class2_kokkos.cpp
lammps-stable_290ct2020/src/KOKKOS/angle_class2_kokkos.h
lammps-stable_290ct2020/src/KOKKOS/angle_cosine_kokkos.cpp
lammps-stable_290ct2020/src/KOKKOS/angle_cosine_kokkos.h
lammps-stable_290ct2020/src/KOKKOS/angle_harmonic_kokkos.cpp
lammps-stable_290ct2020/src/KOKKOS/angle_harmonic_kokkos.h
lammps-stable_290ct2020/src/KOKKOS/atom_kokkos.cpp
lammps-stable_290ct2020/src/KOKKOS/atom_kokkos.h
lammps-stable_290ct2020/src/KOKKOS/atom_vec_angle_kokkos.cpp
lammps-stable_290ct2020/src/KOKKOS/atom_vec_angle_kokkos.h
lammps-stable_290ct2020/src/KOKKOS/atom_vec_atomic_kokkos.cpp
lammps-stable_290ct2020/src/KOKKOS/atom_vec_atomic_kokkos.h
lammps-stable_290ct2020/src/KOKKOS/atom_vec_bond_kokkos.cpp
lammps-stable_290ct2020/src/KOKKOS/atom_vec_bond_kokkos.h
lammps-stable_290ct2020/src/KOKKOS/atom_vec_charge_kokkos.cpp
lammps-stable_290ct2020/src/KOKKOS/atom_vec_charge_kokkos.h
lammps-stable_290ct2020/src/KOKKOS/atom_vec_dpd_kokkos.cpp
lammps-stable_290ct2020/src/KOKKOS/atom_vec_dpd_kokkos.h
lammps-stable_290ct2020/src/KOKKOS/atom_vec_full_kokkos.cpp
lammps-stable_290ct2020/src/KOKKOS/atom_vec_full_kokkos.h
lammps-stable_290ct2020/src/KOKKOS/atom_vec_hybrid_kokkos.cpp
lammps-stable_290ct2020/src/KOKKOS/atom_vec_hybrid_kokkos.h
lammps-stable_290ct2020/src/KOKKOS/atom_vec_kokkos.cpp
lammps-stable_290ct2020/src/KOKKOS/atom_vec_kokkos.h
lammps-stable_290ct2020/src/KOKKOS/atom_vec_molecular_kokkos.cpp
lammps-stable_290ct2020/src/KOKKOS/atom_vec_molecular_kokkos.h
lammps-stable_290ct2020/src/KOKKOS/atom_vec_sphere_kokkos.cpp
lammps-stable_290ct2020/src/KOKKOS/atom_vec_sphere_kokkos.h
```

lammps-stable\_290ct2020/src/KOKKOS/bond\_class2\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/bond\_class2\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/bond\_fene\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/bond\_fene\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/bond\_harmonic\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/bond\_harmonic\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/comm\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/comm\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/comm\_tiled\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/comm\_tiled\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/compute\_coord\_atom\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/compute\_coord\_atom\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/compute\_orientorder\_atom\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/compute\_orientorder\_atom\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/compute\_temp\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/compute\_temp\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/dihedral\_charmm\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/dihedral\_charmm\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/dihedral\_class2\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/dihedral\_class2\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/dihedral\_harmonic\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/dihedral\_harmonic\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/dihedral\_opls\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/dihedral\_opls\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/domain\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/domain\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/fft3d\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/fft3d\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/fftdata\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/fix\_deform\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/fix\_deform\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/fix\_dpd\_energy\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/fix\_dpd\_energy\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/fix\_enforce2d\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/fix\_enforce2d\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/fix\_eos\_table\_rx\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/fix\_eos\_table\_rx\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/fix\_freeze\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/fix\_freeze\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/fix\_gravity\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/fix\_gravity\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/fix\_langevin\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/fix\_langevin\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/fix\_minimize\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/fix\_minimize\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/fix\_momentum\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/fix\_momentum\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/fix\_neigh\_history\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/fix\_neigh\_history\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/fix\_nh\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/fix\_nh\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/fix\_nph\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/fix\_nph\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/fix\_npt\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/fix\_npt\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/fix\_nve\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/fix\_nve\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/fix\_nve\_sphere\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/fix\_nve\_sphere\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/fix\_nvt\_kokkos.cpp

lammps-stable\_290ct2020/src/KOKKOS/fix\_nvt\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/fix\_property\_atom\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/fix\_property\_atom\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/fix\_qeq\_reax\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/fix\_qeq\_reax\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/fix\_reaxc\_bonds\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/fix\_reaxc\_bonds\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/fix\_reaxc\_species\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/fix\_reaxc\_species\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/fix\_rx\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/fix\_rx\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/fix\_setforce\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/fix\_setforce\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/fix\_shardlow\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/fix\_shardlow\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/fix\_wall\_lj93\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/fix\_wall\_lj93\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/fix\_wall\_reflect\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/fix\_wall\_reflect\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/gridcomm\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/gridcomm\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/improper\_class2\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/improper\_class2\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/improper\_harmonic\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/improper\_harmonic\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/kissfft\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/kissfft\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/kokkos\_base.h  
lammps-stable\_290ct2020/src/KOKKOS/kokkos\_base\_fft.h  
lammps-stable\_290ct2020/src/KOKKOS/kokkos\_few.h  
lammps-stable\_290ct2020/src/KOKKOS/kokkos\_type.h  
lammps-stable\_290ct2020/src/KOKKOS/math\_special\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/math\_special\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/memory\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/min\_cg\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/min\_cg\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/min\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/min\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/min\_linesearch\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/min\_linesearch\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/modify\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/modify\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/nbin\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/nbin\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/nbin\_ssa\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/nbin\_ssa\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/neigh\_bond\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/neigh\_bond\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/neigh\_list\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/neigh\_list\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/neighbor\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/neighbor\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/npair\_copy\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/npair\_copy\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/npair\_halffull\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/npair\_halffull\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/npair\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/npair\_kokkos.h

lammps-stable\_290ct2020/src/KOKKOS/npair\_skip\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/npair\_skip\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/npair\_ssa\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/npair\_ssa\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/pack\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/pair\_buck\_coul\_cut\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/pair\_buck\_coul\_cut\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/pair\_buck\_coul\_long\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/pair\_buck\_coul\_long\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/pair\_buck\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/pair\_buck\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/pair\_coul\_cut\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/pair\_coul\_cut\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/pair\_coul\_debye\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/pair\_coul\_debye\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/pair\_coul\_dsf\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/pair\_coul\_dsf\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/pair\_coul\_long\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/pair\_coul\_long\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/pair\_coul\_wolf\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/pair\_coul\_wolf\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/pair\_dpd\_fdt\_energy\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/pair\_dpd\_fdt\_energy\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/pair\_eam\_alloy\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/pair\_eam\_alloy\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/pair\_eam\_fs\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/pair\_eam\_fs\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/pair\_eam\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/pair\_eam\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/pair\_exp6\_rx\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/pair\_exp6\_rx\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/pair\_gran\_hooke\_history\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/pair\_gran\_hooke\_history\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/pair\_hybrid\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/pair\_hybrid\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/pair\_hybrid\_overlay\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/pair\_hybrid\_overlay\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/pair\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/pair\_lj\_charmm\_coul\_charmm\_implicit\_kokko  
s.cpp  
lammps-stable\_290ct2020/src/KOKKOS/pair\_lj\_charmm\_coul\_charmm\_implicit\_kokko  
s.h  
lammps-stable\_290ct2020/src/KOKKOS/pair\_lj\_charmm\_coul\_charmm\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/pair\_lj\_charmm\_coul\_charmm\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/pair\_lj\_charmm\_coul\_long\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/pair\_lj\_charmm\_coul\_long\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/pair\_lj\_class2\_coul\_cut\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/pair\_lj\_class2\_coul\_cut\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/pair\_lj\_class2\_coul\_long\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/pair\_lj\_class2\_coul\_long\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/pair\_lj\_class2\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/pair\_lj\_class2\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/pair\_lj\_cut\_coul\_cut\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/pair\_lj\_cut\_coul\_cut\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/pair\_lj\_cut\_coul\_debye\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/pair\_lj\_cut\_coul\_debye\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/pair\_lj\_cut\_coul\_dsf\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/pair\_lj\_cut\_coul\_dsf\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/pair\_lj\_cut\_coul\_long\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/pair\_lj\_cut\_coul\_long\_kokkos.h

lammps-stable\_290ct2020/src/KOKKOS/pair\_lj\_cut\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/pair\_lj\_cut\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/pair\_lj\_expand\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/pair\_lj\_expand\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/pair\_lj\_gromacs\_coul\_gromacs\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/pair\_lj\_gromacs\_coul\_gromacs\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/pair\_lj\_gromacs\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/pair\_lj\_gromacs\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/pair\_lj\_sdk\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/pair\_lj\_sdk\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/pair\_morse\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/pair\_morse\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/pair\_multi\_lucy\_rx\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/pair\_multi\_lucy\_rx\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/pair\_reaxc\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/pair\_reaxc\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/pair\_snap\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/pair\_snap\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/pair\_snap\_kokkos\_impl.h  
lammps-stable\_290ct2020/src/KOKKOS/pair\_sw\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/pair\_sw\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/pair\_table\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/pair\_table\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/pair\_table\_rx\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/pair\_table\_rx\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/pair\_tersoff\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/pair\_tersoff\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/pair\_tersoff\_mod\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/pair\_tersoff\_mod\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/pair\_tersoff\_zbl\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/pair\_tersoff\_zbl\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/pair\_vashishta\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/pair\_vashishta\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/pair\_yukawa\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/pair\_yukawa\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/pair\_zbl\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/pair\_zbl\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/pppm\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/pppm\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/rand\_pool\_wrap\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/rand\_pool\_wrap\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/region\_block\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/region\_block\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/remap\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/remap\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/sna\_kokkos.h  
lammps-stable\_290ct2020/src/KOKKOS/sna\_kokkos\_impl.h  
lammps-stable\_290ct2020/src/KOKKOS/verlet\_kokkos.cpp  
lammps-stable\_290ct2020/src/KOKKOS/verlet\_kokkos.h  
lammps-stable\_290ct2020/src/KSPACE/  
lammps-stable\_290ct2020/src/KSPACE/ewald.cpp  
lammps-stable\_290ct2020/src/KSPACE/ewald.h  
lammps-stable\_290ct2020/src/KSPACE/ewald\_dipole.cpp  
lammps-stable\_290ct2020/src/KSPACE/ewald\_dipole.h  
lammps-stable\_290ct2020/src/KSPACE/ewald\_dipole\_spin.cpp  
lammps-stable\_290ct2020/src/KSPACE/ewald\_dipole\_spin.h  
lammps-stable\_290ct2020/src/KSPACE/ewald\_disp.cpp  
lammps-stable\_290ct2020/src/KSPACE/ewald\_disp.h  
lammps-stable\_290ct2020/src/KSPACE/fft3d.cpp  
lammps-stable\_290ct2020/src/KSPACE/fft3d.h

```
lammps-stable_290ct2020/src/KSPACE/fft3d_wrap.cpp
lammps-stable_290ct2020/src/KSPACE/fft3d_wrap.h
lammps-stable_290ct2020/src/KSPACE/fix_tune_kspace.cpp
lammps-stable_290ct2020/src/KSPACE/fix_tune_kspace.h
lammps-stable_290ct2020/src/KSPACE/gridcomm.cpp
lammps-stable_290ct2020/src/KSPACE/gridcomm.h
lammps-stable_290ct2020/src/KSPACE/kissfft.h
lammps-stable_290ct2020/src/KSPACE/msm.cpp
lammps-stable_290ct2020/src/KSPACE/msm.h
lammps-stable_290ct2020/src/KSPACE/msm_cg.cpp
lammps-stable_290ct2020/src/KSPACE/msm_cg.h
lammps-stable_290ct2020/src/KSPACE/pair_born_coul_long.cpp
lammps-stable_290ct2020/src/KSPACE/pair_born_coul_long.h
lammps-stable_290ct2020/src/KSPACE/pair_born_coul_msm.cpp
lammps-stable_290ct2020/src/KSPACE/pair_born_coul_msm.h
lammps-stable_290ct2020/src/KSPACE/pair_buck_coul_long.cpp
lammps-stable_290ct2020/src/KSPACE/pair_buck_coul_long.h
lammps-stable_290ct2020/src/KSPACE/pair_buck_coul_msm.cpp
lammps-stable_290ct2020/src/KSPACE/pair_buck_coul_msm.h
lammps-stable_290ct2020/src/KSPACE/pair_buck_long_coul_long.cpp
lammps-stable_290ct2020/src/KSPACE/pair_buck_long_coul_long.h
lammps-stable_290ct2020/src/KSPACE/pair_coul_long.cpp
lammps-stable_290ct2020/src/KSPACE/pair_coul_long.h
lammps-stable_290ct2020/src/KSPACE/pair_coul_msm.cpp
lammps-stable_290ct2020/src/KSPACE/pair_coul_msm.h
lammps-stable_290ct2020/src/KSPACE/pair_lj_charmm_coul_long.cpp
lammps-stable_290ct2020/src/KSPACE/pair_lj_charmm_coul_long.h
lammps-stable_290ct2020/src/KSPACE/pair_lj_charmm_coul_msm.cpp
lammps-stable_290ct2020/src/KSPACE/pair_lj_charmm_coul_msm.h
lammps-stable_290ct2020/src/KSPACE/pair_lj_charmmfsw_coul_long.cpp
lammps-stable_290ct2020/src/KSPACE/pair_lj_charmmfsw_coul_long.h
lammps-stable_290ct2020/src/KSPACE/pair_lj_cut_coul_long.cpp
lammps-stable_290ct2020/src/KSPACE/pair_lj_cut_coul_long.h
lammps-stable_290ct2020/src/KSPACE/pair_lj_cut_coul_msm.cpp
lammps-stable_290ct2020/src/KSPACE/pair_lj_cut_coul_msm.h
lammps-stable_290ct2020/src/KSPACE/pair_lj_cut_tip4p_long.cpp
lammps-stable_290ct2020/src/KSPACE/pair_lj_cut_tip4p_long.h
lammps-stable_290ct2020/src/KSPACE/pair_lj_long_coul_long.cpp
lammps-stable_290ct2020/src/KSPACE/pair_lj_long_coul_long.h
lammps-stable_290ct2020/src/KSPACE/pair_lj_long_tip4p_long.cpp
lammps-stable_290ct2020/src/KSPACE/pair_lj_long_tip4p_long.h
lammps-stable_290ct2020/src/KSPACE/pair_tip4p_long.cpp
lammps-stable_290ct2020/src/KSPACE/pair_tip4p_long.h
lammps-stable_290ct2020/src/KSPACE/pppm.cpp
lammps-stable_290ct2020/src/KSPACE/pppm.h
lammps-stable_290ct2020/src/KSPACE/pppm_cg.cpp
lammps-stable_290ct2020/src/KSPACE/pppm_cg.h
lammps-stable_290ct2020/src/KSPACE/pppm_dipole.cpp
lammps-stable_290ct2020/src/KSPACE/pppm_dipole.h
lammps-stable_290ct2020/src/KSPACE/pppm_dipole_spin.cpp
lammps-stable_290ct2020/src/KSPACE/pppm_dipole_spin.h
lammps-stable_290ct2020/src/KSPACE/pppm_disp.cpp
lammps-stable_290ct2020/src/KSPACE/pppm_disp.h
lammps-stable_290ct2020/src/KSPACE/pppm_disp_tip4p.cpp
lammps-stable_290ct2020/src/KSPACE/pppm_disp_tip4p.h
lammps-stable_290ct2020/src/KSPACE/pppm_stagger.cpp
lammps-stable_290ct2020/src/KSPACE/pppm_stagger.h
lammps-stable_290ct2020/src/KSPACE/pppm_tip4p.cpp
lammps-stable_290ct2020/src/KSPACE/pppm_tip4p.h
lammps-stable_290ct2020/src/KSPACE/remap.cpp
```

```
lammps-stable_290ct2020/src/KSPACE/remap.h
lammps-stable_290ct2020/src/KSPACE/remap_wrap.cpp
lammps-stable_290ct2020/src/KSPACE/remap_wrap.h
lammps-stable_290ct2020/src/LATTE/
lammps-stable_290ct2020/src/LATTE/Install.sh
lammps-stable_290ct2020/src/LATTE/README
lammps-stable_290ct2020/src/LATTE/fix_latte.cpp
lammps-stable_290ct2020/src/LATTE/fix_latte.h
lammps-stable_290ct2020/src/MAKE/
lammps-stable_290ct2020/src/MAKE/MACHINES/
lammps-stable_290ct2020/src/MAKE/MACHINES/Makefile.aarch64_arm_openmpi_armpl
lammps-stable_290ct2020/src/MAKE/MACHINES/Makefile.aarch64_arm_serial_armpl
lammps-stable_290ct2020/src/MAKE/MACHINES/Makefile.aarch64_g++_openmpi_armpl
lammps-stable_290ct2020/src/MAKE/MACHINES/Makefile.aarch64_g++_serial_armpl
lammps-stable_290ct2020/src/MAKE/MACHINES/Makefile.astra_arm
lammps-stable_290ct2020/src/MAKE/MACHINES/Makefile.bgq
lammps-stable_290ct2020/src/MAKE/MACHINES/Makefile.cori2
lammps-stable_290ct2020/src/MAKE/MACHINES/Makefile.cygwin
lammps-stable_290ct2020/src/MAKE/MACHINES/Makefile.mac
lammps-stable_290ct2020/src/MAKE/MACHINES/Makefile.mac_mpi
lammps-stable_290ct2020/src/MAKE/MACHINES/Makefile.power
lammps-stable_290ct2020/src/MAKE/MACHINES/Makefile.summit_kokkos
lammps-stable_290ct2020/src/MAKE/MACHINES/Makefile.theta
lammps-stable_290ct2020/src/MAKE/MACHINES/Makefile.ubuntu
lammps-stable_290ct2020/src/MAKE/MACHINES/Makefile.ubuntu_simple
lammps-stable_290ct2020/src/MAKE/MACHINES/Makefile.white
lammps-stable_290ct2020/src/MAKE/MACHINES/Makefile.xe6
lammps-stable_290ct2020/src/MAKE/MACHINES/bgq.make.details
lammps-stable_290ct2020/src/MAKE/MINE/
lammps-stable_290ct2020/src/MAKE/Makefile.mpi
lammps-stable_290ct2020/src/MAKE/Makefile.serial
lammps-stable_290ct2020/src/MAKE/OPTIONS/
lammps-stable_290ct2020/src/MAKE/OPTIONS/Makefile.big
lammps-stable_290ct2020/src/MAKE/OPTIONS/Makefile.fftw
lammps-stable_290ct2020/src/MAKE/OPTIONS/Makefile.g++_mpich
lammps-stable_290ct2020/src/MAKE/OPTIONS/Makefile.g++_mpich_link
lammps-stable_290ct2020/src/MAKE/OPTIONS/Makefile.g++_openmpi
lammps-stable_290ct2020/src/MAKE/OPTIONS/Makefile.g++_openmpi_link
lammps-stable_290ct2020/src/MAKE/OPTIONS/Makefile.g++_serial
lammps-stable_290ct2020/src/MAKE/OPTIONS/Makefile.gpu
lammps-stable_290ct2020/src/MAKE/OPTIONS/Makefile.hip
lammps-stable_290ct2020/src/MAKE/OPTIONS/Makefile.icc_mpich
lammps-stable_290ct2020/src/MAKE/OPTIONS/Makefile.icc_mpich_link
lammps-stable_290ct2020/src/MAKE/OPTIONS/Makefile.icc_openmpi
lammps-stable_290ct2020/src/MAKE/OPTIONS/Makefile.icc_openmpi_link
lammps-stable_290ct2020/src/MAKE/OPTIONS/Makefile.icc_serial
lammps-stable_290ct2020/src/MAKE/OPTIONS/Makefile.intel_coprocessor
lammps-stable_290ct2020/src/MAKE/OPTIONS/Makefile.intel_cpu_intelmpi
lammps-stable_290ct2020/src/MAKE/OPTIONS/Makefile.intel_cpu_mpich
lammps-stable_290ct2020/src/MAKE/OPTIONS/Makefile.intel_cpu_openmpi
lammps-stable_290ct2020/src/MAKE/OPTIONS/Makefile.jpeg
lammps-stable_290ct2020/src/MAKE/OPTIONS/Makefile.knl
lammps-stable_290ct2020/src/MAKE/OPTIONS/Makefile.kokkos_cuda_mpi
lammps-stable_290ct2020/src/MAKE/OPTIONS/Makefile.kokkos_mpi_only
lammps-stable_290ct2020/src/MAKE/OPTIONS/Makefile.kokkos_omp
lammps-stable_290ct2020/src/MAKE/OPTIONS/Makefile.kokkos_phi
lammps-stable_290ct2020/src/MAKE/OPTIONS/Makefile.mgptfast
lammps-stable_290ct2020/src/MAKE/OPTIONS/Makefile.omp
lammps-stable_290ct2020/src/MAKE/OPTIONS/Makefile.opt
lammps-stable_290ct2020/src/MAKE/OPTIONS/Makefile.pgi_mpich_link
```

```
lammps-stable_290ct2020/src/MAKE/OPTIONS/Makefile.png
lammps-stable_290ct2020/src/MAKE/README
lammps-stable_290ct2020/src/MANYBODY/
lammps-stable_290ct2020/src/MANYBODY/fix_qeq_comb.cpp
lammps-stable_290ct2020/src/MANYBODY/fix_qeq_comb.h
lammps-stable_290ct2020/src/MANYBODY/pair_adp.cpp
lammps-stable_290ct2020/src/MANYBODY/pair_adp.h
lammps-stable_290ct2020/src/MANYBODY/pair_airebo.cpp
lammps-stable_290ct2020/src/MANYBODY/pair_airebo.h
lammps-stable_290ct2020/src/MANYBODY/pair_airebo_morse.cpp
lammps-stable_290ct2020/src/MANYBODY/pair_airebo_morse.h
lammps-stable_290ct2020/src/MANYBODY/pair_atm.cpp
lammps-stable_290ct2020/src/MANYBODY/pair_atm.h
lammps-stable_290ct2020/src/MANYBODY/pair_bop.cpp
lammps-stable_290ct2020/src/MANYBODY/pair_bop.h
lammps-stable_290ct2020/src/MANYBODY/pair_comb.cpp
lammps-stable_290ct2020/src/MANYBODY/pair_comb.h
lammps-stable_290ct2020/src/MANYBODY/pair_comb3.cpp
lammps-stable_290ct2020/src/MANYBODY/pair_comb3.h
lammps-stable_290ct2020/src/MANYBODY/pair_eam.cpp
lammps-stable_290ct2020/src/MANYBODY/pair_eam.h
lammps-stable_290ct2020/src/MANYBODY/pair_eam_alloy.cpp
lammps-stable_290ct2020/src/MANYBODY/pair_eam_alloy.h
lammps-stable_290ct2020/src/MANYBODY/pair_eam_cd.cpp
lammps-stable_290ct2020/src/MANYBODY/pair_eam_cd.h
lammps-stable_290ct2020/src/MANYBODY/pair_eam_fs.cpp
lammps-stable_290ct2020/src/MANYBODY/pair_eam_fs.h
lammps-stable_290ct2020/src/MANYBODY/pair_eim.cpp
lammps-stable_290ct2020/src/MANYBODY/pair_eim.h
lammps-stable_290ct2020/src/MANYBODY/pair_gw.cpp
lammps-stable_290ct2020/src/MANYBODY/pair_gw.h
lammps-stable_290ct2020/src/MANYBODY/pair_gw_zbl.cpp
lammps-stable_290ct2020/src/MANYBODY/pair_gw_zbl.h
lammps-stable_290ct2020/src/MANYBODY/pair_lcbop.cpp
lammps-stable_290ct2020/src/MANYBODY/pair_lcbop.h
lammps-stable_290ct2020/src/MANYBODY/pair_nb3b_harmonic.cpp
lammps-stable_290ct2020/src/MANYBODY/pair_nb3b_harmonic.h
lammps-stable_290ct2020/src/MANYBODY/pair_polymorphic.cpp
lammps-stable_290ct2020/src/MANYBODY/pair_polymorphic.h
lammps-stable_290ct2020/src/MANYBODY/pair_rebo.cpp
lammps-stable_290ct2020/src/MANYBODY/pair_rebo.h
lammps-stable_290ct2020/src/MANYBODY/pair_sw.cpp
lammps-stable_290ct2020/src/MANYBODY/pair_sw.h
lammps-stable_290ct2020/src/MANYBODY/pair_tersoff.cpp
lammps-stable_290ct2020/src/MANYBODY/pair_tersoff.h
lammps-stable_290ct2020/src/MANYBODY/pair_tersoff_mod.cpp
lammps-stable_290ct2020/src/MANYBODY/pair_tersoff_mod.h
lammps-stable_290ct2020/src/MANYBODY/pair_tersoff_mod_c.cpp
lammps-stable_290ct2020/src/MANYBODY/pair_tersoff_mod_c.h
lammps-stable_290ct2020/src/MANYBODY/pair_tersoff_zbl.cpp
lammps-stable_290ct2020/src/MANYBODY/pair_tersoff_zbl.h
lammps-stable_290ct2020/src/MANYBODY/pair_vashishta.cpp
lammps-stable_290ct2020/src/MANYBODY/pair_vashishta.h
lammps-stable_290ct2020/src/MANYBODY/pair_vashishta_table.cpp
lammps-stable_290ct2020/src/MANYBODY/pair_vashishta_table.h
lammps-stable_290ct2020/src/MC/
lammps-stable_290ct2020/src/MC/fix_atom_swap.cpp
lammps-stable_290ct2020/src/MC/fix_atom_swap.h
lammps-stable_290ct2020/src/MC/fix_bond_break.cpp
lammps-stable_290ct2020/src/MC/fix_bond_break.h
```



```
lammps-stable_290ct2020/src/MC/fix_bond_create.cpp
lammps-stable_290ct2020/src/MC/fix_bond_create.h
lammps-stable_290ct2020/src/MC/fix_bond_create_angle.cpp
lammps-stable_290ct2020/src/MC/fix_bond_create_angle.h
lammps-stable_290ct2020/src/MC/fix_bond_swap.cpp
lammps-stable_290ct2020/src/MC/fix_bond_swap.h
lammps-stable_290ct2020/src/MC/fix_gcmc.cpp
lammps-stable_290ct2020/src/MC/fix_gcmc.h
lammps-stable_290ct2020/src/MC/fix_tfmc.cpp
lammps-stable_290ct2020/src/MC/fix_tfmc.h
lammps-stable_290ct2020/src/MC/fix_widom.cpp
lammps-stable_290ct2020/src/MC/fix_widom.h
lammps-stable_290ct2020/src/MC/pair_dsmc.cpp
lammps-stable_290ct2020/src/MC/pair_dsmc.h
lammps-stable_290ct2020/src/MESSAGE/
lammps-stable_290ct2020/src/MESSAGE/Install.sh
lammps-stable_290ct2020/src/MESSAGE/fix_client_md.cpp
lammps-stable_290ct2020/src/MESSAGE/fix_client_md.h
lammps-stable_290ct2020/src/MESSAGE/message.cpp
lammps-stable_290ct2020/src/MESSAGE/message.h
lammps-stable_290ct2020/src/MESSAGE/server.cpp
lammps-stable_290ct2020/src/MESSAGE/server.h
lammps-stable_290ct2020/src/MESSAGE/server_mc.cpp
lammps-stable_290ct2020/src/MESSAGE/server_mc.h
lammps-stable_290ct2020/src/MESSAGE/server_md.cpp
lammps-stable_290ct2020/src/MESSAGE/server_md.h
lammps-stable_290ct2020/src/MISC/
lammps-stable_290ct2020/src/MISC/compute_msd_nongauss.cpp
lammps-stable_290ct2020/src/MISC/compute_msd_nongauss.h
lammps-stable_290ct2020/src/MISC/compute_ti.cpp
lammps-stable_290ct2020/src/MISC/compute_ti.h
lammps-stable_290ct2020/src/MISC/dump_xtc.cpp
lammps-stable_290ct2020/src/MISC/dump_xtc.h
lammps-stable_290ct2020/src/MISC/fix_deposit.cpp
lammps-stable_290ct2020/src/MISC/fix_deposit.h
lammps-stable_290ct2020/src/MISC/fix_efield.cpp
lammps-stable_290ct2020/src/MISC/fix_efield.h
lammps-stable_290ct2020/src/MISC/fix_evaporate.cpp
lammps-stable_290ct2020/src/MISC/fix_evaporate.h
lammps-stable_290ct2020/src/MISC/fix_gld.cpp
lammps-stable_290ct2020/src/MISC/fix_gld.h
lammps-stable_290ct2020/src/MISC/fix_oneway.cpp
lammps-stable_290ct2020/src/MISC/fix_oneway.h
lammps-stable_290ct2020/src/MISC/fix_orient_bcc.cpp
lammps-stable_290ct2020/src/MISC/fix_orient_bcc.h
lammps-stable_290ct2020/src/MISC/fix_orient_fcc.cpp
lammps-stable_290ct2020/src/MISC/fix_orient_fcc.h
lammps-stable_290ct2020/src/MISC/fix_thermal_conductivity.cpp
lammps-stable_290ct2020/src/MISC/fix_thermal_conductivity.h
lammps-stable_290ct2020/src/MISC/fix_ttm.cpp
lammps-stable_290ct2020/src/MISC/fix_ttm.h
lammps-stable_290ct2020/src/MISC/fix_viscosity.cpp
lammps-stable_290ct2020/src/MISC/fix_viscosity.h
lammps-stable_290ct2020/src/MISC/pair_nm_cut.cpp
lammps-stable_290ct2020/src/MISC/pair_nm_cut.h
lammps-stable_290ct2020/src/MISC/pair_nm_cut_coul_cut.cpp
lammps-stable_290ct2020/src/MISC/pair_nm_cut_coul_cut.h
lammps-stable_290ct2020/src/MISC/pair_nm_cut_coul_long.cpp
lammps-stable_290ct2020/src/MISC/pair_nm_cut_coul_long.h
lammps-stable_290ct2020/src/MISC/xdr_compat.cpp
```

```
lammps-stable_290ct2020/src/MISC/xdr_compat.h
lammps-stable_290ct2020/src/MLIAP/
lammps-stable_290ct2020/src/MLIAP/README
lammps-stable_290ct2020/src/MLIAP/compute_mliap.cpp
lammps-stable_290ct2020/src/MLIAP/compute_mliap.h
lammps-stable_290ct2020/src/MLIAP/mliap_data.cpp
lammps-stable_290ct2020/src/MLIAP/mliap_data.h
lammps-stable_290ct2020/src/MLIAP/mliap_descriptor.cpp
lammps-stable_290ct2020/src/MLIAP/mliap_descriptor.h
lammps-stable_290ct2020/src/MLIAP/mliap_descriptor_snap.cpp
lammps-stable_290ct2020/src/MLIAP/mliap_descriptor_snap.h
lammps-stable_290ct2020/src/MLIAP/mliap_model.cpp
lammps-stable_290ct2020/src/MLIAP/mliap_model.h
lammps-stable_290ct2020/src/MLIAP/mliap_model_linear.cpp
lammps-stable_290ct2020/src/MLIAP/mliap_model_linear.h
lammps-stable_290ct2020/src/MLIAP/mliap_model_quadratic.cpp
lammps-stable_290ct2020/src/MLIAP/mliap_model_quadratic.h
lammps-stable_290ct2020/src/MLIAP/pair_mliap.cpp
lammps-stable_290ct2020/src/MLIAP/pair_mliap.h
lammps-stable_290ct2020/src/MOLECULE/
lammps-stable_290ct2020/src/MOLECULE/angle_charmm.cpp
lammps-stable_290ct2020/src/MOLECULE/angle_charmm.h
lammps-stable_290ct2020/src/MOLECULE/angle_cosine.cpp
lammps-stable_290ct2020/src/MOLECULE/angle_cosine.h
lammps-stable_290ct2020/src/MOLECULE/angle_cosine_delta.cpp
lammps-stable_290ct2020/src/MOLECULE/angle_cosine_delta.h
lammps-stable_290ct2020/src/MOLECULE/angle_cosine_periodic.cpp
lammps-stable_290ct2020/src/MOLECULE/angle_cosine_periodic.h
lammps-stable_290ct2020/src/MOLECULE/angle_cosine_squared.cpp
lammps-stable_290ct2020/src/MOLECULE/angle_cosine_squared.h
lammps-stable_290ct2020/src/MOLECULE/angle_harmonic.cpp
lammps-stable_290ct2020/src/MOLECULE/angle_harmonic.h
lammps-stable_290ct2020/src/MOLECULE/angle_table.cpp
lammps-stable_290ct2020/src/MOLECULE/angle_table.h
lammps-stable_290ct2020/src/MOLECULE/atom_vec_angle.cpp
lammps-stable_290ct2020/src/MOLECULE/atom_vec_angle.h
lammps-stable_290ct2020/src/MOLECULE/atom_vec_bond.cpp
lammps-stable_290ct2020/src/MOLECULE/atom_vec_bond.h
lammps-stable_290ct2020/src/MOLECULE/atom_vec_full.cpp
lammps-stable_290ct2020/src/MOLECULE/atom_vec_full.h
lammps-stable_290ct2020/src/MOLECULE/atom_vec_molecular.cpp
lammps-stable_290ct2020/src/MOLECULE/atom_vec_molecular.h
lammps-stable_290ct2020/src/MOLECULE/atom_vec_template.cpp
lammps-stable_290ct2020/src/MOLECULE/atom_vec_template.h
lammps-stable_290ct2020/src/MOLECULE/bond_fene.cpp
lammps-stable_290ct2020/src/MOLECULE/bond_fene.h
lammps-stable_290ct2020/src/MOLECULE/bond_fene_expand.cpp
lammps-stable_290ct2020/src/MOLECULE/bond_fene_expand.h
lammps-stable_290ct2020/src/MOLECULE/bond_gromos.cpp
lammps-stable_290ct2020/src/MOLECULE/bond_gromos.h
lammps-stable_290ct2020/src/MOLECULE/bond_harmonic.cpp
lammps-stable_290ct2020/src/MOLECULE/bond_harmonic.h
lammps-stable_290ct2020/src/MOLECULE/bond_morse.cpp
lammps-stable_290ct2020/src/MOLECULE/bond_morse.h
lammps-stable_290ct2020/src/MOLECULE/bond_nonlinear.cpp
lammps-stable_290ct2020/src/MOLECULE/bond_nonlinear.h
lammps-stable_290ct2020/src/MOLECULE/bond_quartic.cpp
lammps-stable_290ct2020/src/MOLECULE/bond_quartic.h
lammps-stable_290ct2020/src/MOLECULE/bond_table.cpp
lammps-stable_290ct2020/src/MOLECULE/bond_table.h
```

```
lammps-stable_290ct2020/src/MOLECULE/dihedral_charmm.cpp
lammps-stable_290ct2020/src/MOLECULE/dihedral_charmm.h
lammps-stable_290ct2020/src/MOLECULE/dihedral_charmmfsw.cpp
lammps-stable_290ct2020/src/MOLECULE/dihedral_charmmfsw.h
lammps-stable_290ct2020/src/MOLECULE/dihedral_harmonic.cpp
lammps-stable_290ct2020/src/MOLECULE/dihedral_harmonic.h
lammps-stable_290ct2020/src/MOLECULE/dihedral_helix.cpp
lammps-stable_290ct2020/src/MOLECULE/dihedral_helix.h
lammps-stable_290ct2020/src/MOLECULE/dihedral_multi_harmonic.cpp
lammps-stable_290ct2020/src/MOLECULE/dihedral_multi_harmonic.h
lammps-stable_290ct2020/src/MOLECULE/dihedral_opls.cpp
lammps-stable_290ct2020/src/MOLECULE/dihedral_opls.h
lammps-stable_290ct2020/src/MOLECULE/fix_cmap.cpp
lammps-stable_290ct2020/src/MOLECULE/fix_cmap.h
lammps-stable_290ct2020/src/MOLECULE/improper_cvff.cpp
lammps-stable_290ct2020/src/MOLECULE/improper_cvff.h
lammps-stable_290ct2020/src/MOLECULE/improper_harmonic.cpp
lammps-stable_290ct2020/src/MOLECULE/improper_harmonic.h
lammps-stable_290ct2020/src/MOLECULE/improper_umbrella.cpp
lammps-stable_290ct2020/src/MOLECULE/improper_umbrella.h
lammps-stable_290ct2020/src/MOLECULE/pair_hbond_dreiding_lj.cpp
lammps-stable_290ct2020/src/MOLECULE/pair_hbond_dreiding_lj.h
lammps-stable_290ct2020/src/MOLECULE/pair_hbond_dreiding_morse.cpp
lammps-stable_290ct2020/src/MOLECULE/pair_hbond_dreiding_morse.h
lammps-stable_290ct2020/src/MOLECULE/pair_lj_charmm_coul_charmm.cpp
lammps-stable_290ct2020/src/MOLECULE/pair_lj_charmm_coul_charmm.h
lammps-stable_290ct2020/src/MOLECULE/pair_lj_charmm_coul_charmm_implicit.cpp
lammps-stable_290ct2020/src/MOLECULE/pair_lj_charmm_coul_charmm_implicit.h
lammps-stable_290ct2020/src/MOLECULE/pair_lj_charmmfsw_coul_charmmfsh.cpp
lammps-stable_290ct2020/src/MOLECULE/pair_lj_charmmfsw_coul_charmmfsh.h
lammps-stable_290ct2020/src/MOLECULE/pair_lj_cut_tip4p_cut.cpp
lammps-stable_290ct2020/src/MOLECULE/pair_lj_cut_tip4p_cut.h
lammps-stable_290ct2020/src/MOLECULE/pair_tip4p_cut.cpp
lammps-stable_290ct2020/src/MOLECULE/pair_tip4p_cut.h
lammps-stable_290ct2020/src/MPIIO/
lammps-stable_290ct2020/src/MPIIO/Install.sh
lammps-stable_290ct2020/src/MPIIO/dump_atom_mpiio.cpp
lammps-stable_290ct2020/src/MPIIO/dump_atom_mpiio.h
lammps-stable_290ct2020/src/MPIIO/dump_cfg_mpiio.cpp
lammps-stable_290ct2020/src/MPIIO/dump_cfg_mpiio.h
lammps-stable_290ct2020/src/MPIIO/dump_custom_mpiio.cpp
lammps-stable_290ct2020/src/MPIIO/dump_custom_mpiio.h
lammps-stable_290ct2020/src/MPIIO/dump_xyz_mpiio.cpp
lammps-stable_290ct2020/src/MPIIO/dump_xyz_mpiio.h
lammps-stable_290ct2020/src/MPIIO/restart_mpiio.cpp
lammps-stable_290ct2020/src/MPIIO/restart_mpiio.h
lammps-stable_290ct2020/src/MSCG/
lammps-stable_290ct2020/src/MSCG/Install.sh
lammps-stable_290ct2020/src/MSCG/README
lammps-stable_290ct2020/src/MSCG/fix_mscg.cpp
lammps-stable_290ct2020/src/MSCG/fix_mscg.h
lammps-stable_290ct2020/src/Make.sh
lammps-stable_290ct2020/src/Makefile
lammps-stable_290ct2020/src/Makefile.list
lammps-stable_290ct2020/src/Makefile.package.empty
lammps-stable_290ct2020/src/Makefile.package.settings.empty
lammps-stable_290ct2020/src/Makefile.print
lammps-stable_290ct2020/src/OPT/
lammps-stable_290ct2020/src/OPT/Install.sh
lammps-stable_290ct2020/src/OPT/pair_eam_alloy_opt.cpp
```

```
lammps-stable_290ct2020/src/OPT/pair_eam_alloy_opt.h
lammps-stable_290ct2020/src/OPT/pair_eam_fs_opt.cpp
lammps-stable_290ct2020/src/OPT/pair_eam_fs_opt.h
lammps-stable_290ct2020/src/OPT/pair_eam_opt.cpp
lammps-stable_290ct2020/src/OPT/pair_eam_opt.h
lammps-stable_290ct2020/src/OPT/pair_lj_charmm_coul_long_opt.cpp
lammps-stable_290ct2020/src/OPT/pair_lj_charmm_coul_long_opt.h
lammps-stable_290ct2020/src/OPT/pair_lj_cut_coul_long_opt.cpp
lammps-stable_290ct2020/src/OPT/pair_lj_cut_coul_long_opt.h
lammps-stable_290ct2020/src/OPT/pair_lj_cut_opt.cpp
lammps-stable_290ct2020/src/OPT/pair_lj_cut_opt.h
lammps-stable_290ct2020/src/OPT/pair_lj_cut_tip4p_long_opt.cpp
lammps-stable_290ct2020/src/OPT/pair_lj_cut_tip4p_long_opt.h
lammps-stable_290ct2020/src/OPT/pair_lj_long_coul_long_opt.cpp
lammps-stable_290ct2020/src/OPT/pair_lj_long_coul_long_opt.h
lammps-stable_290ct2020/src/OPT/pair_morse_opt.cpp
lammps-stable_290ct2020/src/OPT/pair_morse_opt.h
lammps-stable_290ct2020/src/OPT/pair_uhm_opt.cpp
lammps-stable_290ct2020/src/OPT/pair_uhm_opt.h
lammps-stable_290ct2020/src/PERI/
lammps-stable_290ct2020/src/PERI/atom_vec_peri.cpp
lammps-stable_290ct2020/src/PERI/atom_vec_peri.h
lammps-stable_290ct2020/src/PERI/compute_damage_atom.cpp
lammps-stable_290ct2020/src/PERI/compute_damage_atom.h
lammps-stable_290ct2020/src/PERI/compute_dilatation_atom.cpp
lammps-stable_290ct2020/src/PERI/compute_dilatation_atom.h
lammps-stable_290ct2020/src/PERI/compute_plasticity_atom.cpp
lammps-stable_290ct2020/src/PERI/compute_plasticity_atom.h
lammps-stable_290ct2020/src/PERI/fix_peri_neigh.cpp
lammps-stable_290ct2020/src/PERI/fix_peri_neigh.h
lammps-stable_290ct2020/src/PERI/pair_peri_eps.cpp
lammps-stable_290ct2020/src/PERI/pair_peri_eps.h
lammps-stable_290ct2020/src/PERI/pair_peri_lps.cpp
lammps-stable_290ct2020/src/PERI/pair_peri_lps.h
lammps-stable_290ct2020/src/PERI/pair_peri_pmb.cpp
lammps-stable_290ct2020/src/PERI/pair_peri_pmb.h
lammps-stable_290ct2020/src/PERI/pair_peri_ves.cpp
lammps-stable_290ct2020/src/PERI/pair_peri_ves.h
lammps-stable_290ct2020/src/POEMS/
lammps-stable_290ct2020/src/POEMS/Install.sh
lammps-stable_290ct2020/src/POEMS/README
lammps-stable_290ct2020/src/POEMS/fix_poems.cpp
lammps-stable_290ct2020/src/POEMS/fix_poems.h
lammps-stable_290ct2020/src/PYTHON/
lammps-stable_290ct2020/src/PYTHON/Install.sh
lammps-stable_290ct2020/src/PYTHON/fix_python_invoke.cpp
lammps-stable_290ct2020/src/PYTHON/fix_python_invoke.h
lammps-stable_290ct2020/src/PYTHON/fix_python_move.cpp
lammps-stable_290ct2020/src/PYTHON/fix_python_move.h
lammps-stable_290ct2020/src/PYTHON/pair_python.cpp
lammps-stable_290ct2020/src/PYTHON/pair_python.h
lammps-stable_290ct2020/src/PYTHON/python_compat.h
lammps-stable_290ct2020/src/PYTHON/python_impl.cpp
lammps-stable_290ct2020/src/PYTHON/python_impl.h
lammps-stable_290ct2020/src/Package.sh
lammps-stable_290ct2020/src/Purge.list
lammps-stable_290ct2020/src/QEQ/
lammps-stable_290ct2020/src/QEQ/Install.sh
lammps-stable_290ct2020/src/QEQ/fix_qeq.cpp
lammps-stable_290ct2020/src/QEQ/fix_qeq.h
```

```
lammps-stable_290ct2020/src/QEQ/fix_qeq_dynamic.cpp
lammps-stable_290ct2020/src/QEQ/fix_qeq_dynamic.h
lammps-stable_290ct2020/src/QEQ/fix_qeq_fire.cpp
lammps-stable_290ct2020/src/QEQ/fix_qeq_fire.h
lammps-stable_290ct2020/src/QEQ/fix_qeq_point.cpp
lammps-stable_290ct2020/src/QEQ/fix_qeq_point.h
lammps-stable_290ct2020/src/QEQ/fix_qeq_shielded.cpp
lammps-stable_290ct2020/src/QEQ/fix_qeq_shielded.h
lammps-stable_290ct2020/src/QEQ/fix_qeq_slater.cpp
lammps-stable_290ct2020/src/QEQ/fix_qeq_slater.h
lammps-stable_290ct2020/src/REPLICA/
lammps-stable_290ct2020/src/REPLICA/compute_event_displace.cpp
lammps-stable_290ct2020/src/REPLICA/compute_event_displace.h
lammps-stable_290ct2020/src/REPLICA/fix_event.cpp
lammps-stable_290ct2020/src/REPLICA/fix_event.h
lammps-stable_290ct2020/src/REPLICA/fix_event_hyper.cpp
lammps-stable_290ct2020/src/REPLICA/fix_event_hyper.h
lammps-stable_290ct2020/src/REPLICA/fix_event_prd.cpp
lammps-stable_290ct2020/src/REPLICA/fix_event_prd.h
lammps-stable_290ct2020/src/REPLICA/fix_event_tad.cpp
lammps-stable_290ct2020/src/REPLICA/fix_event_tad.h
lammps-stable_290ct2020/src/REPLICA/fix_hyper.cpp
lammps-stable_290ct2020/src/REPLICA/fix_hyper.h
lammps-stable_290ct2020/src/REPLICA/fix_hyper_global.cpp
lammps-stable_290ct2020/src/REPLICA/fix_hyper_global.h
lammps-stable_290ct2020/src/REPLICA/fix_hyper_local.cpp
lammps-stable_290ct2020/src/REPLICA/fix_hyper_local.h
lammps-stable_290ct2020/src/REPLICA/fix_neb.cpp
lammps-stable_290ct2020/src/REPLICA/fix_neb.h
lammps-stable_290ct2020/src/REPLICA/hyper.cpp
lammps-stable_290ct2020/src/REPLICA/hyper.h
lammps-stable_290ct2020/src/REPLICA/neb.cpp
lammps-stable_290ct2020/src/REPLICA/neb.h
lammps-stable_290ct2020/src/REPLICA/prd.cpp
lammps-stable_290ct2020/src/REPLICA/prd.h
lammps-stable_290ct2020/src/REPLICA/tad.cpp
lammps-stable_290ct2020/src/REPLICA/tad.h
lammps-stable_290ct2020/src/REPLICA/temper.cpp
lammps-stable_290ct2020/src/REPLICA/temper.h
lammps-stable_290ct2020/src/REPLICA/verlet_split.cpp
lammps-stable_290ct2020/src/REPLICA/verlet_split.h
lammps-stable_290ct2020/src/RIGID/
lammps-stable_290ct2020/src/RIGID/compute_erotate_rigid.cpp
lammps-stable_290ct2020/src/RIGID/compute_erotate_rigid.h
lammps-stable_290ct2020/src/RIGID/compute_ke_rigid.cpp
lammps-stable_290ct2020/src/RIGID/compute_ke_rigid.h
lammps-stable_290ct2020/src/RIGID/compute_rigid_local.cpp
lammps-stable_290ct2020/src/RIGID/compute_rigid_local.h
lammps-stable_290ct2020/src/RIGID/fix_ehex.cpp
lammps-stable_290ct2020/src/RIGID/fix_ehex.h
lammps-stable_290ct2020/src/RIGID/fix_rattle.cpp
lammps-stable_290ct2020/src/RIGID/fix_rattle.h
lammps-stable_290ct2020/src/RIGID/fix_rigid.cpp
lammps-stable_290ct2020/src/RIGID/fix_rigid.h
lammps-stable_290ct2020/src/RIGID/fix_rigid_nh.cpp
lammps-stable_290ct2020/src/RIGID/fix_rigid_nh.h
lammps-stable_290ct2020/src/RIGID/fix_rigid_nh_small.cpp
lammps-stable_290ct2020/src/RIGID/fix_rigid_nh_small.h
lammps-stable_290ct2020/src/RIGID/fix_rigid_nph.cpp
lammps-stable_290ct2020/src/RIGID/fix_rigid_nph.h
```

lammps-stable\_290ct2020/src/RIGID/fix\_rigid\_nph\_small.cpp  
lammps-stable\_290ct2020/src/RIGID/fix\_rigid\_nph\_small.h  
lammps-stable\_290ct2020/src/RIGID/fix\_rigid\_npt.cpp  
lammps-stable\_290ct2020/src/RIGID/fix\_rigid\_npt.h  
lammps-stable\_290ct2020/src/RIGID/fix\_rigid\_npt\_small.cpp  
lammps-stable\_290ct2020/src/RIGID/fix\_rigid\_npt\_small.h  
lammps-stable\_290ct2020/src/RIGID/fix\_rigid\_nve.cpp  
lammps-stable\_290ct2020/src/RIGID/fix\_rigid\_nve.h  
lammps-stable\_290ct2020/src/RIGID/fix\_rigid\_nve\_small.cpp  
lammps-stable\_290ct2020/src/RIGID/fix\_rigid\_nve\_small.h  
lammps-stable\_290ct2020/src/RIGID/fix\_rigid\_nvt.cpp  
lammps-stable\_290ct2020/src/RIGID/fix\_rigid\_nvt.h  
lammps-stable\_290ct2020/src/RIGID/fix\_rigid\_nvt\_small.cpp  
lammps-stable\_290ct2020/src/RIGID/fix\_rigid\_nvt\_small.h  
lammps-stable\_290ct2020/src/RIGID/fix\_rigid\_small.cpp  
lammps-stable\_290ct2020/src/RIGID/fix\_rigid\_small.h  
lammps-stable\_290ct2020/src/RIGID/fix\_shake.cpp  
lammps-stable\_290ct2020/src/RIGID/fix\_shake.h  
lammps-stable\_290ct2020/src/RIGID/rigid\_const.h  
lammps-stable\_290ct2020/src/SHOCK/  
lammps-stable\_290ct2020/src/SHOCK/fix\_append\_atoms.cpp  
lammps-stable\_290ct2020/src/SHOCK/fix\_append\_atoms.h  
lammps-stable\_290ct2020/src/SHOCK/fix\_msst.cpp  
lammps-stable\_290ct2020/src/SHOCK/fix\_msst.h  
lammps-stable\_290ct2020/src/SHOCK/fix\_nphug.cpp  
lammps-stable\_290ct2020/src/SHOCK/fix\_nphug.h  
lammps-stable\_290ct2020/src/SHOCK/fix\_wall\_piston.cpp  
lammps-stable\_290ct2020/src/SHOCK/fix\_wall\_piston.h  
lammps-stable\_290ct2020/src/SNAP/  
lammps-stable\_290ct2020/src/SNAP/compute\_sna\_atom.cpp  
lammps-stable\_290ct2020/src/SNAP/compute\_sna\_atom.h  
lammps-stable\_290ct2020/src/SNAP/compute\_snad\_atom.cpp  
lammps-stable\_290ct2020/src/SNAP/compute\_snad\_atom.h  
lammps-stable\_290ct2020/src/SNAP/compute\_snap.cpp  
lammps-stable\_290ct2020/src/SNAP/compute\_snap.h  
lammps-stable\_290ct2020/src/SNAP/compute\_snav\_atom.cpp  
lammps-stable\_290ct2020/src/SNAP/compute\_snav\_atom.h  
lammps-stable\_290ct2020/src/SNAP/pair\_snap.cpp  
lammps-stable\_290ct2020/src/SNAP/pair\_snap.h  
lammps-stable\_290ct2020/src/SNAP/sna.cpp  
lammps-stable\_290ct2020/src/SNAP/sna.h  
lammps-stable\_290ct2020/src/SPIN/  
lammps-stable\_290ct2020/src/SPIN/README  
lammps-stable\_290ct2020/src/SPIN/atom\_vec\_spin.cpp  
lammps-stable\_290ct2020/src/SPIN/atom\_vec\_spin.h  
lammps-stable\_290ct2020/src/SPIN/compute\_spin.cpp  
lammps-stable\_290ct2020/src/SPIN/compute\_spin.h  
lammps-stable\_290ct2020/src/SPIN/fix\_langevin\_spin.cpp  
lammps-stable\_290ct2020/src/SPIN/fix\_langevin\_spin.h  
lammps-stable\_290ct2020/src/SPIN/fix\_neb\_spin.cpp  
lammps-stable\_290ct2020/src/SPIN/fix\_neb\_spin.h  
lammps-stable\_290ct2020/src/SPIN/fix\_nve\_spin.cpp  
lammps-stable\_290ct2020/src/SPIN/fix\_nve\_spin.h  
lammps-stable\_290ct2020/src/SPIN/fix\_precession\_spin.cpp  
lammps-stable\_290ct2020/src/SPIN/fix\_precession\_spin.h  
lammps-stable\_290ct2020/src/SPIN/fix\_setforce\_spin.cpp  
lammps-stable\_290ct2020/src/SPIN/fix\_setforce\_spin.h  
lammps-stable\_290ct2020/src/SPIN/min\_spin.cpp  
lammps-stable\_290ct2020/src/SPIN/min\_spin.h  
lammps-stable\_290ct2020/src/SPIN/min\_spin\_cg.cpp

```
lammps-stable_290ct2020/src/SPIN/min_spin_cg.h
lammps-stable_290ct2020/src/SPIN/min_spin_lbfgs.cpp
lammps-stable_290ct2020/src/SPIN/min_spin_lbfgs.h
lammps-stable_290ct2020/src/SPIN/neb_spin.cpp
lammps-stable_290ct2020/src/SPIN/neb_spin.h
lammps-stable_290ct2020/src/SPIN/pair_spin.cpp
lammps-stable_290ct2020/src/SPIN/pair_spin.h
lammps-stable_290ct2020/src/SPIN/pair_spin_dipole_cut.cpp
lammps-stable_290ct2020/src/SPIN/pair_spin_dipole_cut.h
lammps-stable_290ct2020/src/SPIN/pair_spin_dipole_long.cpp
lammps-stable_290ct2020/src/SPIN/pair_spin_dipole_long.h
lammps-stable_290ct2020/src/SPIN/pair_spin_dmi.cpp
lammps-stable_290ct2020/src/SPIN/pair_spin_dmi.h
lammps-stable_290ct2020/src/SPIN/pair_spin_exchange.cpp
lammps-stable_290ct2020/src/SPIN/pair_spin_exchange.h
lammps-stable_290ct2020/src/SPIN/pair_spin_magelec.cpp
lammps-stable_290ct2020/src/SPIN/pair_spin_magelec.h
lammps-stable_290ct2020/src/SPIN/pair_spin_neel.cpp
lammps-stable_290ct2020/src/SPIN/pair_spin_neel.h
lammps-stable_290ct2020/src/SRD/
lammps-stable_290ct2020/src/SRD/fix_srd.cpp
lammps-stable_290ct2020/src/SRD/fix_srd.h
lammps-stable_290ct2020/src/SRD/fix_wall_srd.cpp
lammps-stable_290ct2020/src/SRD/fix_wall_srd.h
lammps-stable_290ct2020/src/STUBS/
lammps-stable_290ct2020/src/STUBS/Makefile
lammps-stable_290ct2020/src/STUBS/Makefile.mingw32-cross
lammps-stable_290ct2020/src/STUBS/Makefile.mingw64-cross
lammps-stable_290ct2020/src/STUBS/mpi.c
lammps-stable_290ct2020/src/STUBS/mpi.h
lammps-stable_290ct2020/src/USER-ADIOS/
lammps-stable_290ct2020/src/USER-ADIOS/Install.sh
lammps-stable_290ct2020/src/USER-ADIOS/README
lammps-stable_290ct2020/src/USER-ADIOS/dump_atom_adios.cpp
lammps-stable_290ct2020/src/USER-ADIOS/dump_atom_adios.h
lammps-stable_290ct2020/src/USER-ADIOS/dump_custom_adios.cpp
lammps-stable_290ct2020/src/USER-ADIOS/dump_custom_adios.h
lammps-stable_290ct2020/src/USER-ADIOS/reader_adios.cpp
lammps-stable_290ct2020/src/USER-ADIOS/reader_adios.h
lammps-stable_290ct2020/src/USER-ATC/
lammps-stable_290ct2020/src/USER-ATC/Install.sh
lammps-stable_290ct2020/src/USER-ATC/README
lammps-stable_290ct2020/src/USER-ATC/fix_atc.cpp
lammps-stable_290ct2020/src/USER-ATC/fix_atc.h
lammps-stable_290ct2020/src/USER-AWPMO/
lammps-stable_290ct2020/src/USER-AWPMO/Install.sh
lammps-stable_290ct2020/src/USER-AWPMO/README
lammps-stable_290ct2020/src/USER-AWPMO/atom_vec_wavepacket.cpp
lammps-stable_290ct2020/src/USER-AWPMO/atom_vec_wavepacket.h
lammps-stable_290ct2020/src/USER-AWPMO/fix_nve_awpmd.cpp
lammps-stable_290ct2020/src/USER-AWPMO/fix_nve_awpmd.h
lammps-stable_290ct2020/src/USER-AWPMO/pair_awpmd_cut.cpp
lammps-stable_290ct2020/src/USER-AWPMO/pair_awpmd_cut.h
lammps-stable_290ct2020/src/USER-BOCS/
lammps-stable_290ct2020/src/USER-BOCS/README
lammps-stable_290ct2020/src/USER-BOCS/compute_pressure_bocs.cpp
lammps-stable_290ct2020/src/USER-BOCS/compute_pressure_bocs.h
lammps-stable_290ct2020/src/USER-BOCS/fix_bocs.cpp
lammps-stable_290ct2020/src/USER-BOCS/fix_bocs.h
lammps-stable_290ct2020/src/USER-CGDNA/
```

```
lammps-stable_290ct2020/src/USER-CGDNA/Install.sh
lammps-stable_290ct2020/src/USER-CGDNA/README.md
lammps-stable_290ct2020/src/USER-CGDNA/bond_oxdna2_fene.cpp
lammps-stable_290ct2020/src/USER-CGDNA/bond_oxdna2_fene.h
lammps-stable_290ct2020/src/USER-CGDNA/bond_oxdna_fene.cpp
lammps-stable_290ct2020/src/USER-CGDNA/bond_oxdna_fene.h
lammps-stable_290ct2020/src/USER-CGDNA/bond_oxrna2_fene.cpp
lammps-stable_290ct2020/src/USER-CGDNA/bond_oxrna2_fene.h
lammps-stable_290ct2020/src/USER-CGDNA/fix_nve_dot.cpp
lammps-stable_290ct2020/src/USER-CGDNA/fix_nve_dot.h
lammps-stable_290ct2020/src/USER-CGDNA/fix_nve_dotc_langevin.cpp
lammps-stable_290ct2020/src/USER-CGDNA/fix_nve_dotc_langevin.h
lammps-stable_290ct2020/src/USER-CGDNA/mf_oxdna.h
lammps-stable_290ct2020/src/USER-CGDNA/pair_oxdna2_coaxstk.cpp
lammps-stable_290ct2020/src/USER-CGDNA/pair_oxdna2_coaxstk.h
lammps-stable_290ct2020/src/USER-CGDNA/pair_oxdna2_dh.cpp
lammps-stable_290ct2020/src/USER-CGDNA/pair_oxdna2_dh.h
lammps-stable_290ct2020/src/USER-CGDNA/pair_oxdna2_excw.cpp
lammps-stable_290ct2020/src/USER-CGDNA/pair_oxdna2_excw.h
lammps-stable_290ct2020/src/USER-CGDNA/pair_oxdna_coaxstk.cpp
lammps-stable_290ct2020/src/USER-CGDNA/pair_oxdna_coaxstk.h
lammps-stable_290ct2020/src/USER-CGDNA/pair_oxdna_excw.cpp
lammps-stable_290ct2020/src/USER-CGDNA/pair_oxdna_excw.h
lammps-stable_290ct2020/src/USER-CGDNA/pair_oxdna_hbond.cpp
lammps-stable_290ct2020/src/USER-CGDNA/pair_oxdna_hbond.h
lammps-stable_290ct2020/src/USER-CGDNA/pair_oxdna_stk.cpp
lammps-stable_290ct2020/src/USER-CGDNA/pair_oxdna_stk.h
lammps-stable_290ct2020/src/USER-CGDNA/pair_oxdna_xstk.cpp
lammps-stable_290ct2020/src/USER-CGDNA/pair_oxdna_xstk.h
lammps-stable_290ct2020/src/USER-CGDNA/pair_oxrna2_dh.cpp
lammps-stable_290ct2020/src/USER-CGDNA/pair_oxrna2_dh.h
lammps-stable_290ct2020/src/USER-CGDNA/pair_oxrna2_excw.cpp
lammps-stable_290ct2020/src/USER-CGDNA/pair_oxrna2_excw.h
lammps-stable_290ct2020/src/USER-CGDNA/pair_oxrna2_hbond.cpp
lammps-stable_290ct2020/src/USER-CGDNA/pair_oxrna2_hbond.h
lammps-stable_290ct2020/src/USER-CGDNA/pair_oxrna2_stk.cpp
lammps-stable_290ct2020/src/USER-CGDNA/pair_oxrna2_stk.h
lammps-stable_290ct2020/src/USER-CGDNA/pair_oxrna2_xstk.cpp
lammps-stable_290ct2020/src/USER-CGDNA/pair_oxrna2_xstk.h
lammps-stable_290ct2020/src/USER-CGSDK/
lammps-stable_290ct2020/src/USER-CGSDK/Install.sh
lammps-stable_290ct2020/src/USER-CGSDK/README
lammps-stable_290ct2020/src/USER-CGSDK/angle_sdk.cpp
lammps-stable_290ct2020/src/USER-CGSDK/angle_sdk.h
lammps-stable_290ct2020/src/USER-CGSDK/lj_sdk_common.h
lammps-stable_290ct2020/src/USER-CGSDK/pair_lj_sdk.cpp
lammps-stable_290ct2020/src/USER-CGSDK/pair_lj_sdk.h
lammps-stable_290ct2020/src/USER-CGSDK/pair_lj_sdk_coul_long.cpp
lammps-stable_290ct2020/src/USER-CGSDK/pair_lj_sdk_coul_long.h
lammps-stable_290ct2020/src/USER-CGSDK/pair_lj_sdk_coul_msm.cpp
lammps-stable_290ct2020/src/USER-CGSDK/pair_lj_sdk_coul_msm.h
lammps-stable_290ct2020/src/USER-COLVARS/
lammps-stable_290ct2020/src/USER-COLVARS/Install.sh
lammps-stable_290ct2020/src/USER-COLVARS/README
lammps-stable_290ct2020/src/USER-COLVARS/colvarproxy_lammps.cpp
lammps-stable_290ct2020/src/USER-COLVARS/colvarproxy_lammps.h
lammps-stable_290ct2020/src/USER-COLVARS/colvarproxy_lammps_version.h
lammps-stable_290ct2020/src/USER-COLVARS/fix_colvars.cpp
lammps-stable_290ct2020/src/USER-COLVARS/fix_colvars.h
lammps-stable_290ct2020/src/USER-COLVARS/group_ndx.cpp
```



```
lammps-stable_290ct2020/src/USER-COLVARS/group_ndx.h
lammps-stable_290ct2020/src/USER-COLVARS/ndx_group.cpp
lammps-stable_290ct2020/src/USER-COLVARS/ndx_group.h
lammps-stable_290ct2020/src/USER-DIFFRACTION/
lammps-stable_290ct2020/src/USER-DIFFRACTION/README
lammps-stable_290ct2020/src/USER-DIFFRACTION/compute_saed.cpp
lammps-stable_290ct2020/src/USER-DIFFRACTION/compute_saed.h
lammps-stable_290ct2020/src/USER-DIFFRACTION/compute_saed_consts.h
lammps-stable_290ct2020/src/USER-DIFFRACTION/compute_xrd.cpp
lammps-stable_290ct2020/src/USER-DIFFRACTION/compute_xrd.h
lammps-stable_290ct2020/src/USER-DIFFRACTION/compute_xrd_consts.h
lammps-stable_290ct2020/src/USER-DIFFRACTION/fix_saed_vtk.cpp
lammps-stable_290ct2020/src/USER-DIFFRACTION/fix_saed_vtk.h
lammps-stable_290ct2020/src/USER-DPD/
lammps-stable_290ct2020/src/USER-DPD/README
lammps-stable_290ct2020/src/USER-DPD/atom_vec_dpd.cpp
lammps-stable_290ct2020/src/USER-DPD/atom_vec_dpd.h
lammps-stable_290ct2020/src/USER-DPD/compute_dpd.cpp
lammps-stable_290ct2020/src/USER-DPD/compute_dpd.h
lammps-stable_290ct2020/src/USER-DPD/compute_dpd_atom.cpp
lammps-stable_290ct2020/src/USER-DPD/compute_dpd_atom.h
lammps-stable_290ct2020/src/USER-DPD/fix_dpd_energy.cpp
lammps-stable_290ct2020/src/USER-DPD/fix_dpd_energy.h
lammps-stable_290ct2020/src/USER-DPD/fix_eos_cv.cpp
lammps-stable_290ct2020/src/USER-DPD/fix_eos_cv.h
lammps-stable_290ct2020/src/USER-DPD/fix_eos_table.cpp
lammps-stable_290ct2020/src/USER-DPD/fix_eos_table.h
lammps-stable_290ct2020/src/USER-DPD/fix_eos_table_rx.cpp
lammps-stable_290ct2020/src/USER-DPD/fix_eos_table_rx.h
lammps-stable_290ct2020/src/USER-DPD/fix_rx.cpp
lammps-stable_290ct2020/src/USER-DPD/fix_rx.h
lammps-stable_290ct2020/src/USER-DPD/fix_shardlow.cpp
lammps-stable_290ct2020/src/USER-DPD/fix_shardlow.h
lammps-stable_290ct2020/src/USER-DPD/nbin_ssa.cpp
lammps-stable_290ct2020/src/USER-DPD/nbin_ssa.h
lammps-stable_290ct2020/src/USER-DPD/npair_half_bin_newton_ssa.cpp
lammps-stable_290ct2020/src/USER-DPD/npair_half_bin_newton_ssa.h
lammps-stable_290ct2020/src/USER-DPD/nstencil_half_bin_2d_newton_ssa.cpp
lammps-stable_290ct2020/src/USER-DPD/nstencil_half_bin_2d_newton_ssa.h
lammps-stable_290ct2020/src/USER-DPD/nstencil_half_bin_3d_newton_ssa.cpp
lammps-stable_290ct2020/src/USER-DPD/nstencil_half_bin_3d_newton_ssa.h
lammps-stable_290ct2020/src/USER-DPD/nstencil_ssa.h
lammps-stable_290ct2020/src/USER-DPD/pair_dpd_fdt.cpp
lammps-stable_290ct2020/src/USER-DPD/pair_dpd_fdt.h
lammps-stable_290ct2020/src/USER-DPD/pair_dpd_fdt_energy.cpp
lammps-stable_290ct2020/src/USER-DPD/pair_dpd_fdt_energy.h
lammps-stable_290ct2020/src/USER-DPD/pair_exp6_rx.cpp
lammps-stable_290ct2020/src/USER-DPD/pair_exp6_rx.h
lammps-stable_290ct2020/src/USER-DPD/pair_multi_lucy.cpp
lammps-stable_290ct2020/src/USER-DPD/pair_multi_lucy.h
lammps-stable_290ct2020/src/USER-DPD/pair_multi_lucy_rx.cpp
lammps-stable_290ct2020/src/USER-DPD/pair_multi_lucy_rx.h
lammps-stable_290ct2020/src/USER-DPD/pair_table_rx.cpp
lammps-stable_290ct2020/src/USER-DPD/pair_table_rx.h
lammps-stable_290ct2020/src/USER-DPD/random_external_state.h
lammps-stable_290ct2020/src/USER-DRUDE/
lammps-stable_290ct2020/src/USER-DRUDE/README
lammps-stable_290ct2020/src/USER-DRUDE/compute_temp_drude.cpp
lammps-stable_290ct2020/src/USER-DRUDE/compute_temp_drude.h
lammps-stable_290ct2020/src/USER-DRUDE/fix_drude.cpp
```

```
lammps-stable_290ct2020/src/USER-DRUDE/fix_drude.h
lammps-stable_290ct2020/src/USER-DRUDE/fix_drude_transform.cpp
lammps-stable_290ct2020/src/USER-DRUDE/fix_drude_transform.h
lammps-stable_290ct2020/src/USER-DRUDE/fix_langevin_drude.cpp
lammps-stable_290ct2020/src/USER-DRUDE/fix_langevin_drude.h
lammps-stable_290ct2020/src/USER-DRUDE/pair_coul_tt.cpp
lammps-stable_290ct2020/src/USER-DRUDE/pair_coul_tt.h
lammps-stable_290ct2020/src/USER-DRUDE/pair_lj_cut_thole_long.cpp
lammps-stable_290ct2020/src/USER-DRUDE/pair_lj_cut_thole_long.h
lammps-stable_290ct2020/src/USER-DRUDE/pair_thole.cpp
lammps-stable_290ct2020/src/USER-DRUDE/pair_thole.h
lammps-stable_290ct2020/src/USER-EFF/
lammps-stable_290ct2020/src/USER-EFF/README
lammps-stable_290ct2020/src/USER-EFF/atom_vec_electron.cpp
lammps-stable_290ct2020/src/USER-EFF/atom_vec_electron.h
lammps-stable_290ct2020/src/USER-EFF/compute_ke_atom_eff.cpp
lammps-stable_290ct2020/src/USER-EFF/compute_ke_atom_eff.h
lammps-stable_290ct2020/src/USER-EFF/compute_ke_eff.cpp
lammps-stable_290ct2020/src/USER-EFF/compute_ke_eff.h
lammps-stable_290ct2020/src/USER-EFF/compute_temp_deform_eff.cpp
lammps-stable_290ct2020/src/USER-EFF/compute_temp_deform_eff.h
lammps-stable_290ct2020/src/USER-EFF/compute_temp_eff.cpp
lammps-stable_290ct2020/src/USER-EFF/compute_temp_eff.h
lammps-stable_290ct2020/src/USER-EFF/compute_temp_region_eff.cpp
lammps-stable_290ct2020/src/USER-EFF/compute_temp_region_eff.h
lammps-stable_290ct2020/src/USER-EFF/fix_langevin_eff.cpp
lammps-stable_290ct2020/src/USER-EFF/fix_langevin_eff.h
lammps-stable_290ct2020/src/USER-EFF/fix_nh_eff.cpp
lammps-stable_290ct2020/src/USER-EFF/fix_nh_eff.h
lammps-stable_290ct2020/src/USER-EFF/fix_nph_eff.cpp
lammps-stable_290ct2020/src/USER-EFF/fix_nph_eff.h
lammps-stable_290ct2020/src/USER-EFF/fix_npt_eff.cpp
lammps-stable_290ct2020/src/USER-EFF/fix_npt_eff.h
lammps-stable_290ct2020/src/USER-EFF/fix_nve_eff.cpp
lammps-stable_290ct2020/src/USER-EFF/fix_nve_eff.h
lammps-stable_290ct2020/src/USER-EFF/fix_nvt_eff.cpp
lammps-stable_290ct2020/src/USER-EFF/fix_nvt_eff.h
lammps-stable_290ct2020/src/USER-EFF/fix_nvt_sllod_eff.cpp
lammps-stable_290ct2020/src/USER-EFF/fix_nvt_sllod_eff.h
lammps-stable_290ct2020/src/USER-EFF/fix_temp_rescale_eff.cpp
lammps-stable_290ct2020/src/USER-EFF/fix_temp_rescale_eff.h
lammps-stable_290ct2020/src/USER-EFF/pair_eff_cut.cpp
lammps-stable_290ct2020/src/USER-EFF/pair_eff_cut.h
lammps-stable_290ct2020/src/USER-EFF/pair_eff_inline.h
lammps-stable_290ct2020/src/USER-FEP/
lammps-stable_290ct2020/src/USER-FEP/Install.sh
lammps-stable_290ct2020/src/USER-FEP/README
lammps-stable_290ct2020/src/USER-FEP/compute_fep.cpp
lammps-stable_290ct2020/src/USER-FEP/compute_fep.h
lammps-stable_290ct2020/src/USER-FEP/fix_adapt_fep.cpp
lammps-stable_290ct2020/src/USER-FEP/fix_adapt_fep.h
lammps-stable_290ct2020/src/USER-FEP/pair_coul_cut_soft.cpp
lammps-stable_290ct2020/src/USER-FEP/pair_coul_cut_soft.h
lammps-stable_290ct2020/src/USER-FEP/pair_coul_long_soft.cpp
lammps-stable_290ct2020/src/USER-FEP/pair_coul_long_soft.h
lammps-stable_290ct2020/src/USER-FEP/pair_lj_charmm_coul_long_soft.cpp
lammps-stable_290ct2020/src/USER-FEP/pair_lj_charmm_coul_long_soft.h
lammps-stable_290ct2020/src/USER-FEP/pair_lj_class2_coul_cut_soft.cpp
lammps-stable_290ct2020/src/USER-FEP/pair_lj_class2_coul_cut_soft.h
lammps-stable_290ct2020/src/USER-FEP/pair_lj_class2_coul_long_soft.cpp
```

```
lammps-stable_290ct2020/src/USER-FEP/pair_lj_class2_coul_long_soft.h
lammps-stable_290ct2020/src/USER-FEP/pair_lj_class2_soft.cpp
lammps-stable_290ct2020/src/USER-FEP/pair_lj_class2_soft.h
lammps-stable_290ct2020/src/USER-FEP/pair_lj_cut_coul_cut_soft.cpp
lammps-stable_290ct2020/src/USER-FEP/pair_lj_cut_coul_cut_soft.h
lammps-stable_290ct2020/src/USER-FEP/pair_lj_cut_coul_long_soft.cpp
lammps-stable_290ct2020/src/USER-FEP/pair_lj_cut_coul_long_soft.h
lammps-stable_290ct2020/src/USER-FEP/pair_lj_cut_soft.cpp
lammps-stable_290ct2020/src/USER-FEP/pair_lj_cut_soft.h
lammps-stable_290ct2020/src/USER-FEP/pair_lj_cut_tip4p_long_soft.cpp
lammps-stable_290ct2020/src/USER-FEP/pair_lj_cut_tip4p_long_soft.h
lammps-stable_290ct2020/src/USER-FEP/pair_morse_soft.cpp
lammps-stable_290ct2020/src/USER-FEP/pair_morse_soft.h
lammps-stable_290ct2020/src/USER-FEP/pair_tip4p_long_soft.cpp
lammps-stable_290ct2020/src/USER-FEP/pair_tip4p_long_soft.h
lammps-stable_290ct2020/src/USER-H5MD/
lammps-stable_290ct2020/src/USER-H5MD/Install.sh
lammps-stable_290ct2020/src/USER-H5MD/README
lammps-stable_290ct2020/src/USER-H5MD/dump_h5md.cpp
lammps-stable_290ct2020/src/USER-H5MD/dump_h5md.h
lammps-stable_290ct2020/src/USER-INTEL/
lammps-stable_290ct2020/src/USER-INTEL/Install.sh
lammps-stable_290ct2020/src/USER-INTEL/README
lammps-stable_290ct2020/src/USER-INTEL/TEST/
lammps-stable_290ct2020/src/USER-INTEL/TEST/README
lammps-stable_290ct2020/src/USER-INTEL/TEST/in.intel.airebo
lammps-stable_290ct2020/src/USER-INTEL/TEST/in.intel.dpd
lammps-stable_290ct2020/src/USER-INTEL/TEST/in.intel.eam
lammps-stable_290ct2020/src/USER-INTEL/TEST/in.intel.lc
lammps-stable_290ct2020/src/USER-INTEL/TEST/in.intel.lj
lammps-stable_290ct2020/src/USER-INTEL/TEST/in.intel.rhodo
lammps-stable_290ct2020/src/USER-INTEL/TEST/in.intel.sw
lammps-stable_290ct2020/src/USER-INTEL/TEST/in.intel.tersoff
lammps-stable_290ct2020/src/USER-INTEL/TEST/in.intel.water
lammps-stable_290ct2020/src/USER-INTEL/TEST/in.lc_generate_restart
lammps-stable_290ct2020/src/USER-INTEL/TEST/mW.sw
lammps-stable_290ct2020/src/USER-INTEL/TEST/mW_32k_cube.data
lammps-stable_290ct2020/src/USER-INTEL/TEST/run_benchmarks.sh
lammps-stable_290ct2020/src/USER-INTEL/angle_charmm_intel.cpp
lammps-stable_290ct2020/src/USER-INTEL/angle_charmm_intel.h
lammps-stable_290ct2020/src/USER-INTEL/angle_harmonic_intel.cpp
lammps-stable_290ct2020/src/USER-INTEL/angle_harmonic_intel.h
lammps-stable_290ct2020/src/USER-INTEL/bond_fene_intel.cpp
lammps-stable_290ct2020/src/USER-INTEL/bond_fene_intel.h
lammps-stable_290ct2020/src/USER-INTEL/bond_harmonic_intel.cpp
lammps-stable_290ct2020/src/USER-INTEL/bond_harmonic_intel.h
lammps-stable_290ct2020/src/USER-INTEL/dihedral_charmm_intel.cpp
lammps-stable_290ct2020/src/USER-INTEL/dihedral_charmm_intel.h
lammps-stable_290ct2020/src/USER-INTEL/dihedral_fourier_intel.cpp
lammps-stable_290ct2020/src/USER-INTEL/dihedral_fourier_intel.h
lammps-stable_290ct2020/src/USER-INTEL/dihedral_harmonic_intel.cpp
lammps-stable_290ct2020/src/USER-INTEL/dihedral_harmonic_intel.h
lammps-stable_290ct2020/src/USER-INTEL/dihedral_opls_intel.cpp
lammps-stable_290ct2020/src/USER-INTEL/dihedral_opls_intel.h
lammps-stable_290ct2020/src/USER-INTEL/fix_intel.cpp
lammps-stable_290ct2020/src/USER-INTEL/fix_intel.h
lammps-stable_290ct2020/src/USER-INTEL/fix_nh_intel.cpp
lammps-stable_290ct2020/src/USER-INTEL/fix_nh_intel.h
lammps-stable_290ct2020/src/USER-INTEL/fix_npt_intel.cpp
lammps-stable_290ct2020/src/USER-INTEL/fix_npt_intel.h
```

lammps-stable\_290ct2020/src/USER-INTEL/fix\_nve\_asphere\_intel.cpp  
lammps-stable\_290ct2020/src/USER-INTEL/fix\_nve\_asphere\_intel.h  
lammps-stable\_290ct2020/src/USER-INTEL/fix\_nve\_intel.cpp  
lammps-stable\_290ct2020/src/USER-INTEL/fix\_nve\_intel.h  
lammps-stable\_290ct2020/src/USER-INTEL/fix\_nvt\_intel.cpp  
lammps-stable\_290ct2020/src/USER-INTEL/fix\_nvt\_intel.h  
lammps-stable\_290ct2020/src/USER-INTEL/fix\_nvt\_sllod\_intel.cpp  
lammps-stable\_290ct2020/src/USER-INTEL/fix\_nvt\_sllod\_intel.h  
lammps-stable\_290ct2020/src/USER-INTEL/improper\_cvff\_intel.cpp  
lammps-stable\_290ct2020/src/USER-INTEL/improper\_cvff\_intel.h  
lammps-stable\_290ct2020/src/USER-INTEL/improper\_harmonic\_intel.cpp  
lammps-stable\_290ct2020/src/USER-INTEL/improper\_harmonic\_intel.h  
lammps-stable\_290ct2020/src/USER-INTEL/intel\_buffers.cpp  
lammps-stable\_290ct2020/src/USER-INTEL/intel\_buffers.h  
lammps-stable\_290ct2020/src/USER-INTEL/intel\_intrinsics.h  
lammps-stable\_290ct2020/src/USER-INTEL/intel\_intrinsics\_airebo.h  
lammps-stable\_290ct2020/src/USER-INTEL/intel\_preprocess.h  
lammps-stable\_290ct2020/src/USER-INTEL/intel\_simd.h  
lammps-stable\_290ct2020/src/USER-INTEL/math\_extra\_intel.h  
lammps-stable\_290ct2020/src/USER-INTEL/nbin\_intel.cpp  
lammps-stable\_290ct2020/src/USER-INTEL/nbin\_intel.h  
lammps-stable\_290ct2020/src/USER-INTEL/npair\_full\_bin\_ghost\_intel.cpp  
lammps-stable\_290ct2020/src/USER-INTEL/npair\_full\_bin\_ghost\_intel.h  
lammps-stable\_290ct2020/src/USER-INTEL/npair\_full\_bin\_intel.cpp  
lammps-stable\_290ct2020/src/USER-INTEL/npair\_full\_bin\_intel.h  
lammps-stable\_290ct2020/src/USER-INTEL/npair\_half\_bin\_newton\_intel.cpp  
lammps-stable\_290ct2020/src/USER-INTEL/npair\_half\_bin\_newton\_intel.h  
lammps-stable\_290ct2020/src/USER-INTEL/npair\_half\_bin\_newton\_tri\_intel.cpp  
lammps-stable\_290ct2020/src/USER-INTEL/npair\_half\_bin\_newton\_tri\_intel.h  
lammps-stable\_290ct2020/src/USER-INTEL/npair\_halffull\_newtoff\_intel.h  
lammps-stable\_290ct2020/src/USER-INTEL/npair\_halffull\_newton\_intel.cpp  
lammps-stable\_290ct2020/src/USER-INTEL/npair\_halffull\_newton\_intel.h  
lammps-stable\_290ct2020/src/USER-INTEL/npair\_intel.cpp  
lammps-stable\_290ct2020/src/USER-INTEL/npair\_intel.h  
lammps-stable\_290ct2020/src/USER-INTEL/npair\_skip\_intel.cpp  
lammps-stable\_290ct2020/src/USER-INTEL/npair\_skip\_intel.h  
lammps-stable\_290ct2020/src/USER-INTEL/pair\_airebo\_intel.cpp  
lammps-stable\_290ct2020/src/USER-INTEL/pair\_airebo\_intel.h  
lammps-stable\_290ct2020/src/USER-INTEL/pair\_airebo\_morse\_intel.cpp  
lammps-stable\_290ct2020/src/USER-INTEL/pair\_airebo\_morse\_intel.h  
lammps-stable\_290ct2020/src/USER-INTEL/pair\_buck\_coul\_cut\_intel.cpp  
lammps-stable\_290ct2020/src/USER-INTEL/pair\_buck\_coul\_cut\_intel.h  
lammps-stable\_290ct2020/src/USER-INTEL/pair\_buck\_coul\_long\_intel.cpp  
lammps-stable\_290ct2020/src/USER-INTEL/pair\_buck\_coul\_long\_intel.h  
lammps-stable\_290ct2020/src/USER-INTEL/pair\_buck\_intel.cpp  
lammps-stable\_290ct2020/src/USER-INTEL/pair\_buck\_intel.h  
lammps-stable\_290ct2020/src/USER-INTEL/pair\_dpd\_intel.cpp  
lammps-stable\_290ct2020/src/USER-INTEL/pair\_dpd\_intel.h  
lammps-stable\_290ct2020/src/USER-INTEL/pair\_eam\_alloy\_intel.cpp  
lammps-stable\_290ct2020/src/USER-INTEL/pair\_eam\_alloy\_intel.h  
lammps-stable\_290ct2020/src/USER-INTEL/pair\_eam\_fs\_intel.cpp  
lammps-stable\_290ct2020/src/USER-INTEL/pair\_eam\_fs\_intel.h  
lammps-stable\_290ct2020/src/USER-INTEL/pair\_eam\_intel.cpp  
lammps-stable\_290ct2020/src/USER-INTEL/pair\_eam\_intel.h  
lammps-stable\_290ct2020/src/USER-INTEL/pair\_gayberne\_intel.cpp  
lammps-stable\_290ct2020/src/USER-INTEL/pair\_gayberne\_intel.h  
lammps-stable\_290ct2020/src/USER-INTEL/pair\_lj\_charmm\_coul\_charmm\_intel.cpp  
lammps-stable\_290ct2020/src/USER-INTEL/pair\_lj\_charmm\_coul\_charmm\_intel.h  
lammps-stable\_290ct2020/src/USER-INTEL/pair\_lj\_charmm\_coul\_long\_intel.cpp  
lammps-stable\_290ct2020/src/USER-INTEL/pair\_lj\_charmm\_coul\_long\_intel.h

```
lammps-stable_290ct2020/src/USER-INTEL/pair_lj_cut_coul_long_intel.cpp
lammps-stable_290ct2020/src/USER-INTEL/pair_lj_cut_coul_long_intel.h
lammps-stable_290ct2020/src/USER-INTEL/pair_lj_cut_intel.cpp
lammps-stable_290ct2020/src/USER-INTEL/pair_lj_cut_intel.h
lammps-stable_290ct2020/src/USER-INTEL/pair_lj_long_coul_long_intel.cpp
lammps-stable_290ct2020/src/USER-INTEL/pair_lj_long_coul_long_intel.h
lammps-stable_290ct2020/src/USER-INTEL/pair_rebo_intel.cpp
lammps-stable_290ct2020/src/USER-INTEL/pair_rebo_intel.h
lammps-stable_290ct2020/src/USER-INTEL/pair_sw_intel.cpp
lammps-stable_290ct2020/src/USER-INTEL/pair_sw_intel.h
lammps-stable_290ct2020/src/USER-INTEL/pair_tersoff_intel.cpp
lammps-stable_290ct2020/src/USER-INTEL/pair_tersoff_intel.h
lammps-stable_290ct2020/src/USER-INTEL/pppm_disp_intel.cpp
lammps-stable_290ct2020/src/USER-INTEL/pppm_disp_intel.h
lammps-stable_290ct2020/src/USER-INTEL/pppm_intel.cpp
lammps-stable_290ct2020/src/USER-INTEL/pppm_intel.h
lammps-stable_290ct2020/src/USER-INTEL/verlet_lrt_intel.cpp
lammps-stable_290ct2020/src/USER-INTEL/verlet_lrt_intel.h
lammps-stable_290ct2020/src/USER-LB/
lammps-stable_290ct2020/src/USER-LB/README
lammps-stable_290ct2020/src/USER-LB/fix_lb_fluid.cpp
lammps-stable_290ct2020/src/USER-LB/fix_lb_fluid.h
lammps-stable_290ct2020/src/USER-LB/fix_lb_momentum.cpp
lammps-stable_290ct2020/src/USER-LB/fix_lb_momentum.h
lammps-stable_290ct2020/src/USER-LB/fix_lb_pc.cpp
lammps-stable_290ct2020/src/USER-LB/fix_lb_pc.h
lammps-stable_290ct2020/src/USER-LB/fix_lb_rigid_pc_sphere.cpp
lammps-stable_290ct2020/src/USER-LB/fix_lb_rigid_pc_sphere.h
lammps-stable_290ct2020/src/USER-LB/fix_lb_viscous.cpp
lammps-stable_290ct2020/src/USER-LB/fix_lb_viscous.h
lammps-stable_290ct2020/src/USER-MANIFOLD/
lammps-stable_290ct2020/src/USER-MANIFOLD/README
lammps-stable_290ct2020/src/USER-MANIFOLD/fix_manifoldforce.cpp
lammps-stable_290ct2020/src/USER-MANIFOLD/fix_manifoldforce.h
lammps-stable_290ct2020/src/USER-MANIFOLD/fix_nve_manifold_rattle.cpp
lammps-stable_290ct2020/src/USER-MANIFOLD/fix_nve_manifold_rattle.h
lammps-stable_290ct2020/src/USER-MANIFOLD/fix_nvt_manifold_rattle.cpp
lammps-stable_290ct2020/src/USER-MANIFOLD/fix_nvt_manifold_rattle.h
lammps-stable_290ct2020/src/USER-MANIFOLD/manifold.h
lammps-stable_290ct2020/src/USER-MANIFOLD/manifold_cylinder.cpp
lammps-stable_290ct2020/src/USER-MANIFOLD/manifold_cylinder.h
lammps-stable_290ct2020/src/USER-MANIFOLD/manifold_cylinder_dent.cpp
lammps-stable_290ct2020/src/USER-MANIFOLD/manifold_cylinder_dent.h
lammps-stable_290ct2020/src/USER-MANIFOLD/manifold_dumbbell.cpp
lammps-stable_290ct2020/src/USER-MANIFOLD/manifold_dumbbell.h
lammps-stable_290ct2020/src/USER-MANIFOLD/manifold_ellipsoid.cpp
lammps-stable_290ct2020/src/USER-MANIFOLD/manifold_ellipsoid.h
lammps-stable_290ct2020/src/USER-MANIFOLD/manifold_factory.cpp
lammps-stable_290ct2020/src/USER-MANIFOLD/manifold_factory.h
lammps-stable_290ct2020/src/USER-MANIFOLD/manifold_gaussian_bump.cpp
lammps-stable_290ct2020/src/USER-MANIFOLD/manifold_gaussian_bump.h
lammps-stable_290ct2020/src/USER-MANIFOLD/manifold_plane.cpp
lammps-stable_290ct2020/src/USER-MANIFOLD/manifold_plane.h
lammps-stable_290ct2020/src/USER-MANIFOLD/manifold_plane_wiggle.cpp
lammps-stable_290ct2020/src/USER-MANIFOLD/manifold_plane_wiggle.h
lammps-stable_290ct2020/src/USER-MANIFOLD/manifold_sphere.h
lammps-stable_290ct2020/src/USER-MANIFOLD/manifold_spine.cpp
lammps-stable_290ct2020/src/USER-MANIFOLD/manifold_spine.h
lammps-stable_290ct2020/src/USER-MANIFOLD/manifold_supersphere.h
lammps-stable_290ct2020/src/USER-MANIFOLD/manifold_thylakoid.cpp
```

```
lammps-stable_290ct2020/src/USER-MANIFOLD/manifold_thylakoid.h
lammps-stable_290ct2020/src/USER-MANIFOLD/manifold_thylakoid_shared.cpp
lammps-stable_290ct2020/src/USER-MANIFOLD/manifold_thylakoid_shared.h
lammps-stable_290ct2020/src/USER-MANIFOLD/manifold_torus.cpp
lammps-stable_290ct2020/src/USER-MANIFOLD/manifold_torus.h
lammps-stable_290ct2020/src/USER-MEAMC/
lammps-stable_290ct2020/src/USER-MEAMC/README
lammps-stable_290ct2020/src/USER-MEAMC/meam.h
lammps-stable_290ct2020/src/USER-MEAMC/meam_dens_final.cpp
lammps-stable_290ct2020/src/USER-MEAMC/meam_dens_init.cpp
lammps-stable_290ct2020/src/USER-MEAMC/meam_force.cpp
lammps-stable_290ct2020/src/USER-MEAMC/meam_funcs.cpp
lammps-stable_290ct2020/src/USER-MEAMC/meam_impl.cpp
lammps-stable_290ct2020/src/USER-MEAMC/meam_setup_done.cpp
lammps-stable_290ct2020/src/USER-MEAMC/meam_setup_global.cpp
lammps-stable_290ct2020/src/USER-MEAMC/meam_setup_param.cpp
lammps-stable_290ct2020/src/USER-MEAMC/pair_meamc.cpp
lammps-stable_290ct2020/src/USER-MEAMC/pair_meamc.h
lammps-stable_290ct2020/src/USER-MESODPD/
lammps-stable_290ct2020/src/USER-MESODPD/README
lammps-stable_290ct2020/src/USER-MESODPD/atom_vec_edpd.cpp
lammps-stable_290ct2020/src/USER-MESODPD/atom_vec_edpd.h
lammps-stable_290ct2020/src/USER-MESODPD/atom_vec_mdpd.cpp
lammps-stable_290ct2020/src/USER-MESODPD/atom_vec_mdpd.h
lammps-stable_290ct2020/src/USER-MESODPD/atom_vec_tdpd.cpp
lammps-stable_290ct2020/src/USER-MESODPD/atom_vec_tdpd.h
lammps-stable_290ct2020/src/USER-MESODPD/compute_edpd_temp_atom.cpp
lammps-stable_290ct2020/src/USER-MESODPD/compute_edpd_temp_atom.h
lammps-stable_290ct2020/src/USER-MESODPD/compute_tdpd_cc_atom.cpp
lammps-stable_290ct2020/src/USER-MESODPD/compute_tdpd_cc_atom.h
lammps-stable_290ct2020/src/USER-MESODPD/fix_edpd_source.cpp
lammps-stable_290ct2020/src/USER-MESODPD/fix_edpd_source.h
lammps-stable_290ct2020/src/USER-MESODPD/fix_mvv_dpd.cpp
lammps-stable_290ct2020/src/USER-MESODPD/fix_mvv_dpd.h
lammps-stable_290ct2020/src/USER-MESODPD/fix_mvv_edpd.cpp
lammps-stable_290ct2020/src/USER-MESODPD/fix_mvv_edpd.h
lammps-stable_290ct2020/src/USER-MESODPD/fix_mvv_tdpd.cpp
lammps-stable_290ct2020/src/USER-MESODPD/fix_mvv_tdpd.h
lammps-stable_290ct2020/src/USER-MESODPD/fix_tdpd_source.cpp
lammps-stable_290ct2020/src/USER-MESODPD/fix_tdpd_source.h
lammps-stable_290ct2020/src/USER-MESODPD/pair_edpd.cpp
lammps-stable_290ct2020/src/USER-MESODPD/pair_edpd.h
lammps-stable_290ct2020/src/USER-MESODPD/pair_mdpd.cpp
lammps-stable_290ct2020/src/USER-MESODPD/pair_mdpd.h
lammps-stable_290ct2020/src/USER-MESODPD/pair_mdpd_rhosum.cpp
lammps-stable_290ct2020/src/USER-MESODPD/pair_mdpd_rhosum.h
lammps-stable_290ct2020/src/USER-MESODPD/pair_tdpd.cpp
lammps-stable_290ct2020/src/USER-MESODPD/pair_tdpd.h
lammps-stable_290ct2020/src/USER-MESONT/
lammps-stable_290ct2020/src/USER-MESONT/Install.sh
lammps-stable_290ct2020/src/USER-MESONT/README
lammps-stable_290ct2020/src/USER-MESONT/atom_vec_mesont.cpp
lammps-stable_290ct2020/src/USER-MESONT/atom_vec_mesont.h
lammps-stable_290ct2020/src/USER-MESONT/compute_mesont.cpp
lammps-stable_290ct2020/src/USER-MESONT/compute_mesont.h
lammps-stable_290ct2020/src/USER-MESONT/export_mesont.h
lammps-stable_290ct2020/src/USER-MESONT/pair_mesocnt.cpp
lammps-stable_290ct2020/src/USER-MESONT/pair_mesocnt.h
lammps-stable_290ct2020/src/USER-MESONT/pair_mesont_tpm.cpp
lammps-stable_290ct2020/src/USER-MESONT/pair_mesont_tpm.h
```

```
lammps-stable_290ct2020/src/USER-MESONT/potentials.txt
lammps-stable_290ct2020/src/USER-MGPT/
lammps-stable_290ct2020/src/USER-MGPT/README
lammps-stable_290ct2020/src/USER-MGPT/mgpt_bgmul_7.c.h
lammps-stable_290ct2020/src/USER-MGPT/mgpt_linalg.cpp
lammps-stable_290ct2020/src/USER-MGPT/mgpt_linalg.h
lammps-stable_290ct2020/src/USER-MGPT/mgpt_mmul3_538.c.h
lammps-stable_290ct2020/src/USER-MGPT/mgpt_mmul3_748.c.h
lammps-stable_290ct2020/src/USER-MGPT/mgpt_mmul3d_526.c.h
lammps-stable_290ct2020/src/USER-MGPT/mgpt_mmul3d_744.c.h
lammps-stable_290ct2020/src/USER-MGPT/mgpt_mmul_bg_552.c.h
lammps-stable_290ct2020/src/USER-MGPT/mgpt_mmul_bg_722.c.h
lammps-stable_290ct2020/src/USER-MGPT/mgpt_mmul_bgq_n5_lda8_2x8.c.h
lammps-stable_290ct2020/src/USER-MGPT/mgpt_mmul_bgq_n7_lda8_4x8.c.h
lammps-stable_290ct2020/src/USER-MGPT/mgpt_readpot.cpp
lammps-stable_290ct2020/src/USER-MGPT/mgpt_readpot.h
lammps-stable_290ct2020/src/USER-MGPT/mgpt_splinetab.cpp
lammps-stable_290ct2020/src/USER-MGPT/mgpt_splinetab.h
lammps-stable_290ct2020/src/USER-MGPT/mgpt_ttr_5022.c.h
lammps-stable_290ct2020/src/USER-MGPT/mgpt_ttr_5042.c.h
lammps-stable_290ct2020/src/USER-MGPT/mgpt_ttr_5123.c.h
lammps-stable_290ct2020/src/USER-MGPT/mgpt_ttr_5141.c.h
lammps-stable_290ct2020/src/USER-MGPT/mgpt_ttr_7022.c.h
lammps-stable_290ct2020/src/USER-MGPT/mgpt_ttr_7042.c.h
lammps-stable_290ct2020/src/USER-MGPT/mgpt_ttr_7123.c.h
lammps-stable_290ct2020/src/USER-MGPT/mgpt_ttr_7141.c.h
lammps-stable_290ct2020/src/USER-MGPT/pair_mgpt.cpp
lammps-stable_290ct2020/src/USER-MGPT/pair_mgpt.h
lammps-stable_290ct2020/src/USER-MISC/
lammps-stable_290ct2020/src/USER-MISC/README
lammps-stable_290ct2020/src/USER-MISC/angle_cosine_shift.cpp
lammps-stable_290ct2020/src/USER-MISC/angle_cosine_shift.h
lammps-stable_290ct2020/src/USER-MISC/angle_cosine_shift_exp.cpp
lammps-stable_290ct2020/src/USER-MISC/angle_cosine_shift_exp.h
lammps-stable_290ct2020/src/USER-MISC/angle_dipole.cpp
lammps-stable_290ct2020/src/USER-MISC/angle_dipole.h
lammps-stable_290ct2020/src/USER-MISC/angle_fourier.cpp
lammps-stable_290ct2020/src/USER-MISC/angle_fourier.h
lammps-stable_290ct2020/src/USER-MISC/angle_fourier_simple.cpp
lammps-stable_290ct2020/src/USER-MISC/angle_fourier_simple.h
lammps-stable_290ct2020/src/USER-MISC/angle_quartic.cpp
lammps-stable_290ct2020/src/USER-MISC/angle_quartic.h
lammps-stable_290ct2020/src/USER-MISC/bond_harmonic_shift.cpp
lammps-stable_290ct2020/src/USER-MISC/bond_harmonic_shift.h
lammps-stable_290ct2020/src/USER-MISC/bond_harmonic_shift_cut.cpp
lammps-stable_290ct2020/src/USER-MISC/bond_harmonic_shift_cut.h
lammps-stable_290ct2020/src/USER-MISC/bond_special.cpp
lammps-stable_290ct2020/src/USER-MISC/bond_special.h
lammps-stable_290ct2020/src/USER-MISC/compute_ackland_atom.cpp
lammps-stable_290ct2020/src/USER-MISC/compute_ackland_atom.h
lammps-stable_290ct2020/src/USER-MISC/compute_basal_atom.cpp
lammps-stable_290ct2020/src/USER-MISC/compute_basal_atom.h
lammps-stable_290ct2020/src/USER-MISC/compute_cnp_atom.cpp
lammps-stable_290ct2020/src/USER-MISC/compute_cnp_atom.h
lammps-stable_290ct2020/src/USER-MISC/compute_entropy_atom.cpp
lammps-stable_290ct2020/src/USER-MISC/compute_entropy_atom.h
lammps-stable_290ct2020/src/USER-MISC/compute_gyration_shape.cpp
lammps-stable_290ct2020/src/USER-MISC/compute_gyration_shape.h
lammps-stable_290ct2020/src/USER-MISC/compute_gyration_shape_chunk.cpp
lammps-stable_290ct2020/src/USER-MISC/compute_gyration_shape_chunk.h
```

lammps-stable\_290ct2020/src/USER-MISC/compute\_hma.cpp  
lammps-stable\_290ct2020/src/USER-MISC/compute\_hma.h  
lammps-stable\_290ct2020/src/USER-MISC/compute\_momentum.cpp  
lammps-stable\_290ct2020/src/USER-MISC/compute\_momentum.h  
lammps-stable\_290ct2020/src/USER-MISC/compute\_pressure\_cylinder.cpp  
lammps-stable\_290ct2020/src/USER-MISC/compute\_pressure\_cylinder.h  
lammps-stable\_290ct2020/src/USER-MISC/compute\_pressure\_grem.cpp  
lammps-stable\_290ct2020/src/USER-MISC/compute\_pressure\_grem.h  
lammps-stable\_290ct2020/src/USER-MISC/compute\_stress\_mop.cpp  
lammps-stable\_290ct2020/src/USER-MISC/compute\_stress\_mop.h  
lammps-stable\_290ct2020/src/USER-MISC/compute\_stress\_mop\_profile.cpp  
lammps-stable\_290ct2020/src/USER-MISC/compute\_stress\_mop\_profile.h  
lammps-stable\_290ct2020/src/USER-MISC/compute\_temp\_rotate.cpp  
lammps-stable\_290ct2020/src/USER-MISC/compute\_temp\_rotate.h  
lammps-stable\_290ct2020/src/USER-MISC/compute\_viscosity\_cos.cpp  
lammps-stable\_290ct2020/src/USER-MISC/compute\_viscosity\_cos.h  
lammps-stable\_290ct2020/src/USER-MISC/dihedral\_cosine\_shift\_exp.cpp  
lammps-stable\_290ct2020/src/USER-MISC/dihedral\_cosine\_shift\_exp.h  
lammps-stable\_290ct2020/src/USER-MISC/dihedral\_fourier.cpp  
lammps-stable\_290ct2020/src/USER-MISC/dihedral\_fourier.h  
lammps-stable\_290ct2020/src/USER-MISC/dihedral\_nharmonic.cpp  
lammps-stable\_290ct2020/src/USER-MISC/dihedral\_nharmonic.h  
lammps-stable\_290ct2020/src/USER-MISC/dihedral\_quadratic.cpp  
lammps-stable\_290ct2020/src/USER-MISC/dihedral\_quadratic.h  
lammps-stable\_290ct2020/src/USER-MISC/dihedral\_spherical.cpp  
lammps-stable\_290ct2020/src/USER-MISC/dihedral\_spherical.h  
lammps-stable\_290ct2020/src/USER-MISC/dihedral\_table.cpp  
lammps-stable\_290ct2020/src/USER-MISC/dihedral\_table.h  
lammps-stable\_290ct2020/src/USER-MISC/dihedral\_table\_cut.cpp  
lammps-stable\_290ct2020/src/USER-MISC/dihedral\_table\_cut.h  
lammps-stable\_290ct2020/src/USER-MISC/fix\_accelerate\_cos.cpp  
lammps-stable\_290ct2020/src/USER-MISC/fix\_accelerate\_cos.h  
lammps-stable\_290ct2020/src/USER-MISC/fix\_addtorque.cpp  
lammps-stable\_290ct2020/src/USER-MISC/fix\_addtorque.h  
lammps-stable\_290ct2020/src/USER-MISC/fix\_ave\_correlate\_long.cpp  
lammps-stable\_290ct2020/src/USER-MISC/fix\_ave\_correlate\_long.h  
lammps-stable\_290ct2020/src/USER-MISC/fix\_electron\_stopping.cpp  
lammps-stable\_290ct2020/src/USER-MISC/fix\_electron\_stopping.h  
lammps-stable\_290ct2020/src/USER-MISC/fix\_ffl.cpp  
lammps-stable\_290ct2020/src/USER-MISC/fix\_ffl.h  
lammps-stable\_290ct2020/src/USER-MISC/fix\_filter\_corotate.cpp  
lammps-stable\_290ct2020/src/USER-MISC/fix\_filter\_corotate.h  
lammps-stable\_290ct2020/src/USER-MISC/fix\_flow\_gauss.cpp  
lammps-stable\_290ct2020/src/USER-MISC/fix\_flow\_gauss.h  
lammps-stable\_290ct2020/src/USER-MISC/fix\_gle.cpp  
lammps-stable\_290ct2020/src/USER-MISC/fix\_gle.h  
lammps-stable\_290ct2020/src/USER-MISC/fix\_grem.cpp  
lammps-stable\_290ct2020/src/USER-MISC/fix\_grem.h  
lammps-stable\_290ct2020/src/USER-MISC/fix\_imd.cpp  
lammps-stable\_290ct2020/src/USER-MISC/fix\_imd.h  
lammps-stable\_290ct2020/src/USER-MISC/fix\_ipi.cpp  
lammps-stable\_290ct2020/src/USER-MISC/fix\_ipi.h  
lammps-stable\_290ct2020/src/USER-MISC/fix\_momentum\_chunk.cpp  
lammps-stable\_290ct2020/src/USER-MISC/fix\_momentum\_chunk.h  
lammps-stable\_290ct2020/src/USER-MISC/fix\_npt\_cauchy.cpp  
lammps-stable\_290ct2020/src/USER-MISC/fix\_npt\_cauchy.h  
lammps-stable\_290ct2020/src/USER-MISC/fix\_nvkc.cpp  
lammps-stable\_290ct2020/src/USER-MISC/fix\_nvkc.h  
lammps-stable\_290ct2020/src/USER-MISC/fix\_orient\_eco.cpp  
lammps-stable\_290ct2020/src/USER-MISC/fix\_orient\_eco.h



lammps-stable\_290ct2020/src/USER-MISC/fix\_pafi.cpp  
lammps-stable\_290ct2020/src/USER-MISC/fix\_pafi.h  
lammps-stable\_290ct2020/src/USER-MISC/fix\_pimd.cpp  
lammps-stable\_290ct2020/src/USER-MISC/fix\_pimd.h  
lammps-stable\_290ct2020/src/USER-MISC/fix\_propel\_self.cpp  
lammps-stable\_290ct2020/src/USER-MISC/fix\_propel\_self.h  
lammps-stable\_290ct2020/src/USER-MISC/fix\_rhok.cpp  
lammps-stable\_290ct2020/src/USER-MISC/fix\_rhok.h  
lammps-stable\_290ct2020/src/USER-MISC/fix\_smd.cpp  
lammps-stable\_290ct2020/src/USER-MISC/fix\_smd.h  
lammps-stable\_290ct2020/src/USER-MISC/fix\_srp.cpp  
lammps-stable\_290ct2020/src/USER-MISC/fix\_srp.h  
lammps-stable\_290ct2020/src/USER-MISC/fix\_ti\_spring.cpp  
lammps-stable\_290ct2020/src/USER-MISC/fix\_ti\_spring.h  
lammps-stable\_290ct2020/src/USER-MISC/fix\_ttm\_mod.cpp  
lammps-stable\_290ct2020/src/USER-MISC/fix\_ttm\_mod.h  
lammps-stable\_290ct2020/src/USER-MISC/fix\_wall\_ees.cpp  
lammps-stable\_290ct2020/src/USER-MISC/fix\_wall\_ees.h  
lammps-stable\_290ct2020/src/USER-MISC/fix\_wall\_reflect\_stochastic.cpp  
lammps-stable\_290ct2020/src/USER-MISC/fix\_wall\_reflect\_stochastic.h  
lammps-stable\_290ct2020/src/USER-MISC/fix\_wall\_region\_ees.cpp  
lammps-stable\_290ct2020/src/USER-MISC/fix\_wall\_region\_ees.h  
lammps-stable\_290ct2020/src/USER-MISC/improper\_cossq.cpp  
lammps-stable\_290ct2020/src/USER-MISC/improper\_cossq.h  
lammps-stable\_290ct2020/src/USER-MISC/improper\_distance.cpp  
lammps-stable\_290ct2020/src/USER-MISC/improper\_distance.h  
lammps-stable\_290ct2020/src/USER-MISC/improper\_fourier.cpp  
lammps-stable\_290ct2020/src/USER-MISC/improper\_fourier.h  
lammps-stable\_290ct2020/src/USER-MISC/improper\_ring.cpp  
lammps-stable\_290ct2020/src/USER-MISC/improper\_ring.h  
lammps-stable\_290ct2020/src/USER-MISC/pair\_agni.cpp  
lammps-stable\_290ct2020/src/USER-MISC/pair\_agni.h  
lammps-stable\_290ct2020/src/USER-MISC/pair\_buck\_mdf.cpp  
lammps-stable\_290ct2020/src/USER-MISC/pair\_buck\_mdf.h  
lammps-stable\_290ct2020/src/USER-MISC/pair\_cosine\_squared.cpp  
lammps-stable\_290ct2020/src/USER-MISC/pair\_cosine\_squared.h  
lammps-stable\_290ct2020/src/USER-MISC/pair\_coul\_diel.cpp  
lammps-stable\_290ct2020/src/USER-MISC/pair\_coul\_diel.h  
lammps-stable\_290ct2020/src/USER-MISC/pair\_coul\_shield.cpp  
lammps-stable\_290ct2020/src/USER-MISC/pair\_coul\_shield.h  
lammps-stable\_290ct2020/src/USER-MISC/pair\_coul\_slater\_cut.cpp  
lammps-stable\_290ct2020/src/USER-MISC/pair\_coul\_slater\_cut.h  
lammps-stable\_290ct2020/src/USER-MISC/pair\_coul\_slater\_long.cpp  
lammps-stable\_290ct2020/src/USER-MISC/pair\_coul\_slater\_long.h  
lammps-stable\_290ct2020/src/USER-MISC/pair\_drip.cpp  
lammps-stable\_290ct2020/src/USER-MISC/pair\_drip.h  
lammps-stable\_290ct2020/src/USER-MISC/pair\_e3b.cpp  
lammps-stable\_290ct2020/src/USER-MISC/pair\_e3b.h  
lammps-stable\_290ct2020/src/USER-MISC/pair\_edip.cpp  
lammps-stable\_290ct2020/src/USER-MISC/pair\_edip.h  
lammps-stable\_290ct2020/src/USER-MISC/pair\_edip\_multi.cpp  
lammps-stable\_290ct2020/src/USER-MISC/pair\_edip\_multi.h  
lammps-stable\_290ct2020/src/USER-MISC/pair\_extep.cpp  
lammps-stable\_290ct2020/src/USER-MISC/pair\_extep.h  
lammps-stable\_290ct2020/src/USER-MISC/pair\_gauss\_cut.cpp  
lammps-stable\_290ct2020/src/USER-MISC/pair\_gauss\_cut.h  
lammps-stable\_290ct2020/src/USER-MISC/pair\_ilp\_graphene\_hbn.cpp  
lammps-stable\_290ct2020/src/USER-MISC/pair\_ilp\_graphene\_hbn.h  
lammps-stable\_290ct2020/src/USER-MISC/pair\_kolmogorov\_crespi\_full.cpp  
lammps-stable\_290ct2020/src/USER-MISC/pair\_kolmogorov\_crespi\_full.h

```
lammps-stable_290ct2020/src/USER-MISC/pair_kolmogorov_crespi_z.cpp
lammps-stable_290ct2020/src/USER-MISC/pair_kolmogorov_crespi_z.h
lammps-stable_290ct2020/src/USER-MISC/pair_lebedeva_z.cpp
lammps-stable_290ct2020/src/USER-MISC/pair_lebedeva_z.h
lammps-stable_290ct2020/src/USER-MISC/pair_lennard_mdf.cpp
lammps-stable_290ct2020/src/USER-MISC/pair_lennard_mdf.h
lammps-stable_290ct2020/src/USER-MISC/pair_list.cpp
lammps-stable_290ct2020/src/USER-MISC/pair_list.h
lammps-stable_290ct2020/src/USER-MISC/pair_lj_expand_coul_long.cpp
lammps-stable_290ct2020/src/USER-MISC/pair_lj_expand_coul_long.h
lammps-stable_290ct2020/src/USER-MISC/pair_lj_mdf.cpp
lammps-stable_290ct2020/src/USER-MISC/pair_lj_mdf.h
lammps-stable_290ct2020/src/USER-MISC/pair_lj_sf_dipole_sf.cpp
lammps-stable_290ct2020/src/USER-MISC/pair_lj_sf_dipole_sf.h
lammps-stable_290ct2020/src/USER-MISC/pair_local_density.cpp
lammps-stable_290ct2020/src/USER-MISC/pair_local_density.h
lammps-stable_290ct2020/src/USER-MISC/pair_meam_spline.cpp
lammps-stable_290ct2020/src/USER-MISC/pair_meam_spline.h
lammps-stable_290ct2020/src/USER-MISC/pair_meam_sw_spline.cpp
lammps-stable_290ct2020/src/USER-MISC/pair_meam_sw_spline.h
lammps-stable_290ct2020/src/USER-MISC/pair_momb.cpp
lammps-stable_290ct2020/src/USER-MISC/pair_momb.h
lammps-stable_290ct2020/src/USER-MISC/pair_morse_smooth_linear.cpp
lammps-stable_290ct2020/src/USER-MISC/pair_morse_smooth_linear.h
lammps-stable_290ct2020/src/USER-MISC/pair_srp.cpp
lammps-stable_290ct2020/src/USER-MISC/pair_srp.h
lammps-stable_290ct2020/src/USER-MISC/pair_tersoff_table.cpp
lammps-stable_290ct2020/src/USER-MISC/pair_tersoff_table.h
lammps-stable_290ct2020/src/USER-MISC/temper_grem.cpp
lammps-stable_290ct2020/src/USER-MISC/temper_grem.h
lammps-stable_290ct2020/src/USER-MISC/temper_npt.cpp
lammps-stable_290ct2020/src/USER-MISC/temper_npt.h
lammps-stable_290ct2020/src/USER-M0FFF/
lammps-stable_290ct2020/src/USER-M0FFF/README
lammps-stable_290ct2020/src/USER-M0FFF/angle_class2_p6.cpp
lammps-stable_290ct2020/src/USER-M0FFF/angle_class2_p6.h
lammps-stable_290ct2020/src/USER-M0FFF/angle_cosine_buck6d.cpp
lammps-stable_290ct2020/src/USER-M0FFF/angle_cosine_buck6d.h
lammps-stable_290ct2020/src/USER-M0FFF/improper_inversion_harmonic.cpp
lammps-stable_290ct2020/src/USER-M0FFF/improper_inversion_harmonic.h
lammps-stable_290ct2020/src/USER-M0FFF/pair_buck6d_coul_gauss_dsfc.cpp
lammps-stable_290ct2020/src/USER-M0FFF/pair_buck6d_coul_gauss_dsfc.h
lammps-stable_290ct2020/src/USER-M0FFF/pair_buck6d_coul_gauss_long.cpp
lammps-stable_290ct2020/src/USER-M0FFF/pair_buck6d_coul_gauss_long.h
lammps-stable_290ct2020/src/USER-MOLFILE/
lammps-stable_290ct2020/src/USER-MOLFILE/Install.sh
lammps-stable_290ct2020/src/USER-MOLFILE/README
lammps-stable_290ct2020/src/USER-MOLFILE/dump_molfile.cpp
lammps-stable_290ct2020/src/USER-MOLFILE/dump_molfile.h
lammps-stable_290ct2020/src/USER-MOLFILE/molfile_interface.cpp
lammps-stable_290ct2020/src/USER-MOLFILE/molfile_interface.h
lammps-stable_290ct2020/src/USER-MOLFILE/reader_molfile.cpp
lammps-stable_290ct2020/src/USER-MOLFILE/reader_molfile.h
lammps-stable_290ct2020/src/USER-NETCDF/
lammps-stable_290ct2020/src/USER-NETCDF/Install.sh
lammps-stable_290ct2020/src/USER-NETCDF/README
lammps-stable_290ct2020/src/USER-NETCDF/dump_netcdf.cpp
lammps-stable_290ct2020/src/USER-NETCDF/dump_netcdf.h
lammps-stable_290ct2020/src/USER-NETCDF/dump_netcdf_mpio.cpp
lammps-stable_290ct2020/src/USER-NETCDF/dump_netcdf_mpio.h
```

```
lammps-stable_290ct2020/src/USER-OMP/  
lammps-stable_290ct2020/src/USER-OMP/Install.sh  
lammps-stable_290ct2020/src/USER-OMP/README  
lammps-stable_290ct2020/src/USER-OMP/angle_charmm_omp.cpp  
lammps-stable_290ct2020/src/USER-OMP/angle_charmm_omp.h  
lammps-stable_290ct2020/src/USER-OMP/angle_class2_omp.cpp  
lammps-stable_290ct2020/src/USER-OMP/angle_class2_omp.h  
lammps-stable_290ct2020/src/USER-OMP/angle_cosine_delta_omp.cpp  
lammps-stable_290ct2020/src/USER-OMP/angle_cosine_delta_omp.h  
lammps-stable_290ct2020/src/USER-OMP/angle_cosine_omp.cpp  
lammps-stable_290ct2020/src/USER-OMP/angle_cosine_omp.h  
lammps-stable_290ct2020/src/USER-OMP/angle_cosine_periodic_omp.cpp  
lammps-stable_290ct2020/src/USER-OMP/angle_cosine_periodic_omp.h  
lammps-stable_290ct2020/src/USER-OMP/angle_cosine_shift_exp_omp.cpp  
lammps-stable_290ct2020/src/USER-OMP/angle_cosine_shift_exp_omp.h  
lammps-stable_290ct2020/src/USER-OMP/angle_cosine_shift_omp.cpp  
lammps-stable_290ct2020/src/USER-OMP/angle_cosine_shift_omp.h  
lammps-stable_290ct2020/src/USER-OMP/angle_cosine_squared_omp.cpp  
lammps-stable_290ct2020/src/USER-OMP/angle_cosine_squared_omp.h  
lammps-stable_290ct2020/src/USER-OMP/angle_dipole_omp.cpp  
lammps-stable_290ct2020/src/USER-OMP/angle_dipole_omp.h  
lammps-stable_290ct2020/src/USER-OMP/angle_fourier_omp.cpp  
lammps-stable_290ct2020/src/USER-OMP/angle_fourier_omp.h  
lammps-stable_290ct2020/src/USER-OMP/angle_fourier_simple_omp.cpp  
lammps-stable_290ct2020/src/USER-OMP/angle_fourier_simple_omp.h  
lammps-stable_290ct2020/src/USER-OMP/angle_harmonic_omp.cpp  
lammps-stable_290ct2020/src/USER-OMP/angle_harmonic_omp.h  
lammps-stable_290ct2020/src/USER-OMP/angle_quartic_omp.cpp  
lammps-stable_290ct2020/src/USER-OMP/angle_quartic_omp.h  
lammps-stable_290ct2020/src/USER-OMP/angle_sdk_omp.cpp  
lammps-stable_290ct2020/src/USER-OMP/angle_sdk_omp.h  
lammps-stable_290ct2020/src/USER-OMP/angle_table_omp.cpp  
lammps-stable_290ct2020/src/USER-OMP/angle_table_omp.h  
lammps-stable_290ct2020/src/USER-OMP/bond_class2_omp.cpp  
lammps-stable_290ct2020/src/USER-OMP/bond_class2_omp.h  
lammps-stable_290ct2020/src/USER-OMP/bond_fene_expand_omp.cpp  
lammps-stable_290ct2020/src/USER-OMP/bond_fene_expand_omp.h  
lammps-stable_290ct2020/src/USER-OMP/bond_fene_omp.cpp  
lammps-stable_290ct2020/src/USER-OMP/bond_fene_omp.h  
lammps-stable_290ct2020/src/USER-OMP/bond_gromos_omp.cpp  
lammps-stable_290ct2020/src/USER-OMP/bond_gromos_omp.h  
lammps-stable_290ct2020/src/USER-OMP/bond_harmonic_omp.cpp  
lammps-stable_290ct2020/src/USER-OMP/bond_harmonic_omp.h  
lammps-stable_290ct2020/src/USER-OMP/bond_harmonic_shift_cut_omp.cpp  
lammps-stable_290ct2020/src/USER-OMP/bond_harmonic_shift_cut_omp.h  
lammps-stable_290ct2020/src/USER-OMP/bond_harmonic_shift_omp.cpp  
lammps-stable_290ct2020/src/USER-OMP/bond_harmonic_shift_omp.h  
lammps-stable_290ct2020/src/USER-OMP/bond_morse_omp.cpp  
lammps-stable_290ct2020/src/USER-OMP/bond_morse_omp.h  
lammps-stable_290ct2020/src/USER-OMP/bond_nonlinear_omp.cpp  
lammps-stable_290ct2020/src/USER-OMP/bond_nonlinear_omp.h  
lammps-stable_290ct2020/src/USER-OMP/bond_quartic_omp.cpp  
lammps-stable_290ct2020/src/USER-OMP/bond_quartic_omp.h  
lammps-stable_290ct2020/src/USER-OMP/bond_table_omp.cpp  
lammps-stable_290ct2020/src/USER-OMP/bond_table_omp.h  
lammps-stable_290ct2020/src/USER-OMP/dihedral_charmm_omp.cpp  
lammps-stable_290ct2020/src/USER-OMP/dihedral_charmm_omp.h  
lammps-stable_290ct2020/src/USER-OMP/dihedral_class2_omp.cpp  
lammps-stable_290ct2020/src/USER-OMP/dihedral_class2_omp.h  
lammps-stable_290ct2020/src/USER-OMP/dihedral_cosine_shift_exp_omp.cpp
```

lammps-stable\_290ct2020/src/USER-OMP/dihedral\_cosine\_shift\_exp\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/dihedral\_fourier\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/dihedral\_fourier\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/dihedral\_harmonic\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/dihedral\_harmonic\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/dihedral\_helix\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/dihedral\_helix\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/dihedral\_multi\_harmonic\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/dihedral\_multi\_harmonic\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/dihedral\_nharmonic\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/dihedral\_nharmonic\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/dihedral\_opls\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/dihedral\_opls\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/dihedral\_quadratic\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/dihedral\_quadratic\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/dihedral\_table\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/dihedral\_table\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/domain\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/ewald\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/ewald\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/fix\_gravity\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/fix\_gravity\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/fix\_neigh\_history\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/fix\_neigh\_history\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/fix\_nh\_asphere\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/fix\_nh\_asphere\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/fix\_nh\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/fix\_nh\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/fix\_nh\_sphere\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/fix\_nh\_sphere\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/fix\_nph\_asphere\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/fix\_nph\_asphere\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/fix\_nph\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/fix\_nph\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/fix\_nph\_sphere\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/fix\_nph\_sphere\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/fix\_npt\_asphere\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/fix\_npt\_asphere\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/fix\_npt\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/fix\_npt\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/fix\_npt\_sphere\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/fix\_npt\_sphere\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/fix\_nve\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/fix\_nve\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/fix\_nve\_sphere\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/fix\_nve\_sphere\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/fix\_nvt\_asphere\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/fix\_nvt\_asphere\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/fix\_nvt\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/fix\_nvt\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/fix\_nvt\_sllod\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/fix\_nvt\_sllod\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/fix\_nvt\_sphere\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/fix\_nvt\_sphere\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/fix\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/fix\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/fix\_peri\_neigh\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/fix\_peri\_neigh\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/fix\_qeq\_comb\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/fix\_qeq\_comb\_omp.h

lammps-stable\_290ct2020/src/USER-OMP/fix\_geq\_reax\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/fix\_geq\_reax\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/fix\_rigid\_nh\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/fix\_rigid\_nh\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/fix\_rigid\_nph\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/fix\_rigid\_nph\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/fix\_rigid\_npt\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/fix\_rigid\_npt\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/fix\_rigid\_nve\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/fix\_rigid\_nve\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/fix\_rigid\_nvt\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/fix\_rigid\_nvt\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/fix\_rigid\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/fix\_rigid\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/fix\_rigid\_small\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/fix\_rigid\_small\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/improper\_class2\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/improper\_class2\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/improper\_cossq\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/improper\_cossq\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/improper\_cvff\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/improper\_cvff\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/improper\_fourier\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/improper\_fourier\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/improper\_harmonic\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/improper\_harmonic\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/improper\_ring\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/improper\_ring\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/improper\_umbrella\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/improper\_umbrella\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/msm\_cg\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/msm\_cg\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/msm\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/msm\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/npair\_full\_bin\_atomonly\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/npair\_full\_bin\_atomonly\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/npair\_full\_bin\_ghost\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/npair\_full\_bin\_ghost\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/npair\_full\_bin\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/npair\_full\_bin\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/npair\_full\_multi\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/npair\_full\_multi\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/npair\_full\_nsq\_ghost\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/npair\_full\_nsq\_ghost\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/npair\_full\_nsq\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/npair\_full\_nsq\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/npair\_half\_bin\_atomonly\_newton\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/npair\_half\_bin\_atomonly\_newton\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/npair\_half\_bin\_newtoff\_ghost\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/npair\_half\_bin\_newtoff\_ghost\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/npair\_half\_bin\_newtoff\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/npair\_half\_bin\_newtoff\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/npair\_half\_bin\_newton\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/npair\_half\_bin\_newton\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/npair\_half\_bin\_newton\_tri\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/npair\_half\_bin\_newton\_tri\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/npair\_half\_multi\_newtoff\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/npair\_half\_multi\_newtoff\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/npair\_half\_multi\_newton\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/npair\_half\_multi\_newton\_omp.h

lammps-stable\_290ct2020/src/USER-OMP/npair\_half\_multi\_newton\_tri\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/npair\_half\_multi\_newton\_tri\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/npair\_half\_nsq\_newtoff\_ghost\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/npair\_half\_nsq\_newtoff\_ghost\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/npair\_half\_nsq\_newtoff\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/npair\_half\_nsq\_newtoff\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/npair\_half\_nsq\_newton\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/npair\_half\_nsq\_newton\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/npair\_half\_respa\_bin\_newtoff\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/npair\_half\_respa\_bin\_newtoff\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/npair\_half\_respa\_bin\_newton\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/npair\_half\_respa\_bin\_newton\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/npair\_half\_respa\_bin\_newton\_tri\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/npair\_half\_respa\_bin\_newton\_tri\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/npair\_half\_respa\_nsq\_newtoff\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/npair\_half\_respa\_nsq\_newtoff\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/npair\_half\_respa\_nsq\_newton\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/npair\_half\_respa\_nsq\_newton\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/npair\_half\_size\_bin\_newtoff\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/npair\_half\_size\_bin\_newtoff\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/npair\_half\_size\_bin\_newton\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/npair\_half\_size\_bin\_newton\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/npair\_half\_size\_bin\_newton\_tri\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/npair\_half\_size\_bin\_newton\_tri\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/npair\_half\_size\_nsq\_newtoff\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/npair\_half\_size\_nsq\_newtoff\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/npair\_half\_size\_nsq\_newton\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/npair\_half\_size\_nsq\_newton\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/npair\_halffull\_newtoff\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/npair\_halffull\_newtoff\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/npair\_halffull\_newton\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/npair\_halffull\_newton\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/npair\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/npair\_skip\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_adp\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_adp\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_agni\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_agni\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_airebo\_morse\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_airebo\_morse\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_airebo\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_airebo\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_beck\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_beck\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_born\_coul\_long\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_born\_coul\_long\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_born\_coul\_msm\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_born\_coul\_msm\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_born\_coul\_wolf\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_born\_coul\_wolf\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_born\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_born\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_brownian\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_brownian\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_brownian\_poly\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_brownian\_poly\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_buck\_coul\_cut\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_buck\_coul\_cut\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_buck\_coul\_long\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_buck\_coul\_long\_omp.h

lammps-stable\_290ct2020/src/USER-OMP/pair\_buck\_coul\_msm\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_buck\_coul\_msm\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_buck\_long\_coul\_long\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_buck\_long\_coul\_long\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_buck\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_buck\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_colloid\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_colloid\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_comb\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_comb\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_coul\_cut\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_coul\_cut\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_coul\_cut\_soft\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_coul\_cut\_soft\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_coul\_debye\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_coul\_debye\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_coul\_diel\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_coul\_diel\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_coul\_dsf\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_coul\_dsf\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_coul\_long\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_coul\_long\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_coul\_long\_soft\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_coul\_long\_soft\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_coul\_msm\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_coul\_msm\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_coul\_wolf\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_coul\_wolf\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_dpd\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_dpd\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_dpd\_tstat\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_dpd\_tstat\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_eam\_alloy\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_eam\_alloy\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_eam\_fs\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_eam\_fs\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_eam\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_eam\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_edip\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_edip\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_eim\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_eim\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_gauss\_cut\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_gauss\_cut\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_gauss\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_gauss\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_gayberne\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_gayberne\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_gran\_hertz\_history\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_gran\_hertz\_history\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_gran\_hooke\_history\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_gran\_hooke\_history\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_gran\_hooke\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_gran\_hooke\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_hbond\_dreiding\_lj\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_hbond\_dreiding\_lj\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_hbond\_dreiding\_morse\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_hbond\_dreiding\_morse\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj96\_cut\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj96\_cut\_omp.h

lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_charmm\_coul\_charmm\_implicit\_omp.  
cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_charmm\_coul\_charmm\_implicit\_omp.  
h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_charmm\_coul\_charmm\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_charmm\_coul\_charmm\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_charmm\_coul\_long\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_charmm\_coul\_long\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_charmm\_coul\_long\_soft\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_charmm\_coul\_long\_soft\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_charmm\_coul\_msm\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_charmm\_coul\_msm\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_class2\_coul\_cut\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_class2\_coul\_cut\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_class2\_coul\_long\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_class2\_coul\_long\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_class2\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_class2\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_cubic\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_cubic\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_cut\_coul\_cut\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_cut\_coul\_cut\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_cut\_coul\_cut\_soft\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_cut\_coul\_cut\_soft\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_cut\_coul\_debye\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_cut\_coul\_debye\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_cut\_coul\_dsf\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_cut\_coul\_dsf\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_cut\_coul\_long\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_cut\_coul\_long\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_cut\_coul\_long\_soft\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_cut\_coul\_long\_soft\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_cut\_coul\_msm\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_cut\_coul\_msm\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_cut\_coul\_wolf\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_cut\_coul\_wolf\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_cut\_dipole\_cut\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_cut\_dipole\_cut\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_cut\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_cut\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_cut\_soft\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_cut\_soft\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_cut\_thole\_long\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_cut\_thole\_long\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_cut\_tip4p\_cut\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_cut\_tip4p\_cut\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_cut\_tip4p\_long\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_cut\_tip4p\_long\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_cut\_tip4p\_long\_soft\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_cut\_tip4p\_long\_soft\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_expand\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_expand\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_gromacs\_coul\_gromacs\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_gromacs\_coul\_gromacs\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_gromacs\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_gromacs\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_long\_coul\_long\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_long\_coul\_long\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_long\_tip4p\_long\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_long\_tip4p\_long\_omp.h



lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_sdk\_coul\_long\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_sdk\_coul\_long\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_sdk\_coul\_msm\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_sdk\_coul\_msm\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_sdk\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_sdk\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_sf\_dipole\_sf\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_sf\_dipole\_sf\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_smooth\_linear\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_smooth\_linear\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_smooth\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lj\_smooth\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lubricate\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lubricate\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lubricate\_poly\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_lubricate\_poly\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_meam\_spline\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_meam\_spline\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_morse\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_morse\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_morse\_smooth\_linear\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_morse\_smooth\_linear\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_nm\_cut\_coul\_cut\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_nm\_cut\_coul\_cut\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_nm\_cut\_coul\_long\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_nm\_cut\_coul\_long\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_nm\_cut\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_nm\_cut\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_peri\_lps\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_peri\_lps\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_peri\_pmb\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_peri\_pmb\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_reaxc\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_reaxc\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_rebo\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_rebo\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_resquared\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_resquared\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_soft\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_soft\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_sw\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_sw\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_table\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_table\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_tersoff\_mod\_c\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_tersoff\_mod\_c\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_tersoff\_mod\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_tersoff\_mod\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_tersoff\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_tersoff\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_tersoff\_table\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_tersoff\_table\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_tersoff\_zbl\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_tersoff\_zbl\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_tip4p\_cut\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_tip4p\_cut\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_tip4p\_long\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_tip4p\_long\_omp.h  
lammps-stable\_290ct2020/src/USER-OMP/pair\_tip4p\_long\_soft\_omp.cpp  
lammps-stable\_290ct2020/src/USER-OMP/pair\_tip4p\_long\_soft\_omp.h

```
lammps-stable_290ct2020/src/USER-OMP/pair_uhm_omp.cpp
lammps-stable_290ct2020/src/USER-OMP/pair_uhm_omp.h
lammps-stable_290ct2020/src/USER-OMP/pair_vashishta_omp.cpp
lammps-stable_290ct2020/src/USER-OMP/pair_vashishta_omp.h
lammps-stable_290ct2020/src/USER-OMP/pair_vashishta_table_omp.cpp
lammps-stable_290ct2020/src/USER-OMP/pair_vashishta_table_omp.h
lammps-stable_290ct2020/src/USER-OMP/pair_yukawa_colloid_omp.cpp
lammps-stable_290ct2020/src/USER-OMP/pair_yukawa_colloid_omp.h
lammps-stable_290ct2020/src/USER-OMP/pair_yukawa_omp.cpp
lammps-stable_290ct2020/src/USER-OMP/pair_yukawa_omp.h
lammps-stable_290ct2020/src/USER-OMP/pair_zbl_omp.cpp
lammps-stable_290ct2020/src/USER-OMP/pair_zbl_omp.h
lammps-stable_290ct2020/src/USER-OMP/pppm_cg_omp.cpp
lammps-stable_290ct2020/src/USER-OMP/pppm_cg_omp.h
lammps-stable_290ct2020/src/USER-OMP/pppm_disp_omp.cpp
lammps-stable_290ct2020/src/USER-OMP/pppm_disp_omp.h
lammps-stable_290ct2020/src/USER-OMP/pppm_disp_tip4p_omp.cpp
lammps-stable_290ct2020/src/USER-OMP/pppm_disp_tip4p_omp.h
lammps-stable_290ct2020/src/USER-OMP/pppm_omp.cpp
lammps-stable_290ct2020/src/USER-OMP/pppm_omp.h
lammps-stable_290ct2020/src/USER-OMP/pppm_tip4p_omp.cpp
lammps-stable_290ct2020/src/USER-OMP/pppm_tip4p_omp.h
lammps-stable_290ct2020/src/USER-OMP/reaxc_bond_orders_omp.cpp
lammps-stable_290ct2020/src/USER-OMP/reaxc_bond_orders_omp.h
lammps-stable_290ct2020/src/USER-OMP/reaxc_bonds_omp.cpp
lammps-stable_290ct2020/src/USER-OMP/reaxc_bonds_omp.h
lammps-stable_290ct2020/src/USER-OMP/reaxc_forces_omp.cpp
lammps-stable_290ct2020/src/USER-OMP/reaxc_forces_omp.h
lammps-stable_290ct2020/src/USER-OMP/reaxc_hydrogen_bonds_omp.cpp
lammps-stable_290ct2020/src/USER-OMP/reaxc_hydrogen_bonds_omp.h
lammps-stable_290ct2020/src/USER-OMP/reaxc_init_md_omp.cpp
lammps-stable_290ct2020/src/USER-OMP/reaxc_init_md_omp.h
lammps-stable_290ct2020/src/USER-OMP/reaxc_multi_body_omp.cpp
lammps-stable_290ct2020/src/USER-OMP/reaxc_multi_body_omp.h
lammps-stable_290ct2020/src/USER-OMP/reaxc_nonbonded_omp.cpp
lammps-stable_290ct2020/src/USER-OMP/reaxc_nonbonded_omp.h
lammps-stable_290ct2020/src/USER-OMP/reaxc_torsion_angles_omp.cpp
lammps-stable_290ct2020/src/USER-OMP/reaxc_torsion_angles_omp.h
lammps-stable_290ct2020/src/USER-OMP/reaxc_valence_angles_omp.cpp
lammps-stable_290ct2020/src/USER-OMP/reaxc_valence_angles_omp.h
lammps-stable_290ct2020/src/USER-OMP/respa_omp.cpp
lammps-stable_290ct2020/src/USER-OMP/respa_omp.h
lammps-stable_290ct2020/src/USER-OMP/thr_data.cpp
lammps-stable_290ct2020/src/USER-OMP/thr_data.h
lammps-stable_290ct2020/src/USER-OMP/thr_omp.cpp
lammps-stable_290ct2020/src/USER-OMP/thr_omp.h
lammps-stable_290ct2020/src/USER-PHONON/
lammps-stable_290ct2020/src/USER-PHONON/Install.sh
lammps-stable_290ct2020/src/USER-PHONON/README
lammps-stable_290ct2020/src/USER-PHONON/dynamical_matrix.cpp
lammps-stable_290ct2020/src/USER-PHONON/dynamical_matrix.h
lammps-stable_290ct2020/src/USER-PHONON/fix_phonon.cpp
lammps-stable_290ct2020/src/USER-PHONON/fix_phonon.h
lammps-stable_290ct2020/src/USER-PHONON/third_order.cpp
lammps-stable_290ct2020/src/USER-PHONON/third_order.h
lammps-stable_290ct2020/src/USER-PLUMED/
lammps-stable_290ct2020/src/USER-PLUMED/Install.sh
lammps-stable_290ct2020/src/USER-PLUMED/README
lammps-stable_290ct2020/src/USER-PLUMED/fix_plumed.cpp
lammps-stable_290ct2020/src/USER-PLUMED/fix_plumed.h
```

```
lammps-stable_290ct2020/src/USER-PTM/  
lammps-stable_290ct2020/src/USER-PTM/LICENSE  
lammps-stable_290ct2020/src/USER-PTM/README  
lammps-stable_290ct2020/src/USER-PTM/compute_ptm_atom.cpp  
lammps-stable_290ct2020/src/USER-PTM/compute_ptm_atom.h  
lammps-stable_290ct2020/src/USER-PTM/ptm_alloy_types.cpp  
lammps-stable_290ct2020/src/USER-PTM/ptm_alloy_types.h  
lammps-stable_290ct2020/src/USER-PTM/ptm_alt_templates.h  
lammps-stable_290ct2020/src/USER-PTM/ptm_canonical_coloured.cpp  
lammps-stable_290ct2020/src/USER-PTM/ptm_canonical_coloured.h  
lammps-stable_290ct2020/src/USER-PTM/ptm_constants.h  
lammps-stable_290ct2020/src/USER-PTM/ptm_convex_hull_incremental.cpp  
lammps-stable_290ct2020/src/USER-PTM/ptm_convex_hull_incremental.h  
lammps-stable_290ct2020/src/USER-PTM/ptm_deformation_gradient.cpp  
lammps-stable_290ct2020/src/USER-PTM/ptm_deformation_gradient.h  
lammps-stable_290ct2020/src/USER-PTM/ptm_functions.h  
lammps-stable_290ct2020/src/USER-PTM/ptm_fundamental_mappings.h  
lammps-stable_290ct2020/src/USER-PTM/ptm_graph_data.cpp  
lammps-stable_290ct2020/src/USER-PTM/ptm_graph_data.h  
lammps-stable_290ct2020/src/USER-PTM/ptm_graph_tools.cpp  
lammps-stable_290ct2020/src/USER-PTM/ptm_graph_tools.h  
lammps-stable_290ct2020/src/USER-PTM/ptm_index.cpp  
lammps-stable_290ct2020/src/USER-PTM/ptm_initialize_data.cpp  
lammps-stable_290ct2020/src/USER-PTM/ptm_initialize_data.h  
lammps-stable_290ct2020/src/USER-PTM/ptm_neighbour_ordering.cpp  
lammps-stable_290ct2020/src/USER-PTM/ptm_neighbour_ordering.h  
lammps-stable_290ct2020/src/USER-PTM/ptm_normalize_vertices.cpp  
lammps-stable_290ct2020/src/USER-PTM/ptm_normalize_vertices.h  
lammps-stable_290ct2020/src/USER-PTM/ptm_polar.cpp  
lammps-stable_290ct2020/src/USER-PTM/ptm_polar.h  
lammps-stable_290ct2020/src/USER-PTM/ptm_quat.cpp  
lammps-stable_290ct2020/src/USER-PTM/ptm_quat.h  
lammps-stable_290ct2020/src/USER-PTM/ptm_structure_matcher.cpp  
lammps-stable_290ct2020/src/USER-PTM/ptm_structure_matcher.h  
lammps-stable_290ct2020/src/USER-PTM/ptm_voronoi_cell.cpp  
lammps-stable_290ct2020/src/USER-PTM/ptm_voronoi_cell.h  
lammps-stable_290ct2020/src/USER-PTM/ptm_voronoi_config.h  
lammps-stable_290ct2020/src/USER-QMMM/  
lammps-stable_290ct2020/src/USER-QMMM/Install.sh  
lammps-stable_290ct2020/src/USER-QMMM/README  
lammps-stable_290ct2020/src/USER-QMMM/fix_qmmm.cpp  
lammps-stable_290ct2020/src/USER-QMMM/fix_qmmm.h  
lammps-stable_290ct2020/src/USER-QTB/  
lammps-stable_290ct2020/src/USER-QTB/README  
lammps-stable_290ct2020/src/USER-QTB/fix_qbmsst.cpp  
lammps-stable_290ct2020/src/USER-QTB/fix_qbmsst.h  
lammps-stable_290ct2020/src/USER-QTB/fix_qtb.cpp  
lammps-stable_290ct2020/src/USER-QTB/fix_qtb.h  
lammps-stable_290ct2020/src/USER-QUIP/  
lammps-stable_290ct2020/src/USER-QUIP/Install.sh  
lammps-stable_290ct2020/src/USER-QUIP/README  
lammps-stable_290ct2020/src/USER-QUIP/pair_quip.cpp  
lammps-stable_290ct2020/src/USER-QUIP/pair_quip.h  
lammps-stable_290ct2020/src/USER-REACTION/  
lammps-stable_290ct2020/src/USER-REACTION/README  
lammps-stable_290ct2020/src/USER-REACTION/fix_bond_react.cpp  
lammps-stable_290ct2020/src/USER-REACTION/fix_bond_react.h  
lammps-stable_290ct2020/src/USER-REACTION/superpose3d.h  
lammps-stable_290ct2020/src/USER-REAXC/  
lammps-stable_290ct2020/src/USER-REAXC/README
```

```
lammps-stable_290ct2020/src/USER-REAXC/compute_spec_atom.cpp
lammps-stable_290ct2020/src/USER-REAXC/compute_spec_atom.h
lammps-stable_290ct2020/src/USER-REAXC/fix_geq_reax.cpp
lammps-stable_290ct2020/src/USER-REAXC/fix_geq_reax.h
lammps-stable_290ct2020/src/USER-REAXC/fix_reaxc.cpp
lammps-stable_290ct2020/src/USER-REAXC/fix_reaxc.h
lammps-stable_290ct2020/src/USER-REAXC/fix_reaxc_bonds.cpp
lammps-stable_290ct2020/src/USER-REAXC/fix_reaxc_bonds.h
lammps-stable_290ct2020/src/USER-REAXC/fix_reaxc_species.cpp
lammps-stable_290ct2020/src/USER-REAXC/fix_reaxc_species.h
lammps-stable_290ct2020/src/USER-REAXC/pair_reaxc.cpp
lammps-stable_290ct2020/src/USER-REAXC/pair_reaxc.h
lammps-stable_290ct2020/src/USER-REAXC/reaxc_allocate.cpp
lammps-stable_290ct2020/src/USER-REAXC/reaxc_allocate.h
lammps-stable_290ct2020/src/USER-REAXC/reaxc_bond_orders.cpp
lammps-stable_290ct2020/src/USER-REAXC/reaxc_bond_orders.h
lammps-stable_290ct2020/src/USER-REAXC/reaxc_bonds.cpp
lammps-stable_290ct2020/src/USER-REAXC/reaxc_bonds.h
lammps-stable_290ct2020/src/USER-REAXC/reaxc_control.cpp
lammps-stable_290ct2020/src/USER-REAXC/reaxc_control.h
lammps-stable_290ct2020/src/USER-REAXC/reaxc_defs.h
lammps-stable_290ct2020/src/USER-REAXC/reaxc_ffield.cpp
lammps-stable_290ct2020/src/USER-REAXC/reaxc_ffield.h
lammps-stable_290ct2020/src/USER-REAXC/reaxc_forces.cpp
lammps-stable_290ct2020/src/USER-REAXC/reaxc_forces.h
lammps-stable_290ct2020/src/USER-REAXC/reaxc_hydrogen_bonds.cpp
lammps-stable_290ct2020/src/USER-REAXC/reaxc_hydrogen_bonds.h
lammps-stable_290ct2020/src/USER-REAXC/reaxc_init_md.cpp
lammps-stable_290ct2020/src/USER-REAXC/reaxc_init_md.h
lammps-stable_290ct2020/src/USER-REAXC/reaxc_io_tools.cpp
lammps-stable_290ct2020/src/USER-REAXC/reaxc_io_tools.h
lammps-stable_290ct2020/src/USER-REAXC/reaxc_list.cpp
lammps-stable_290ct2020/src/USER-REAXC/reaxc_list.h
lammps-stable_290ct2020/src/USER-REAXC/reaxc_lookup.cpp
lammps-stable_290ct2020/src/USER-REAXC/reaxc_lookup.h
lammps-stable_290ct2020/src/USER-REAXC/reaxc_multi_body.cpp
lammps-stable_290ct2020/src/USER-REAXC/reaxc_multi_body.h
lammps-stable_290ct2020/src/USER-REAXC/reaxc_nonbonded.cpp
lammps-stable_290ct2020/src/USER-REAXC/reaxc_nonbonded.h
lammps-stable_290ct2020/src/USER-REAXC/reaxc_reset_tools.cpp
lammps-stable_290ct2020/src/USER-REAXC/reaxc_reset_tools.h
lammps-stable_290ct2020/src/USER-REAXC/reaxc_system_props.cpp
lammps-stable_290ct2020/src/USER-REAXC/reaxc_system_props.h
lammps-stable_290ct2020/src/USER-REAXC/reaxc_tool_box.cpp
lammps-stable_290ct2020/src/USER-REAXC/reaxc_tool_box.h
lammps-stable_290ct2020/src/USER-REAXC/reaxc_torsion_angles.cpp
lammps-stable_290ct2020/src/USER-REAXC/reaxc_torsion_angles.h
lammps-stable_290ct2020/src/USER-REAXC/reaxc_traj.cpp
lammps-stable_290ct2020/src/USER-REAXC/reaxc_traj.h
lammps-stable_290ct2020/src/USER-REAXC/reaxc_types.h
lammps-stable_290ct2020/src/USER-REAXC/reaxc_valence_angles.cpp
lammps-stable_290ct2020/src/USER-REAXC/reaxc_valence_angles.h
lammps-stable_290ct2020/src/USER-REAXC/reaxc_vector.cpp
lammps-stable_290ct2020/src/USER-REAXC/reaxc_vector.h
lammps-stable_290ct2020/src/USER-SCAFACOS/
lammps-stable_290ct2020/src/USER-SCAFACOS/Install.sh
lammps-stable_290ct2020/src/USER-SCAFACOS/README
lammps-stable_290ct2020/src/USER-SCAFACOS/scafacos.cpp
lammps-stable_290ct2020/src/USER-SCAFACOS/scafacos.h
lammps-stable_290ct2020/src/USER-SDPD/
```

```
lammps-stable_290ct2020/src/USER-SDPD/Install.sh
lammps-stable_290ct2020/src/USER-SDPD/README
lammps-stable_290ct2020/src/USER-SDPD/fix_meso_move.cpp
lammps-stable_290ct2020/src/USER-SDPD/fix_meso_move.h
lammps-stable_290ct2020/src/USER-SDPD/fix_rigid_meso.cpp
lammps-stable_290ct2020/src/USER-SDPD/fix_rigid_meso.h
lammps-stable_290ct2020/src/USER-SDPD/pair_sdpd_taitwater_isothermal.cpp
lammps-stable_290ct2020/src/USER-SDPD/pair_sdpd_taitwater_isothermal.h
lammps-stable_290ct2020/src/USER-SMD/
lammps-stable_290ct2020/src/USER-SMD/Install.sh
lammps-stable_290ct2020/src/USER-SMD/README
lammps-stable_290ct2020/src/USER-SMD/atom_vec_smd.cpp
lammps-stable_290ct2020/src/USER-SMD/atom_vec_smd.h
lammps-stable_290ct2020/src/USER-SMD/compute_smd_contact_radius.cpp
lammps-stable_290ct2020/src/USER-SMD/compute_smd_contact_radius.h
lammps-stable_290ct2020/src/USER-SMD/compute_smd_damage.cpp
lammps-stable_290ct2020/src/USER-SMD/compute_smd_damage.h
lammps-stable_290ct2020/src/USER-SMD/compute_smd_hourglass_error.cpp
lammps-stable_290ct2020/src/USER-SMD/compute_smd_hourglass_error.h
lammps-stable_290ct2020/src/USER-SMD/compute_smd_internal_energy.cpp
lammps-stable_290ct2020/src/USER-SMD/compute_smd_internal_energy.h
lammps-stable_290ct2020/src/USER-SMD/compute_smd_plastic_strain.cpp
lammps-stable_290ct2020/src/USER-SMD/compute_smd_plastic_strain.h
lammps-stable_290ct2020/src/USER-SMD/compute_smd_plastic_strain_rate.cpp
lammps-stable_290ct2020/src/USER-SMD/compute_smd_plastic_strain_rate.h
lammps-stable_290ct2020/src/USER-SMD/compute_smd_rho.cpp
lammps-stable_290ct2020/src/USER-SMD/compute_smd_rho.h
lammps-stable_290ct2020/src/USER-SMD/compute_smd_tlsph_defgrad.cpp
lammps-stable_290ct2020/src/USER-SMD/compute_smd_tlsph_defgrad.h
lammps-stable_290ct2020/src/USER-SMD/compute_smd_tlsph_dt.cpp
lammps-stable_290ct2020/src/USER-SMD/compute_smd_tlsph_dt.h
lammps-stable_290ct2020/src/USER-SMD/compute_smd_tlsph_num_neighs.cpp
lammps-stable_290ct2020/src/USER-SMD/compute_smd_tlsph_num_neighs.h
lammps-stable_290ct2020/src/USER-SMD/compute_smd_tlsph_shape.cpp
lammps-stable_290ct2020/src/USER-SMD/compute_smd_tlsph_shape.h
lammps-stable_290ct2020/src/USER-SMD/compute_smd_tlsph_strain.cpp
lammps-stable_290ct2020/src/USER-SMD/compute_smd_tlsph_strain.h
lammps-stable_290ct2020/src/USER-SMD/compute_smd_tlsph_strain_rate.cpp
lammps-stable_290ct2020/src/USER-SMD/compute_smd_tlsph_strain_rate.h
lammps-stable_290ct2020/src/USER-SMD/compute_smd_tlsph_stress.cpp
lammps-stable_290ct2020/src/USER-SMD/compute_smd_tlsph_stress.h
lammps-stable_290ct2020/src/USER-SMD/compute_smd_triangle_vertices.cpp
lammps-stable_290ct2020/src/USER-SMD/compute_smd_triangle_vertices.h
lammps-stable_290ct2020/src/USER-SMD/compute_smd_ulsph_effm.cpp
lammps-stable_290ct2020/src/USER-SMD/compute_smd_ulsph_effm.h
lammps-stable_290ct2020/src/USER-SMD/compute_smd_ulsph_num_neighs.cpp
lammps-stable_290ct2020/src/USER-SMD/compute_smd_ulsph_num_neighs.h
lammps-stable_290ct2020/src/USER-SMD/compute_smd_ulsph_strain.cpp
lammps-stable_290ct2020/src/USER-SMD/compute_smd_ulsph_strain.h
lammps-stable_290ct2020/src/USER-SMD/compute_smd_ulsph_strain_rate.cpp
lammps-stable_290ct2020/src/USER-SMD/compute_smd_ulsph_strain_rate.h
lammps-stable_290ct2020/src/USER-SMD/compute_smd_ulsph_stress.cpp
lammps-stable_290ct2020/src/USER-SMD/compute_smd_ulsph_stress.h
lammps-stable_290ct2020/src/USER-SMD/compute_smd_vol.cpp
lammps-stable_290ct2020/src/USER-SMD/compute_smd_vol.h
lammps-stable_290ct2020/src/USER-SMD/fix_smd_adjust_dt.cpp
lammps-stable_290ct2020/src/USER-SMD/fix_smd_adjust_dt.h
lammps-stable_290ct2020/src/USER-SMD/fix_smd_integrate_tlsph.cpp
lammps-stable_290ct2020/src/USER-SMD/fix_smd_integrate_tlsph.h
lammps-stable_290ct2020/src/USER-SMD/fix_smd_integrate_ulsph.cpp
```

lammps-stable\_290ct2020/src/USER-SMD/fix\_smd\_integrate\_ulsph.h  
lammps-stable\_290ct2020/src/USER-SMD/fix\_smd\_move\_triangulated\_surface.cpp  
lammps-stable\_290ct2020/src/USER-SMD/fix\_smd\_move\_triangulated\_surface.h  
lammps-stable\_290ct2020/src/USER-SMD/fix\_smd\_setvel.cpp  
lammps-stable\_290ct2020/src/USER-SMD/fix\_smd\_setvel.h  
lammps-stable\_290ct2020/src/USER-SMD/fix\_smd\_tlsph\_reference\_configuration.cp  
p  
lammps-stable\_290ct2020/src/USER-SMD/fix\_smd\_tlsph\_reference\_configuration.h  
lammps-stable\_290ct2020/src/USER-SMD/fix\_smd\_wall\_surface.cpp  
lammps-stable\_290ct2020/src/USER-SMD/fix\_smd\_wall\_surface.h  
lammps-stable\_290ct2020/src/USER-SMD/pair\_smd\_hertz.cpp  
lammps-stable\_290ct2020/src/USER-SMD/pair\_smd\_hertz.h  
lammps-stable\_290ct2020/src/USER-SMD/pair\_smd\_tlsph.cpp  
lammps-stable\_290ct2020/src/USER-SMD/pair\_smd\_tlsph.h  
lammps-stable\_290ct2020/src/USER-SMD/pair\_smd\_triangulated\_surface.cpp  
lammps-stable\_290ct2020/src/USER-SMD/pair\_smd\_triangulated\_surface.h  
lammps-stable\_290ct2020/src/USER-SMD/pair\_smd\_ulsph.cpp  
lammps-stable\_290ct2020/src/USER-SMD/pair\_smd\_ulsph.h  
lammps-stable\_290ct2020/src/USER-SMD/smd\_kernels.h  
lammps-stable\_290ct2020/src/USER-SMD/smd\_material\_models.cpp  
lammps-stable\_290ct2020/src/USER-SMD/smd\_material\_models.h  
lammps-stable\_290ct2020/src/USER-SMD/smd\_math.h  
lammps-stable\_290ct2020/src/USER-SMTBQ/  
lammps-stable\_290ct2020/src/USER-SMTBQ/README  
lammps-stable\_290ct2020/src/USER-SMTBQ/pair\_smtbq.cpp  
lammps-stable\_290ct2020/src/USER-SMTBQ/pair\_smtbq.h  
lammps-stable\_290ct2020/src/USER-SPH/  
lammps-stable\_290ct2020/src/USER-SPH/README  
lammps-stable\_290ct2020/src/USER-SPH/atom\_vec\_sph.cpp  
lammps-stable\_290ct2020/src/USER-SPH/atom\_vec\_sph.h  
lammps-stable\_290ct2020/src/USER-SPH/compute\_sph\_e\_atom.cpp  
lammps-stable\_290ct2020/src/USER-SPH/compute\_sph\_e\_atom.h  
lammps-stable\_290ct2020/src/USER-SPH/compute\_sph\_rho\_atom.cpp  
lammps-stable\_290ct2020/src/USER-SPH/compute\_sph\_rho\_atom.h  
lammps-stable\_290ct2020/src/USER-SPH/compute\_sph\_t\_atom.cpp  
lammps-stable\_290ct2020/src/USER-SPH/compute\_sph\_t\_atom.h  
lammps-stable\_290ct2020/src/USER-SPH/fix\_sph.cpp  
lammps-stable\_290ct2020/src/USER-SPH/fix\_sph.h  
lammps-stable\_290ct2020/src/USER-SPH/fix\_sph\_stationary.cpp  
lammps-stable\_290ct2020/src/USER-SPH/fix\_sph\_stationary.h  
lammps-stable\_290ct2020/src/USER-SPH/pair\_sph\_heatconduction.cpp  
lammps-stable\_290ct2020/src/USER-SPH/pair\_sph\_heatconduction.h  
lammps-stable\_290ct2020/src/USER-SPH/pair\_sph\_idealgas.cpp  
lammps-stable\_290ct2020/src/USER-SPH/pair\_sph\_idealgas.h  
lammps-stable\_290ct2020/src/USER-SPH/pair\_sph\_lj.cpp  
lammps-stable\_290ct2020/src/USER-SPH/pair\_sph\_lj.h  
lammps-stable\_290ct2020/src/USER-SPH/pair\_sph\_rhosum.cpp  
lammps-stable\_290ct2020/src/USER-SPH/pair\_sph\_rhosum.h  
lammps-stable\_290ct2020/src/USER-SPH/pair\_sph\_taitwater.cpp  
lammps-stable\_290ct2020/src/USER-SPH/pair\_sph\_taitwater.h  
lammps-stable\_290ct2020/src/USER-SPH/pair\_sph\_taitwater\_morris.cpp  
lammps-stable\_290ct2020/src/USER-SPH/pair\_sph\_taitwater\_morris.h  
lammps-stable\_290ct2020/src/USER-TALLY/  
lammps-stable\_290ct2020/src/USER-TALLY/README  
lammps-stable\_290ct2020/src/USER-TALLY/compute\_force\_tally.cpp  
lammps-stable\_290ct2020/src/USER-TALLY/compute\_force\_tally.h  
lammps-stable\_290ct2020/src/USER-TALLY/compute\_heat\_flux\_tally.cpp  
lammps-stable\_290ct2020/src/USER-TALLY/compute\_heat\_flux\_tally.h  
lammps-stable\_290ct2020/src/USER-TALLY/compute\_pe\_mol\_tally.cpp  
lammps-stable\_290ct2020/src/USER-TALLY/compute\_pe\_mol\_tally.h

```
lammps-stable_290ct2020/src/USER-TALLY/compute_pe_tally.cpp
lammps-stable_290ct2020/src/USER-TALLY/compute_pe_tally.h
lammps-stable_290ct2020/src/USER-TALLY/compute_stress_tally.cpp
lammps-stable_290ct2020/src/USER-TALLY/compute_stress_tally.h
lammps-stable_290ct2020/src/USER-UEF/
lammps-stable_290ct2020/src/USER-UEF/README
lammps-stable_290ct2020/src/USER-UEF/compute_pressure_uef.cpp
lammps-stable_290ct2020/src/USER-UEF/compute_pressure_uef.h
lammps-stable_290ct2020/src/USER-UEF/compute_temp_uef.cpp
lammps-stable_290ct2020/src/USER-UEF/compute_temp_uef.h
lammps-stable_290ct2020/src/USER-UEF/dump_cfg_uef.cpp
lammps-stable_290ct2020/src/USER-UEF/dump_cfg_uef.h
lammps-stable_290ct2020/src/USER-UEF/fix_nh_uef.cpp
lammps-stable_290ct2020/src/USER-UEF/fix_nh_uef.h
lammps-stable_290ct2020/src/USER-UEF/fix_npt_uef.cpp
lammps-stable_290ct2020/src/USER-UEF/fix_npt_uef.h
lammps-stable_290ct2020/src/USER-UEF/fix_nvt_uef.cpp
lammps-stable_290ct2020/src/USER-UEF/fix_nvt_uef.h
lammps-stable_290ct2020/src/USER-UEF/uef_utils.cpp
lammps-stable_290ct2020/src/USER-UEF/uef_utils.h
lammps-stable_290ct2020/src/USER-VTK/
lammps-stable_290ct2020/src/USER-VTK/Install.sh
lammps-stable_290ct2020/src/USER-VTK/README
lammps-stable_290ct2020/src/USER-VTK/dump_vtk.cpp
lammps-stable_290ct2020/src/USER-VTK/dump_vtk.h
lammps-stable_290ct2020/src/USER-YAFF/
lammps-stable_290ct2020/src/USER-YAFF/README
lammps-stable_290ct2020/src/USER-YAFF/angle_cross.cpp
lammps-stable_290ct2020/src/USER-YAFF/angle_cross.h
lammps-stable_290ct2020/src/USER-YAFF/angle_mm3.cpp
lammps-stable_290ct2020/src/USER-YAFF/angle_mm3.h
lammps-stable_290ct2020/src/USER-YAFF/bond_mm3.cpp
lammps-stable_290ct2020/src/USER-YAFF/bond_mm3.h
lammps-stable_290ct2020/src/USER-YAFF/improper_distharm.cpp
lammps-stable_290ct2020/src/USER-YAFF/improper_distharm.h
lammps-stable_290ct2020/src/USER-YAFF/improper_sqdistharm.cpp
lammps-stable_290ct2020/src/USER-YAFF/improper_sqdistharm.h
lammps-stable_290ct2020/src/USER-YAFF/pair_lj_switch3_coulgauss_long.cpp
lammps-stable_290ct2020/src/USER-YAFF/pair_lj_switch3_coulgauss_long.h
lammps-stable_290ct2020/src/USER-YAFF/pair_mm3_switch3_coulgauss_long.cpp
lammps-stable_290ct2020/src/USER-YAFF/pair_mm3_switch3_coulgauss_long.h
lammps-stable_290ct2020/src/VORONOI/
lammps-stable_290ct2020/src/VORONOI/Install.sh
lammps-stable_290ct2020/src/VORONOI/README
lammps-stable_290ct2020/src/VORONOI/compute_voronoi_atom.cpp
lammps-stable_290ct2020/src/VORONOI/compute_voronoi_atom.h
lammps-stable_290ct2020/src/accelerator_kokkos.h
lammps-stable_290ct2020/src/accelerator_omp.h
lammps-stable_290ct2020/src/angle.cpp
lammps-stable_290ct2020/src/angle.h
lammps-stable_290ct2020/src/angle_deprecated.cpp
lammps-stable_290ct2020/src/angle_deprecated.h
lammps-stable_290ct2020/src/angle_hybrid.cpp
lammps-stable_290ct2020/src/angle_hybrid.h
lammps-stable_290ct2020/src/angle_zero.cpp
lammps-stable_290ct2020/src/angle_zero.h
lammps-stable_290ct2020/src/atom.cpp
lammps-stable_290ct2020/src/atom.h
lammps-stable_290ct2020/src/atom_map.cpp
lammps-stable_290ct2020/src/atom_map.h
```

lammps-stable\_290ct2020/src/atom\_masks.h  
lammps-stable\_290ct2020/src/atom\_vec.cpp  
lammps-stable\_290ct2020/src/atom\_vec.h  
lammps-stable\_290ct2020/src/atom\_vec\_atomic.cpp  
lammps-stable\_290ct2020/src/atom\_vec\_atomic.h  
lammps-stable\_290ct2020/src/atom\_vec\_body.cpp  
lammps-stable\_290ct2020/src/atom\_vec\_body.h  
lammps-stable\_290ct2020/src/atom\_vec\_charge.cpp  
lammps-stable\_290ct2020/src/atom\_vec\_charge.h  
lammps-stable\_290ct2020/src/atom\_vec\_ellipsoid.cpp  
lammps-stable\_290ct2020/src/atom\_vec\_ellipsoid.h  
lammps-stable\_290ct2020/src/atom\_vec\_hybrid.cpp  
lammps-stable\_290ct2020/src/atom\_vec\_hybrid.h  
lammps-stable\_290ct2020/src/atom\_vec\_line.cpp  
lammps-stable\_290ct2020/src/atom\_vec\_line.h  
lammps-stable\_290ct2020/src/atom\_vec\_sphere.cpp  
lammps-stable\_290ct2020/src/atom\_vec\_sphere.h  
lammps-stable\_290ct2020/src/atom\_vec\_tri.cpp  
lammps-stable\_290ct2020/src/atom\_vec\_tri.h  
lammps-stable\_290ct2020/src/balance.cpp  
lammps-stable\_290ct2020/src/balance.h  
lammps-stable\_290ct2020/src/body.cpp  
lammps-stable\_290ct2020/src/body.h  
lammps-stable\_290ct2020/src/bond.cpp  
lammps-stable\_290ct2020/src/bond.h  
lammps-stable\_290ct2020/src/bond\_deprecated.cpp  
lammps-stable\_290ct2020/src/bond\_deprecated.h  
lammps-stable\_290ct2020/src/bond\_hybrid.cpp  
lammps-stable\_290ct2020/src/bond\_hybrid.h  
lammps-stable\_290ct2020/src/bond\_zero.cpp  
lammps-stable\_290ct2020/src/bond\_zero.h  
lammps-stable\_290ct2020/src/change\_box.cpp  
lammps-stable\_290ct2020/src/change\_box.h  
lammps-stable\_290ct2020/src/citeme.cpp  
lammps-stable\_290ct2020/src/citeme.h  
lammps-stable\_290ct2020/src/comm.cpp  
lammps-stable\_290ct2020/src/comm.h  
lammps-stable\_290ct2020/src/comm\_brick.cpp  
lammps-stable\_290ct2020/src/comm\_brick.h  
lammps-stable\_290ct2020/src/comm\_tiled.cpp  
lammps-stable\_290ct2020/src/comm\_tiled.h  
lammps-stable\_290ct2020/src/compute.cpp  
lammps-stable\_290ct2020/src/compute.h  
lammps-stable\_290ct2020/src/compute\_adf.cpp  
lammps-stable\_290ct2020/src/compute\_adf.h  
lammps-stable\_290ct2020/src/compute\_aggregate\_atom.cpp  
lammps-stable\_290ct2020/src/compute\_aggregate\_atom.h  
lammps-stable\_290ct2020/src/compute\_angle.cpp  
lammps-stable\_290ct2020/src/compute\_angle.h  
lammps-stable\_290ct2020/src/compute\_angle\_local.cpp  
lammps-stable\_290ct2020/src/compute\_angle\_local.h  
lammps-stable\_290ct2020/src/compute\_angmom\_chunk.cpp  
lammps-stable\_290ct2020/src/compute\_angmom\_chunk.h  
lammps-stable\_290ct2020/src/compute\_bond.cpp  
lammps-stable\_290ct2020/src/compute\_bond.h  
lammps-stable\_290ct2020/src/compute\_bond\_local.cpp  
lammps-stable\_290ct2020/src/compute\_bond\_local.h  
lammps-stable\_290ct2020/src/compute\_centro\_atom.cpp  
lammps-stable\_290ct2020/src/compute\_centro\_atom.h  
lammps-stable\_290ct2020/src/compute\_centroid\_stress\_atom.cpp



lammps-stable\_290ct2020/src/compute\_centroid\_stress\_atom.h  
lammps-stable\_290ct2020/src/compute\_chunk\_atom.cpp  
lammps-stable\_290ct2020/src/compute\_chunk\_atom.h  
lammps-stable\_290ct2020/src/compute\_chunk\_spread\_atom.cpp  
lammps-stable\_290ct2020/src/compute\_chunk\_spread\_atom.h  
lammps-stable\_290ct2020/src/compute\_cluster\_atom.cpp  
lammps-stable\_290ct2020/src/compute\_cluster\_atom.h  
lammps-stable\_290ct2020/src/compute\_cna\_atom.cpp  
lammps-stable\_290ct2020/src/compute\_cna\_atom.h  
lammps-stable\_290ct2020/src/compute\_com.cpp  
lammps-stable\_290ct2020/src/compute\_com.h  
lammps-stable\_290ct2020/src/compute\_com\_chunk.cpp  
lammps-stable\_290ct2020/src/compute\_com\_chunk.h  
lammps-stable\_290ct2020/src/compute\_contact\_atom.cpp  
lammps-stable\_290ct2020/src/compute\_contact\_atom.h  
lammps-stable\_290ct2020/src/compute\_coord\_atom.cpp  
lammps-stable\_290ct2020/src/compute\_coord\_atom.h  
lammps-stable\_290ct2020/src/compute\_deprecated.cpp  
lammps-stable\_290ct2020/src/compute\_deprecated.h  
lammps-stable\_290ct2020/src/compute\_dihedral.cpp  
lammps-stable\_290ct2020/src/compute\_dihedral.h  
lammps-stable\_290ct2020/src/compute\_dihedral\_local.cpp  
lammps-stable\_290ct2020/src/compute\_dihedral\_local.h  
lammps-stable\_290ct2020/src/compute\_dipole\_chunk.cpp  
lammps-stable\_290ct2020/src/compute\_dipole\_chunk.h  
lammps-stable\_290ct2020/src/compute\_displace\_atom.cpp  
lammps-stable\_290ct2020/src/compute\_displace\_atom.h  
lammps-stable\_290ct2020/src/compute\_erotate\_sphere.cpp  
lammps-stable\_290ct2020/src/compute\_erotate\_sphere.h  
lammps-stable\_290ct2020/src/compute\_erotate\_sphere\_atom.cpp  
lammps-stable\_290ct2020/src/compute\_erotate\_sphere\_atom.h  
lammps-stable\_290ct2020/src/compute\_fragment\_atom.cpp  
lammps-stable\_290ct2020/src/compute\_fragment\_atom.h  
lammps-stable\_290ct2020/src/compute\_global\_atom.cpp  
lammps-stable\_290ct2020/src/compute\_global\_atom.h  
lammps-stable\_290ct2020/src/compute\_group\_group.cpp  
lammps-stable\_290ct2020/src/compute\_group\_group.h  
lammps-stable\_290ct2020/src/compute\_gyration.cpp  
lammps-stable\_290ct2020/src/compute\_gyration.h  
lammps-stable\_290ct2020/src/compute\_gyration\_chunk.cpp  
lammps-stable\_290ct2020/src/compute\_gyration\_chunk.h  
lammps-stable\_290ct2020/src/compute\_heat\_flux.cpp  
lammps-stable\_290ct2020/src/compute\_heat\_flux.h  
lammps-stable\_290ct2020/src/compute\_hexorder\_atom.cpp  
lammps-stable\_290ct2020/src/compute\_hexorder\_atom.h  
lammps-stable\_290ct2020/src/compute\_improper.cpp  
lammps-stable\_290ct2020/src/compute\_improper.h  
lammps-stable\_290ct2020/src/compute\_improper\_local.cpp  
lammps-stable\_290ct2020/src/compute\_improper\_local.h  
lammps-stable\_290ct2020/src/compute\_inertia\_chunk.cpp  
lammps-stable\_290ct2020/src/compute\_inertia\_chunk.h  
lammps-stable\_290ct2020/src/compute\_ke.cpp  
lammps-stable\_290ct2020/src/compute\_ke.h  
lammps-stable\_290ct2020/src/compute\_ke\_atom.cpp  
lammps-stable\_290ct2020/src/compute\_ke\_atom.h  
lammps-stable\_290ct2020/src/compute\_msd.cpp  
lammps-stable\_290ct2020/src/compute\_msd.h  
lammps-stable\_290ct2020/src/compute\_msd\_chunk.cpp  
lammps-stable\_290ct2020/src/compute\_msd\_chunk.h  
lammps-stable\_290ct2020/src/compute\_omega\_chunk.cpp

lammps-stable\_290ct2020/src/compute\_omega\_chunk.h  
lammps-stable\_290ct2020/src/compute\_orientorder\_atom.cpp  
lammps-stable\_290ct2020/src/compute\_orientorder\_atom.h  
lammps-stable\_290ct2020/src/compute\_pair.cpp  
lammps-stable\_290ct2020/src/compute\_pair.h  
lammps-stable\_290ct2020/src/compute\_pair\_local.cpp  
lammps-stable\_290ct2020/src/compute\_pair\_local.h  
lammps-stable\_290ct2020/src/compute\_pe.cpp  
lammps-stable\_290ct2020/src/compute\_pe.h  
lammps-stable\_290ct2020/src/compute\_pe\_atom.cpp  
lammps-stable\_290ct2020/src/compute\_pe\_atom.h  
lammps-stable\_290ct2020/src/compute\_pressure.cpp  
lammps-stable\_290ct2020/src/compute\_pressure.h  
lammps-stable\_290ct2020/src/compute\_property\_atom.cpp  
lammps-stable\_290ct2020/src/compute\_property\_atom.h  
lammps-stable\_290ct2020/src/compute\_property\_chunk.cpp  
lammps-stable\_290ct2020/src/compute\_property\_chunk.h  
lammps-stable\_290ct2020/src/compute\_property\_local.cpp  
lammps-stable\_290ct2020/src/compute\_property\_local.h  
lammps-stable\_290ct2020/src/compute\_rdf.cpp  
lammps-stable\_290ct2020/src/compute\_rdf.h  
lammps-stable\_290ct2020/src/compute\_reduce.cpp  
lammps-stable\_290ct2020/src/compute\_reduce.h  
lammps-stable\_290ct2020/src/compute\_reduce\_chunk.cpp  
lammps-stable\_290ct2020/src/compute\_reduce\_chunk.h  
lammps-stable\_290ct2020/src/compute\_reduce\_region.cpp  
lammps-stable\_290ct2020/src/compute\_reduce\_region.h  
lammps-stable\_290ct2020/src/compute\_slice.cpp  
lammps-stable\_290ct2020/src/compute\_slice.h  
lammps-stable\_290ct2020/src/compute\_stress\_atom.cpp  
lammps-stable\_290ct2020/src/compute\_stress\_atom.h  
lammps-stable\_290ct2020/src/compute\_temp.cpp  
lammps-stable\_290ct2020/src/compute\_temp.h  
lammps-stable\_290ct2020/src/compute\_temp\_chunk.cpp  
lammps-stable\_290ct2020/src/compute\_temp\_chunk.h  
lammps-stable\_290ct2020/src/compute\_temp\_com.cpp  
lammps-stable\_290ct2020/src/compute\_temp\_com.h  
lammps-stable\_290ct2020/src/compute\_temp\_deform.cpp  
lammps-stable\_290ct2020/src/compute\_temp\_deform.h  
lammps-stable\_290ct2020/src/compute\_temp\_partial.cpp  
lammps-stable\_290ct2020/src/compute\_temp\_partial.h  
lammps-stable\_290ct2020/src/compute\_temp\_profile.cpp  
lammps-stable\_290ct2020/src/compute\_temp\_profile.h  
lammps-stable\_290ct2020/src/compute\_temp\_ramp.cpp  
lammps-stable\_290ct2020/src/compute\_temp\_ramp.h  
lammps-stable\_290ct2020/src/compute\_temp\_region.cpp  
lammps-stable\_290ct2020/src/compute\_temp\_region.h  
lammps-stable\_290ct2020/src/compute\_temp\_sphere.cpp  
lammps-stable\_290ct2020/src/compute\_temp\_sphere.h  
lammps-stable\_290ct2020/src/compute\_torque\_chunk.cpp  
lammps-stable\_290ct2020/src/compute\_torque\_chunk.h  
lammps-stable\_290ct2020/src/compute\_vacf.cpp  
lammps-stable\_290ct2020/src/compute\_vacf.h  
lammps-stable\_290ct2020/src/compute\_vcm\_chunk.cpp  
lammps-stable\_290ct2020/src/compute\_vcm\_chunk.h  
lammps-stable\_290ct2020/src/create\_atoms.cpp  
lammps-stable\_290ct2020/src/create\_atoms.h  
lammps-stable\_290ct2020/src/create\_bonds.cpp  
lammps-stable\_290ct2020/src/create\_bonds.h  
lammps-stable\_290ct2020/src/create\_box.cpp

lammps-stable\_290ct2020/src/create\_box.h  
lammps-stable\_290ct2020/src/delete\_atoms.cpp  
lammps-stable\_290ct2020/src/delete\_atoms.h  
lammps-stable\_290ct2020/src/delete\_bonds.cpp  
lammps-stable\_290ct2020/src/delete\_bonds.h  
lammps-stable\_290ct2020/src/deprecated.cpp  
lammps-stable\_290ct2020/src/deprecated.h  
lammps-stable\_290ct2020/src/dihedral.cpp  
lammps-stable\_290ct2020/src/dihedral.h  
lammps-stable\_290ct2020/src/dihedral\_deprecated.cpp  
lammps-stable\_290ct2020/src/dihedral\_deprecated.h  
lammps-stable\_290ct2020/src/dihedral\_hybrid.cpp  
lammps-stable\_290ct2020/src/dihedral\_hybrid.h  
lammps-stable\_290ct2020/src/dihedral\_zero.cpp  
lammps-stable\_290ct2020/src/dihedral\_zero.h  
lammps-stable\_290ct2020/src/displace\_atoms.cpp  
lammps-stable\_290ct2020/src/displace\_atoms.h  
lammps-stable\_290ct2020/src/domain.cpp  
lammps-stable\_290ct2020/src/domain.h  
lammps-stable\_290ct2020/src/dump.cpp  
lammps-stable\_290ct2020/src/dump.h  
lammps-stable\_290ct2020/src/dump\_atom.cpp  
lammps-stable\_290ct2020/src/dump\_atom.h  
lammps-stable\_290ct2020/src/dump\_cfg.cpp  
lammps-stable\_290ct2020/src/dump\_cfg.h  
lammps-stable\_290ct2020/src/dump\_custom.cpp  
lammps-stable\_290ct2020/src/dump\_custom.h  
lammps-stable\_290ct2020/src/dump\_dcd.cpp  
lammps-stable\_290ct2020/src/dump\_dcd.h  
lammps-stable\_290ct2020/src/dump\_deprecated.cpp  
lammps-stable\_290ct2020/src/dump\_deprecated.h  
lammps-stable\_290ct2020/src/dump\_image.cpp  
lammps-stable\_290ct2020/src/dump\_image.h  
lammps-stable\_290ct2020/src/dump\_local.cpp  
lammps-stable\_290ct2020/src/dump\_local.h  
lammps-stable\_290ct2020/src/dump\_movie.cpp  
lammps-stable\_290ct2020/src/dump\_movie.h  
lammps-stable\_290ct2020/src/dump\_xyz.cpp  
lammps-stable\_290ct2020/src/dump\_xyz.h  
lammps-stable\_290ct2020/src/error.cpp  
lammps-stable\_290ct2020/src/error.h  
lammps-stable\_290ct2020/src/exceptions.h  
lammps-stable\_290ct2020/src/file\_writer.h  
lammps-stable\_290ct2020/src/finish.cpp  
lammps-stable\_290ct2020/src/finish.h  
lammps-stable\_290ct2020/src/fix.cpp  
lammps-stable\_290ct2020/src/fix.h  
lammps-stable\_290ct2020/src/fix\_adapt.cpp  
lammps-stable\_290ct2020/src/fix\_adapt.h  
lammps-stable\_290ct2020/src/fix\_addforce.cpp  
lammps-stable\_290ct2020/src/fix\_addforce.h  
lammps-stable\_290ct2020/src/fix\_ave\_atom.cpp  
lammps-stable\_290ct2020/src/fix\_ave\_atom.h  
lammps-stable\_290ct2020/src/fix\_ave\_chunk.cpp  
lammps-stable\_290ct2020/src/fix\_ave\_chunk.h  
lammps-stable\_290ct2020/src/fix\_ave\_correlate.cpp  
lammps-stable\_290ct2020/src/fix\_ave\_correlate.h  
lammps-stable\_290ct2020/src/fix\_ave\_histo.cpp  
lammps-stable\_290ct2020/src/fix\_ave\_histo.h  
lammps-stable\_290ct2020/src/fix\_ave\_histo\_weight.cpp

lammps-stable\_290ct2020/src/fix\_ave\_histo\_weight.h  
lammps-stable\_290ct2020/src/fix\_ave\_time.cpp  
lammps-stable\_290ct2020/src/fix\_ave\_time.h  
lammps-stable\_290ct2020/src/fix\_aveforce.cpp  
lammps-stable\_290ct2020/src/fix\_aveforce.h  
lammps-stable\_290ct2020/src/fix\_balance.cpp  
lammps-stable\_290ct2020/src/fix\_balance.h  
lammps-stable\_290ct2020/src/fix\_box\_relax.cpp  
lammps-stable\_290ct2020/src/fix\_box\_relax.h  
lammps-stable\_290ct2020/src/fix\_controller.cpp  
lammps-stable\_290ct2020/src/fix\_controller.h  
lammps-stable\_290ct2020/src/fix\_deform.cpp  
lammps-stable\_290ct2020/src/fix\_deform.h  
lammps-stable\_290ct2020/src/fix\_deprecated.cpp  
lammps-stable\_290ct2020/src/fix\_deprecated.h  
lammps-stable\_290ct2020/src/fix\_drag.cpp  
lammps-stable\_290ct2020/src/fix\_drag.h  
lammps-stable\_290ct2020/src/fix\_dt\_reset.cpp  
lammps-stable\_290ct2020/src/fix\_dt\_reset.h  
lammps-stable\_290ct2020/src/fix\_dummy.cpp  
lammps-stable\_290ct2020/src/fix\_dummy.h  
lammps-stable\_290ct2020/src/fix\_enforce2d.cpp  
lammps-stable\_290ct2020/src/fix\_enforce2d.h  
lammps-stable\_290ct2020/src/fix\_external.cpp  
lammps-stable\_290ct2020/src/fix\_external.h  
lammps-stable\_290ct2020/src/fix\_gravity.cpp  
lammps-stable\_290ct2020/src/fix\_gravity.h  
lammps-stable\_290ct2020/src/fix\_group.cpp  
lammps-stable\_290ct2020/src/fix\_group.h  
lammps-stable\_290ct2020/src/fix\_halt.cpp  
lammps-stable\_290ct2020/src/fix\_halt.h  
lammps-stable\_290ct2020/src/fix\_heat.cpp  
lammps-stable\_290ct2020/src/fix\_heat.h  
lammps-stable\_290ct2020/src/fix\_indent.cpp  
lammps-stable\_290ct2020/src/fix\_indent.h  
lammps-stable\_290ct2020/src/fix\_langevin.cpp  
lammps-stable\_290ct2020/src/fix\_langevin.h  
lammps-stable\_290ct2020/src/fix\_lineforce.cpp  
lammps-stable\_290ct2020/src/fix\_lineforce.h  
lammps-stable\_290ct2020/src/fix\_minimize.cpp  
lammps-stable\_290ct2020/src/fix\_minimize.h  
lammps-stable\_290ct2020/src/fix\_momentum.cpp  
lammps-stable\_290ct2020/src/fix\_momentum.h  
lammps-stable\_290ct2020/src/fix\_move.cpp  
lammps-stable\_290ct2020/src/fix\_move.h  
lammps-stable\_290ct2020/src/fix\_neigh\_history.cpp  
lammps-stable\_290ct2020/src/fix\_neigh\_history.h  
lammps-stable\_290ct2020/src/fix\_nh.cpp  
lammps-stable\_290ct2020/src/fix\_nh.h  
lammps-stable\_290ct2020/src/fix\_nh\_sphere.cpp  
lammps-stable\_290ct2020/src/fix\_nh\_sphere.h  
lammps-stable\_290ct2020/src/fix\_nph.cpp  
lammps-stable\_290ct2020/src/fix\_nph.h  
lammps-stable\_290ct2020/src/fix\_nph\_sphere.cpp  
lammps-stable\_290ct2020/src/fix\_nph\_sphere.h  
lammps-stable\_290ct2020/src/fix\_npt.cpp  
lammps-stable\_290ct2020/src/fix\_npt.h  
lammps-stable\_290ct2020/src/fix\_npt\_sphere.cpp  
lammps-stable\_290ct2020/src/fix\_npt\_sphere.h  
lammps-stable\_290ct2020/src/fix\_numdiff.cpp

lammps-stable\_290ct2020/src/fix\_numdiff.h  
lammps-stable\_290ct2020/src/fix\_nve.cpp  
lammps-stable\_290ct2020/src/fix\_nve.h  
lammps-stable\_290ct2020/src/fix\_nve\_limit.cpp  
lammps-stable\_290ct2020/src/fix\_nve\_limit.h  
lammps-stable\_290ct2020/src/fix\_nve\_noforce.cpp  
lammps-stable\_290ct2020/src/fix\_nve\_noforce.h  
lammps-stable\_290ct2020/src/fix\_nve\_sphere.cpp  
lammps-stable\_290ct2020/src/fix\_nve\_sphere.h  
lammps-stable\_290ct2020/src/fix\_nvt.cpp  
lammps-stable\_290ct2020/src/fix\_nvt.h  
lammps-stable\_290ct2020/src/fix\_nvt\_sllod.cpp  
lammps-stable\_290ct2020/src/fix\_nvt\_sllod.h  
lammps-stable\_290ct2020/src/fix\_nvt\_sphere.cpp  
lammps-stable\_290ct2020/src/fix\_nvt\_sphere.h  
lammps-stable\_290ct2020/src/fix\_planeforce.cpp  
lammps-stable\_290ct2020/src/fix\_planeforce.h  
lammps-stable\_290ct2020/src/fix\_press\_berendsen.cpp  
lammps-stable\_290ct2020/src/fix\_press\_berendsen.h  
lammps-stable\_290ct2020/src/fix\_print.cpp  
lammps-stable\_290ct2020/src/fix\_print.h  
lammps-stable\_290ct2020/src/fix\_property\_atom.cpp  
lammps-stable\_290ct2020/src/fix\_property\_atom.h  
lammps-stable\_290ct2020/src/fix\_read\_restart.cpp  
lammps-stable\_290ct2020/src/fix\_read\_restart.h  
lammps-stable\_290ct2020/src/fix\_recenter.cpp  
lammps-stable\_290ct2020/src/fix\_recenter.h  
lammps-stable\_290ct2020/src/fix\_respa.cpp  
lammps-stable\_290ct2020/src/fix\_respa.h  
lammps-stable\_290ct2020/src/fix\_restrain.cpp  
lammps-stable\_290ct2020/src/fix\_restrain.h  
lammps-stable\_290ct2020/src/fix\_setforce.cpp  
lammps-stable\_290ct2020/src/fix\_setforce.h  
lammps-stable\_290ct2020/src/fix\_spring.cpp  
lammps-stable\_290ct2020/src/fix\_spring.h  
lammps-stable\_290ct2020/src/fix\_spring\_chunk.cpp  
lammps-stable\_290ct2020/src/fix\_spring\_chunk.h  
lammps-stable\_290ct2020/src/fix\_spring\_rg.cpp  
lammps-stable\_290ct2020/src/fix\_spring\_rg.h  
lammps-stable\_290ct2020/src/fix\_spring\_self.cpp  
lammps-stable\_290ct2020/src/fix\_spring\_self.h  
lammps-stable\_290ct2020/src/fix\_store.cpp  
lammps-stable\_290ct2020/src/fix\_store.h  
lammps-stable\_290ct2020/src/fix\_store\_force.cpp  
lammps-stable\_290ct2020/src/fix\_store\_force.h  
lammps-stable\_290ct2020/src/fix\_store\_state.cpp  
lammps-stable\_290ct2020/src/fix\_store\_state.h  
lammps-stable\_290ct2020/src/fix\_temp\_berendsen.cpp  
lammps-stable\_290ct2020/src/fix\_temp\_berendsen.h  
lammps-stable\_290ct2020/src/fix\_temp\_csld.cpp  
lammps-stable\_290ct2020/src/fix\_temp\_csld.h  
lammps-stable\_290ct2020/src/fix\_temp\_csvr.cpp  
lammps-stable\_290ct2020/src/fix\_temp\_csvr.h  
lammps-stable\_290ct2020/src/fix\_temp\_rescale.cpp  
lammps-stable\_290ct2020/src/fix\_temp\_rescale.h  
lammps-stable\_290ct2020/src/fix\_tmd.cpp  
lammps-stable\_290ct2020/src/fix\_tmd.h  
lammps-stable\_290ct2020/src/fix\_vector.cpp  
lammps-stable\_290ct2020/src/fix\_vector.h  
lammps-stable\_290ct2020/src/fix\_viscous.cpp

```
lammps-stable_290ct2020/src/fix_viscous.h
lammps-stable_290ct2020/src/fix_wall.cpp
lammps-stable_290ct2020/src/fix_wall.h
lammps-stable_290ct2020/src/fix_wall_harmonic.cpp
lammps-stable_290ct2020/src/fix_wall_harmonic.h
lammps-stable_290ct2020/src/fix_wall_lj1043.cpp
lammps-stable_290ct2020/src/fix_wall_lj1043.h
lammps-stable_290ct2020/src/fix_wall_lj126.cpp
lammps-stable_290ct2020/src/fix_wall_lj126.h
lammps-stable_290ct2020/src/fix_wall_lj93.cpp
lammps-stable_290ct2020/src/fix_wall_lj93.h
lammps-stable_290ct2020/src/fix_wall_morse.cpp
lammps-stable_290ct2020/src/fix_wall_morse.h
lammps-stable_290ct2020/src/fix_wall_reflect.cpp
lammps-stable_290ct2020/src/fix_wall_reflect.h
lammps-stable_290ct2020/src/fix_wall_region.cpp
lammps-stable_290ct2020/src/fix_wall_region.h
lammps-stable_290ct2020/src/fmt/
lammps-stable_290ct2020/src/fmt/LICENSE
lammps-stable_290ct2020/src/fmt/chrono.h
lammps-stable_290ct2020/src/fmt/color.h
lammps-stable_290ct2020/src/fmt/compile.h
lammps-stable_290ct2020/src/fmt/core.h
lammps-stable_290ct2020/src/fmt/format-inl.h
lammps-stable_290ct2020/src/fmt/format.h
lammps-stable_290ct2020/src/fmt/locale.h
lammps-stable_290ct2020/src/fmt/os.h
lammps-stable_290ct2020/src/fmt/ostream.h
lammps-stable_290ct2020/src/fmt/printf.h
lammps-stable_290ct2020/src/fmt/ranges.h
lammps-stable_290ct2020/src/fmtlib_format.cpp
lammps-stable_290ct2020/src/fmtlib_os.cpp
lammps-stable_290ct2020/src/force.cpp
lammps-stable_290ct2020/src/force.h
lammps-stable_290ct2020/src/group.cpp
lammps-stable_290ct2020/src/group.h
lammps-stable_290ct2020/src/hashlittle.cpp
lammps-stable_290ct2020/src/hashlittle.h
lammps-stable_290ct2020/src/image.cpp
lammps-stable_290ct2020/src/image.h
lammps-stable_290ct2020/src/imbalance.cpp
lammps-stable_290ct2020/src/imbalance.h
lammps-stable_290ct2020/src/imbalance_group.cpp
lammps-stable_290ct2020/src/imbalance_group.h
lammps-stable_290ct2020/src/imbalance_neigh.cpp
lammps-stable_290ct2020/src/imbalance_neigh.h
lammps-stable_290ct2020/src/imbalance_store.cpp
lammps-stable_290ct2020/src/imbalance_store.h
lammps-stable_290ct2020/src/imbalance_time.cpp
lammps-stable_290ct2020/src/imbalance_time.h
lammps-stable_290ct2020/src/imbalance_var.cpp
lammps-stable_290ct2020/src/imbalance_var.h
lammps-stable_290ct2020/src/improper.cpp
lammps-stable_290ct2020/src/improper.h
lammps-stable_290ct2020/src/improper_deprecated.cpp
lammps-stable_290ct2020/src/improper_deprecated.h
lammps-stable_290ct2020/src/improper_hybrid.cpp
lammps-stable_290ct2020/src/improper_hybrid.h
lammps-stable_290ct2020/src/improper_zero.cpp
lammps-stable_290ct2020/src/improper_zero.h
```

lammps-stable\_290ct2020/src/info.cpp  
lammps-stable\_290ct2020/src/info.h  
lammps-stable\_290ct2020/src/input.cpp  
lammps-stable\_290ct2020/src/input.h  
lammps-stable\_290ct2020/src/integrate.cpp  
lammps-stable\_290ct2020/src/integrate.h  
lammps-stable\_290ct2020/src/irregular.cpp  
lammps-stable\_290ct2020/src/irregular.h  
lammps-stable\_290ct2020/src/kspace.cpp  
lammps-stable\_290ct2020/src/kspace.h  
lammps-stable\_290ct2020/src/kspace\_deprecated.cpp  
lammps-stable\_290ct2020/src/kspace\_deprecated.h  
lammps-stable\_290ct2020/src/lammps.cpp  
lammps-stable\_290ct2020/src/lammps.h  
lammps-stable\_290ct2020/src/lattice.cpp  
lammps-stable\_290ct2020/src/lattice.h  
lammps-stable\_290ct2020/src/library.cpp  
lammps-stable\_290ct2020/src/library.h  
lammps-stable\_290ct2020/src/lmpython.cpp  
lammps-stable\_290ct2020/src/lmpython.h  
lammps-stable\_290ct2020/src/lmprestart.h  
lammps-stable\_290ct2020/src/lmpdtype.h  
lammps-stable\_290ct2020/src/lmpwindows.h  
lammps-stable\_290ct2020/src/main.cpp  
lammps-stable\_290ct2020/src/math\_complex.h  
lammps-stable\_290ct2020/src/math\_const.h  
lammps-stable\_290ct2020/src/math\_eigen.cpp  
lammps-stable\_290ct2020/src/math\_eigen.h  
lammps-stable\_290ct2020/src/math\_eigen\_impl.h  
lammps-stable\_290ct2020/src/math\_extra.cpp  
lammps-stable\_290ct2020/src/math\_extra.h  
lammps-stable\_290ct2020/src/math\_special.cpp  
lammps-stable\_290ct2020/src/math\_special.h  
lammps-stable\_290ct2020/src/math\_vector.h  
lammps-stable\_290ct2020/src/memory.cpp  
lammps-stable\_290ct2020/src/memory.h  
lammps-stable\_290ct2020/src/min.cpp  
lammps-stable\_290ct2020/src/min.h  
lammps-stable\_290ct2020/src/min\_cg.cpp  
lammps-stable\_290ct2020/src/min\_cg.h  
lammps-stable\_290ct2020/src/min\_fire.cpp  
lammps-stable\_290ct2020/src/min\_fire.h  
lammps-stable\_290ct2020/src/min\_fire\_old.cpp  
lammps-stable\_290ct2020/src/min\_fire\_old.h  
lammps-stable\_290ct2020/src/min\_hftn.cpp  
lammps-stable\_290ct2020/src/min\_hftn.h  
lammps-stable\_290ct2020/src/min\_linesearch.cpp  
lammps-stable\_290ct2020/src/min\_linesearch.h  
lammps-stable\_290ct2020/src/min\_quickmin.cpp  
lammps-stable\_290ct2020/src/min\_quickmin.h  
lammps-stable\_290ct2020/src/min\_sd.cpp  
lammps-stable\_290ct2020/src/min\_sd.h  
lammps-stable\_290ct2020/src/minimize.cpp  
lammps-stable\_290ct2020/src/minimize.h  
lammps-stable\_290ct2020/src/modify.cpp  
lammps-stable\_290ct2020/src/modify.h  
lammps-stable\_290ct2020/src/molecule.cpp  
lammps-stable\_290ct2020/src/molecule.h  
lammps-stable\_290ct2020/src/mpiio.h  
lammps-stable\_290ct2020/src/my\_page.cpp

lammps-stable\_290ct2020/src/my\_page.h  
lammps-stable\_290ct2020/src/my\_pool\_chunk.cpp  
lammps-stable\_290ct2020/src/my\_pool\_chunk.h  
lammps-stable\_290ct2020/src/nbin.cpp  
lammps-stable\_290ct2020/src/nbin.h  
lammps-stable\_290ct2020/src/nbin\_standard.cpp  
lammps-stable\_290ct2020/src/nbin\_standard.h  
lammps-stable\_290ct2020/src/neigh\_list.cpp  
lammps-stable\_290ct2020/src/neigh\_list.h  
lammps-stable\_290ct2020/src/neigh\_request.cpp  
lammps-stable\_290ct2020/src/neigh\_request.h  
lammps-stable\_290ct2020/src/neighbor.cpp  
lammps-stable\_290ct2020/src/neighbor.h  
lammps-stable\_290ct2020/src/npair.cpp  
lammps-stable\_290ct2020/src/npair.h  
lammps-stable\_290ct2020/src/npair\_copy.cpp  
lammps-stable\_290ct2020/src/npair\_copy.h  
lammps-stable\_290ct2020/src/npair\_full\_bin.cpp  
lammps-stable\_290ct2020/src/npair\_full\_bin.h  
lammps-stable\_290ct2020/src/npair\_full\_bin\_atomonly.cpp  
lammps-stable\_290ct2020/src/npair\_full\_bin\_atomonly.h  
lammps-stable\_290ct2020/src/npair\_full\_bin\_ghost.cpp  
lammps-stable\_290ct2020/src/npair\_full\_bin\_ghost.h  
lammps-stable\_290ct2020/src/npair\_full\_multi.cpp  
lammps-stable\_290ct2020/src/npair\_full\_multi.h  
lammps-stable\_290ct2020/src/npair\_full\_nsq.cpp  
lammps-stable\_290ct2020/src/npair\_full\_nsq.h  
lammps-stable\_290ct2020/src/npair\_full\_nsq\_ghost.cpp  
lammps-stable\_290ct2020/src/npair\_full\_nsq\_ghost.h  
lammps-stable\_290ct2020/src/npair\_half\_bin\_atomonly\_newton.cpp  
lammps-stable\_290ct2020/src/npair\_half\_bin\_atomonly\_newton.h  
lammps-stable\_290ct2020/src/npair\_half\_bin\_newtoff.cpp  
lammps-stable\_290ct2020/src/npair\_half\_bin\_newtoff.h  
lammps-stable\_290ct2020/src/npair\_half\_bin\_newtoff\_ghost.cpp  
lammps-stable\_290ct2020/src/npair\_half\_bin\_newtoff\_ghost.h  
lammps-stable\_290ct2020/src/npair\_half\_bin\_newton.cpp  
lammps-stable\_290ct2020/src/npair\_half\_bin\_newton.h  
lammps-stable\_290ct2020/src/npair\_half\_bin\_newton\_tri.cpp  
lammps-stable\_290ct2020/src/npair\_half\_bin\_newton\_tri.h  
lammps-stable\_290ct2020/src/npair\_half\_multi\_newtoff.cpp  
lammps-stable\_290ct2020/src/npair\_half\_multi\_newtoff.h  
lammps-stable\_290ct2020/src/npair\_half\_multi\_newton.cpp  
lammps-stable\_290ct2020/src/npair\_half\_multi\_newton.h  
lammps-stable\_290ct2020/src/npair\_half\_multi\_newton\_tri.cpp  
lammps-stable\_290ct2020/src/npair\_half\_multi\_newton\_tri.h  
lammps-stable\_290ct2020/src/npair\_half\_nsq\_newtoff.cpp  
lammps-stable\_290ct2020/src/npair\_half\_nsq\_newtoff.h  
lammps-stable\_290ct2020/src/npair\_half\_nsq\_newtoff\_ghost.cpp  
lammps-stable\_290ct2020/src/npair\_half\_nsq\_newtoff\_ghost.h  
lammps-stable\_290ct2020/src/npair\_half\_nsq\_newton.cpp  
lammps-stable\_290ct2020/src/npair\_half\_nsq\_newton.h  
lammps-stable\_290ct2020/src/npair\_half\_respa\_bin\_newtoff.cpp  
lammps-stable\_290ct2020/src/npair\_half\_respa\_bin\_newtoff.h  
lammps-stable\_290ct2020/src/npair\_half\_respa\_bin\_newton.cpp  
lammps-stable\_290ct2020/src/npair\_half\_respa\_bin\_newton.h  
lammps-stable\_290ct2020/src/npair\_half\_respa\_bin\_newton\_tri.cpp  
lammps-stable\_290ct2020/src/npair\_half\_respa\_bin\_newton\_tri.h  
lammps-stable\_290ct2020/src/npair\_half\_respa\_nsq\_newtoff.cpp  
lammps-stable\_290ct2020/src/npair\_half\_respa\_nsq\_newtoff.h  
lammps-stable\_290ct2020/src/npair\_half\_respa\_nsq\_newton.cpp



lammps-stable\_290ct2020/src/npair\_half\_respa\_nsq\_newton.h  
lammps-stable\_290ct2020/src/npair\_half\_size\_bin\_newtoff.cpp  
lammps-stable\_290ct2020/src/npair\_half\_size\_bin\_newtoff.h  
lammps-stable\_290ct2020/src/npair\_half\_size\_bin\_newton.cpp  
lammps-stable\_290ct2020/src/npair\_half\_size\_bin\_newton.h  
lammps-stable\_290ct2020/src/npair\_half\_size\_bin\_newton\_tri.cpp  
lammps-stable\_290ct2020/src/npair\_half\_size\_bin\_newton\_tri.h  
lammps-stable\_290ct2020/src/npair\_half\_size\_nsq\_newtoff.cpp  
lammps-stable\_290ct2020/src/npair\_half\_size\_nsq\_newtoff.h  
lammps-stable\_290ct2020/src/npair\_half\_size\_nsq\_newton.cpp  
lammps-stable\_290ct2020/src/npair\_half\_size\_nsq\_newton.h  
lammps-stable\_290ct2020/src/npair\_halffull\_newtoff.cpp  
lammps-stable\_290ct2020/src/npair\_halffull\_newtoff.h  
lammps-stable\_290ct2020/src/npair\_halffull\_newton.cpp  
lammps-stable\_290ct2020/src/npair\_halffull\_newton.h  
lammps-stable\_290ct2020/src/npair\_skip.cpp  
lammps-stable\_290ct2020/src/npair\_skip.h  
lammps-stable\_290ct2020/src/npair\_skip\_respa.cpp  
lammps-stable\_290ct2020/src/npair\_skip\_respa.h  
lammps-stable\_290ct2020/src/npair\_skip\_size.cpp  
lammps-stable\_290ct2020/src/npair\_skip\_size.h  
lammps-stable\_290ct2020/src/npair\_skip\_size\_off2on.cpp  
lammps-stable\_290ct2020/src/npair\_skip\_size\_off2on.h  
lammps-stable\_290ct2020/src/npair\_skip\_size\_off2on\_oneside.cpp  
lammps-stable\_290ct2020/src/npair\_skip\_size\_off2on\_oneside.h  
lammps-stable\_290ct2020/src/nstencil.cpp  
lammps-stable\_290ct2020/src/nstencil.h  
lammps-stable\_290ct2020/src/nstencil\_full\_bin\_2d.cpp  
lammps-stable\_290ct2020/src/nstencil\_full\_bin\_2d.h  
lammps-stable\_290ct2020/src/nstencil\_full\_bin\_3d.cpp  
lammps-stable\_290ct2020/src/nstencil\_full\_bin\_3d.h  
lammps-stable\_290ct2020/src/nstencil\_full\_ghost\_bin\_2d.cpp  
lammps-stable\_290ct2020/src/nstencil\_full\_ghost\_bin\_2d.h  
lammps-stable\_290ct2020/src/nstencil\_full\_ghost\_bin\_3d.cpp  
lammps-stable\_290ct2020/src/nstencil\_full\_ghost\_bin\_3d.h  
lammps-stable\_290ct2020/src/nstencil\_full\_multi\_2d.cpp  
lammps-stable\_290ct2020/src/nstencil\_full\_multi\_2d.h  
lammps-stable\_290ct2020/src/nstencil\_full\_multi\_3d.cpp  
lammps-stable\_290ct2020/src/nstencil\_full\_multi\_3d.h  
lammps-stable\_290ct2020/src/nstencil\_half\_bin\_2d\_newtoff.cpp  
lammps-stable\_290ct2020/src/nstencil\_half\_bin\_2d\_newtoff.h  
lammps-stable\_290ct2020/src/nstencil\_half\_bin\_2d\_newton.cpp  
lammps-stable\_290ct2020/src/nstencil\_half\_bin\_2d\_newton.h  
lammps-stable\_290ct2020/src/nstencil\_half\_bin\_2d\_newton\_tri.cpp  
lammps-stable\_290ct2020/src/nstencil\_half\_bin\_2d\_newton\_tri.h  
lammps-stable\_290ct2020/src/nstencil\_half\_bin\_3d\_newtoff.cpp  
lammps-stable\_290ct2020/src/nstencil\_half\_bin\_3d\_newtoff.h  
lammps-stable\_290ct2020/src/nstencil\_half\_bin\_3d\_newton.cpp  
lammps-stable\_290ct2020/src/nstencil\_half\_bin\_3d\_newton.h  
lammps-stable\_290ct2020/src/nstencil\_half\_bin\_3d\_newton\_tri.cpp  
lammps-stable\_290ct2020/src/nstencil\_half\_bin\_3d\_newton\_tri.h  
lammps-stable\_290ct2020/src/nstencil\_half\_ghost\_bin\_2d\_newtoff.cpp  
lammps-stable\_290ct2020/src/nstencil\_half\_ghost\_bin\_2d\_newtoff.h  
lammps-stable\_290ct2020/src/nstencil\_half\_ghost\_bin\_3d\_newtoff.cpp  
lammps-stable\_290ct2020/src/nstencil\_half\_ghost\_bin\_3d\_newtoff.h  
lammps-stable\_290ct2020/src/nstencil\_half\_multi\_2d\_newtoff.cpp  
lammps-stable\_290ct2020/src/nstencil\_half\_multi\_2d\_newtoff.h  
lammps-stable\_290ct2020/src/nstencil\_half\_multi\_2d\_newton.cpp  
lammps-stable\_290ct2020/src/nstencil\_half\_multi\_2d\_newton.h  
lammps-stable\_290ct2020/src/nstencil\_half\_multi\_2d\_newton\_tri.cpp

lammps-stable\_290ct2020/src/nstencil\_half\_multi\_2d\_newton\_tri.h  
lammps-stable\_290ct2020/src/nstencil\_half\_multi\_3d\_newtoff.cpp  
lammps-stable\_290ct2020/src/nstencil\_half\_multi\_3d\_newtoff.h  
lammps-stable\_290ct2020/src/nstencil\_half\_multi\_3d\_newton.cpp  
lammps-stable\_290ct2020/src/nstencil\_half\_multi\_3d\_newton.h  
lammps-stable\_290ct2020/src/nstencil\_half\_multi\_3d\_newton\_tri.cpp  
lammps-stable\_290ct2020/src/nstencil\_half\_multi\_3d\_newton\_tri.h  
lammps-stable\_290ct2020/src/ntopo.cpp  
lammps-stable\_290ct2020/src/ntopo.h  
lammps-stable\_290ct2020/src/ntopo\_angle\_all.cpp  
lammps-stable\_290ct2020/src/ntopo\_angle\_all.h  
lammps-stable\_290ct2020/src/ntopo\_angle\_partial.cpp  
lammps-stable\_290ct2020/src/ntopo\_angle\_partial.h  
lammps-stable\_290ct2020/src/ntopo\_angle\_template.cpp  
lammps-stable\_290ct2020/src/ntopo\_angle\_template.h  
lammps-stable\_290ct2020/src/ntopo\_bond\_all.cpp  
lammps-stable\_290ct2020/src/ntopo\_bond\_all.h  
lammps-stable\_290ct2020/src/ntopo\_bond\_partial.cpp  
lammps-stable\_290ct2020/src/ntopo\_bond\_partial.h  
lammps-stable\_290ct2020/src/ntopo\_bond\_template.cpp  
lammps-stable\_290ct2020/src/ntopo\_bond\_template.h  
lammps-stable\_290ct2020/src/ntopo\_dihedral\_all.cpp  
lammps-stable\_290ct2020/src/ntopo\_dihedral\_all.h  
lammps-stable\_290ct2020/src/ntopo\_dihedral\_partial.cpp  
lammps-stable\_290ct2020/src/ntopo\_dihedral\_partial.h  
lammps-stable\_290ct2020/src/ntopo\_dihedral\_template.cpp  
lammps-stable\_290ct2020/src/ntopo\_dihedral\_template.h  
lammps-stable\_290ct2020/src/ntopo\_improper\_all.cpp  
lammps-stable\_290ct2020/src/ntopo\_improper\_all.h  
lammps-stable\_290ct2020/src/ntopo\_improper\_partial.cpp  
lammps-stable\_290ct2020/src/ntopo\_improper\_partial.h  
lammps-stable\_290ct2020/src/ntopo\_improper\_template.cpp  
lammps-stable\_290ct2020/src/ntopo\_improper\_template.h  
lammps-stable\_290ct2020/src/omp\_compat.h  
lammps-stable\_290ct2020/src/output.cpp  
lammps-stable\_290ct2020/src/output.h  
lammps-stable\_290ct2020/src/pack.h  
lammps-stable\_290ct2020/src/pair.cpp  
lammps-stable\_290ct2020/src/pair.h  
lammps-stable\_290ct2020/src/pair\_beck.cpp  
lammps-stable\_290ct2020/src/pair\_beck.h  
lammps-stable\_290ct2020/src/pair\_born.cpp  
lammps-stable\_290ct2020/src/pair\_born.h  
lammps-stable\_290ct2020/src/pair\_born\_coul\_dsf.cpp  
lammps-stable\_290ct2020/src/pair\_born\_coul\_dsf.h  
lammps-stable\_290ct2020/src/pair\_born\_coul\_wolf.cpp  
lammps-stable\_290ct2020/src/pair\_born\_coul\_wolf.h  
lammps-stable\_290ct2020/src/pair\_buck.cpp  
lammps-stable\_290ct2020/src/pair\_buck.h  
lammps-stable\_290ct2020/src/pair\_buck\_coul\_cut.cpp  
lammps-stable\_290ct2020/src/pair\_buck\_coul\_cut.h  
lammps-stable\_290ct2020/src/pair\_coul\_cut.cpp  
lammps-stable\_290ct2020/src/pair\_coul\_cut.h  
lammps-stable\_290ct2020/src/pair\_coul\_debye.cpp  
lammps-stable\_290ct2020/src/pair\_coul\_debye.h  
lammps-stable\_290ct2020/src/pair\_coul\_dsf.cpp  
lammps-stable\_290ct2020/src/pair\_coul\_dsf.h  
lammps-stable\_290ct2020/src/pair\_coul\_streitz.cpp  
lammps-stable\_290ct2020/src/pair\_coul\_streitz.h  
lammps-stable\_290ct2020/src/pair\_coul\_wolf.cpp

```
lammps-stable_290ct2020/src/pair_coul_wolf.h
lammps-stable_290ct2020/src/pair_deprecated.cpp
lammps-stable_290ct2020/src/pair_deprecated.h
lammps-stable_290ct2020/src/pair_dpd.cpp
lammps-stable_290ct2020/src/pair_dpd.h
lammps-stable_290ct2020/src/pair_dpd_tstat.cpp
lammps-stable_290ct2020/src/pair_dpd_tstat.h
lammps-stable_290ct2020/src/pair_gauss.cpp
lammps-stable_290ct2020/src/pair_gauss.h
lammps-stable_290ct2020/src/pair_hybrid.cpp
lammps-stable_290ct2020/src/pair_hybrid.h
lammps-stable_290ct2020/src/pair_hybrid_overlay.cpp
lammps-stable_290ct2020/src/pair_hybrid_overlay.h
lammps-stable_290ct2020/src/pair_lj96_cut.cpp
lammps-stable_290ct2020/src/pair_lj96_cut.h
lammps-stable_290ct2020/src/pair_lj_cubic.cpp
lammps-stable_290ct2020/src/pair_lj_cubic.h
lammps-stable_290ct2020/src/pair_lj_cut.cpp
lammps-stable_290ct2020/src/pair_lj_cut.h
lammps-stable_290ct2020/src/pair_lj_cut_coul_cut.cpp
lammps-stable_290ct2020/src/pair_lj_cut_coul_cut.h
lammps-stable_290ct2020/src/pair_lj_cut_coul_debye.cpp
lammps-stable_290ct2020/src/pair_lj_cut_coul_debye.h
lammps-stable_290ct2020/src/pair_lj_cut_coul_dsf.cpp
lammps-stable_290ct2020/src/pair_lj_cut_coul_dsf.h
lammps-stable_290ct2020/src/pair_lj_cut_coul_wolf.cpp
lammps-stable_290ct2020/src/pair_lj_cut_coul_wolf.h
lammps-stable_290ct2020/src/pair_lj_expand.cpp
lammps-stable_290ct2020/src/pair_lj_expand.h
lammps-stable_290ct2020/src/pair_lj_gromacs.cpp
lammps-stable_290ct2020/src/pair_lj_gromacs.h
lammps-stable_290ct2020/src/pair_lj_gromacs_coul_gromacs.cpp
lammps-stable_290ct2020/src/pair_lj_gromacs_coul_gromacs.h
lammps-stable_290ct2020/src/pair_lj_smooth.cpp
lammps-stable_290ct2020/src/pair_lj_smooth.h
lammps-stable_290ct2020/src/pair_lj_smooth_linear.cpp
lammps-stable_290ct2020/src/pair_lj_smooth_linear.h
lammps-stable_290ct2020/src/pair_mie_cut.cpp
lammps-stable_290ct2020/src/pair_mie_cut.h
lammps-stable_290ct2020/src/pair_morse.cpp
lammps-stable_290ct2020/src/pair_morse.h
lammps-stable_290ct2020/src/pair_soft.cpp
lammps-stable_290ct2020/src/pair_soft.h
lammps-stable_290ct2020/src/pair_table.cpp
lammps-stable_290ct2020/src/pair_table.h
lammps-stable_290ct2020/src/pair_uvm.cpp
lammps-stable_290ct2020/src/pair_uvm.h
lammps-stable_290ct2020/src/pair_yukawa.cpp
lammps-stable_290ct2020/src/pair_yukawa.h
lammps-stable_290ct2020/src/pair_zbl.cpp
lammps-stable_290ct2020/src/pair_zbl.h
lammps-stable_290ct2020/src/pair_zero.cpp
lammps-stable_290ct2020/src/pair_zero.h
lammps-stable_290ct2020/src/pointers.h
lammps-stable_290ct2020/src/potential_file_reader.cpp
lammps-stable_290ct2020/src/potential_file_reader.h
lammps-stable_290ct2020/src/procmap.cpp
lammps-stable_290ct2020/src/procmap.h
lammps-stable_290ct2020/src/random_mars.cpp
lammps-stable_290ct2020/src/random_mars.h
```

lammps-stable\_290ct2020/src/random\_park.cpp  
lammps-stable\_290ct2020/src/random\_park.h  
lammps-stable\_290ct2020/src/rcb.cpp  
lammps-stable\_290ct2020/src/rcb.h  
lammps-stable\_290ct2020/src/read\_data.cpp  
lammps-stable\_290ct2020/src/read\_data.h  
lammps-stable\_290ct2020/src/read\_dump.cpp  
lammps-stable\_290ct2020/src/read\_dump.h  
lammps-stable\_290ct2020/src/read\_restart.cpp  
lammps-stable\_290ct2020/src/read\_restart.h  
lammps-stable\_290ct2020/src/reader.cpp  
lammps-stable\_290ct2020/src/reader.h  
lammps-stable\_290ct2020/src/reader\_native.cpp  
lammps-stable\_290ct2020/src/reader\_native.h  
lammps-stable\_290ct2020/src/reader\_xyz.cpp  
lammps-stable\_290ct2020/src/reader\_xyz.h  
lammps-stable\_290ct2020/src/region.cpp  
lammps-stable\_290ct2020/src/region.h  
lammps-stable\_290ct2020/src/region\_block.cpp  
lammps-stable\_290ct2020/src/region\_block.h  
lammps-stable\_290ct2020/src/region\_cone.cpp  
lammps-stable\_290ct2020/src/region\_cone.h  
lammps-stable\_290ct2020/src/region\_cylinder.cpp  
lammps-stable\_290ct2020/src/region\_cylinder.h  
lammps-stable\_290ct2020/src/region\_deprecated.cpp  
lammps-stable\_290ct2020/src/region\_deprecated.h  
lammps-stable\_290ct2020/src/region\_intersect.cpp  
lammps-stable\_290ct2020/src/region\_intersect.h  
lammps-stable\_290ct2020/src/region\_plane.cpp  
lammps-stable\_290ct2020/src/region\_plane.h  
lammps-stable\_290ct2020/src/region\_prism.cpp  
lammps-stable\_290ct2020/src/region\_prism.h  
lammps-stable\_290ct2020/src/region\_sphere.cpp  
lammps-stable\_290ct2020/src/region\_sphere.h  
lammps-stable\_290ct2020/src/region\_union.cpp  
lammps-stable\_290ct2020/src/region\_union.h  
lammps-stable\_290ct2020/src/replicate.cpp  
lammps-stable\_290ct2020/src/replicate.h  
lammps-stable\_290ct2020/src/rerun.cpp  
lammps-stable\_290ct2020/src/rerun.h  
lammps-stable\_290ct2020/src/reset\_atom\_ids.cpp  
lammps-stable\_290ct2020/src/reset\_atom\_ids.h  
lammps-stable\_290ct2020/src/reset\_mol\_ids.cpp  
lammps-stable\_290ct2020/src/reset\_mol\_ids.h  
lammps-stable\_290ct2020/src/respa.cpp  
lammps-stable\_290ct2020/src/respa.h  
lammps-stable\_290ct2020/src/run.cpp  
lammps-stable\_290ct2020/src/run.h  
lammps-stable\_290ct2020/src/set.cpp  
lammps-stable\_290ct2020/src/set.h  
lammps-stable\_290ct2020/src/special.cpp  
lammps-stable\_290ct2020/src/special.h  
lammps-stable\_290ct2020/src/suffix.h  
lammps-stable\_290ct2020/src/table\_file\_reader.cpp  
lammps-stable\_290ct2020/src/table\_file\_reader.h  
lammps-stable\_290ct2020/src/text\_file\_reader.cpp  
lammps-stable\_290ct2020/src/text\_file\_reader.h  
lammps-stable\_290ct2020/src/thermo.cpp  
lammps-stable\_290ct2020/src/thermo.h  
lammps-stable\_290ct2020/src/timer.cpp

```
lammps-stable_290ct2020/src/timer.h
lammps-stable_290ct2020/src/tokenizer.cpp
lammps-stable_290ct2020/src/tokenizer.h
lammps-stable_290ct2020/src/universe.cpp
lammps-stable_290ct2020/src/universe.h
lammps-stable_290ct2020/src/update.cpp
lammps-stable_290ct2020/src/update.h
lammps-stable_290ct2020/src/utils.cpp
lammps-stable_290ct2020/src/utils.h
lammps-stable_290ct2020/src/variable.cpp
lammps-stable_290ct2020/src/variable.h
lammps-stable_290ct2020/src/velocity.cpp
lammps-stable_290ct2020/src/velocity.h
lammps-stable_290ct2020/src/verlet.cpp
lammps-stable_290ct2020/src/verlet.h
lammps-stable_290ct2020/src/version.h
lammps-stable_290ct2020/src/write_coeff.cpp
lammps-stable_290ct2020/src/write_coeff.h
lammps-stable_290ct2020/src/write_data.cpp
lammps-stable_290ct2020/src/write_data.h
lammps-stable_290ct2020/src/write_dump.cpp
lammps-stable_290ct2020/src/write_dump.h
lammps-stable_290ct2020/src/write_restart.cpp
lammps-stable_290ct2020/src/write_restart.h
lammps-stable_290ct2020/tools/
lammps-stable_290ct2020/tools/Makefile
lammps-stable_290ct2020/tools/README
lammps-stable_290ct2020/tools/amber2lmp/
lammps-stable_290ct2020/tools/amber2lmp/README
lammps-stable_290ct2020/tools/amber2lmp/amber2lammps.py
lammps-stable_290ct2020/tools/amber2lmp/dump2trj.py
lammps-stable_290ct2020/tools/amber2lmp/dump2trj99.py
lammps-stable_290ct2020/tools/binary2txt.cpp
lammps-stable_290ct2020/tools/ch2lmp/
lammps-stable_290ct2020/tools/ch2lmp/README
lammps-stable_290ct2020/tools/ch2lmp/charmm2lammps.pl
lammps-stable_290ct2020/tools/ch2lmp/example-cmap/
lammps-stable_290ct2020/tools/ch2lmp/example-cmap/1gb1.data
lammps-stable_290ct2020/tools/ch2lmp/example-cmap/1gb1.in
lammps-stable_290ct2020/tools/ch2lmp/example-cmap/1gb1.log
lammps-stable_290ct2020/tools/ch2lmp/example-cmap/1gb1.pdb
lammps-stable_290ct2020/tools/ch2lmp/example-cmap/1gb1.psf
lammps-stable_290ct2020/tools/ch2lmp/example-cmap/1gb1_ctrl.pdb
lammps-stable_290ct2020/tools/ch2lmp/example-cmap/1gb1_ctrl.psf
lammps-stable_290ct2020/tools/ch2lmp/example-cmap/convert.sh
lammps-stable_290ct2020/tools/ch2lmp/example-cmap/par_all36_prot.prm
lammps-stable_290ct2020/tools/ch2lmp/example-cmap/top_all36_prot.rtf
lammps-stable_290ct2020/tools/ch2lmp/example/
lammps-stable_290ct2020/tools/ch2lmp/example/1ac7.data
lammps-stable_290ct2020/tools/ch2lmp/example/1ac7.in
lammps-stable_290ct2020/tools/ch2lmp/example/1ac7.log
lammps-stable_290ct2020/tools/ch2lmp/example/1ac7.pdb
lammps-stable_290ct2020/tools/ch2lmp/example/1ac7.pdb1
lammps-stable_290ct2020/tools/ch2lmp/example/1ac7.pgn
lammps-stable_290ct2020/tools/ch2lmp/example/1ac7.psf
lammps-stable_290ct2020/tools/ch2lmp/example/1ac7_ctrl.pdb
lammps-stable_290ct2020/tools/ch2lmp/example/1ac7_ctrl.psf
lammps-stable_290ct2020/tools/ch2lmp/example/1ac7_pared.pdb
lammps-stable_290ct2020/tools/ch2lmp/example/1ac7_trj.pdb
lammps-stable_290ct2020/tools/ch2lmp/example/1ac7_trj.psf
```

```
lammps-stable_290ct2020/tools/ch2lmp/example/convert.sh
lammps-stable_290ct2020/tools/ch2lmp/example/par_all27_na.prm
lammps-stable_290ct2020/tools/ch2lmp/example/top_all27_na.rtf
lammps-stable_290ct2020/tools/ch2lmp/lammps2pdb.pl
lammps-stable_290ct2020/tools/ch2lmp/other/
lammps-stable_290ct2020/tools/ch2lmp/other/crd2pdb.pl
lammps-stable_290ct2020/tools/ch2lmp/other/in_mkdcd
lammps-stable_290ct2020/tools/ch2lmp/other/in_mkpdb
lammps-stable_290ct2020/tools/ch2lmp/other/mkdcd.f
lammps-stable_290ct2020/tools/ch2lmp/other/mkdcd_f77.f
lammps-stable_290ct2020/tools/ch2lmp/other/mkpdb.f
lammps-stable_290ct2020/tools/ch2lmp/other/pdb_to_crd.f
lammps-stable_290ct2020/tools/chain.f
lammps-stable_290ct2020/tools/cmake/
lammps-stable_290ct2020/tools/cmake/cmbuild
lammps-stable_290ct2020/tools/coding_standard/
lammps-stable_290ct2020/tools/coding_standard/README
lammps-stable_290ct2020/tools/coding_standard/permissions.py
lammps-stable_290ct2020/tools/coding_standard/whitespace.py
lammps-stable_290ct2020/tools/colvars/
lammps-stable_290ct2020/tools/colvars/Makefile
lammps-stable_290ct2020/tools/colvars/abf_data.cpp
lammps-stable_290ct2020/tools/colvars/abf_data.h
lammps-stable_290ct2020/tools/colvars/abf_integrate.cpp
lammps-stable_290ct2020/tools/createatoms/
lammps-stable_290ct2020/tools/createatoms/Manual.pdf
lammps-stable_290ct2020/tools/createatoms/README
lammps-stable_290ct2020/tools/createatoms/create.input
lammps-stable_290ct2020/tools/createatoms/createAtoms.f
lammps-stable_290ct2020/tools/createatoms/createAtoms.h
lammps-stable_290ct2020/tools/def.chain
lammps-stable_290ct2020/tools/def.chain.ab
lammps-stable_290ct2020/tools/def.micelle2d
lammps-stable_290ct2020/tools/drude/
lammps-stable_290ct2020/tools/drude/drude.dff
lammps-stable_290ct2020/tools/drude/polarizer.py
lammps-stable_290ct2020/tools/drude/schwerdtfeger.dff
lammps-stable_290ct2020/tools/eam_database/
lammps-stable_290ct2020/tools/eam_database/EAM.input
lammps-stable_290ct2020/tools/eam_database/EAM_code
lammps-stable_290ct2020/tools/eam_database/README
lammps-stable_290ct2020/tools/eam_database/create.f
lammps-stable_290ct2020/tools/eam_generate/
lammps-stable_290ct2020/tools/eam_generate/Al_Zhou.c
lammps-stable_290ct2020/tools/eam_generate/Cu_Mishin1.c
lammps-stable_290ct2020/tools/eam_generate/Cu_Zhou.c
lammps-stable_290ct2020/tools/eam_generate/README
lammps-stable_290ct2020/tools/eam_generate/W_Zhou.c
lammps-stable_290ct2020/tools/eff/
lammps-stable_290ct2020/tools/eff/README
lammps-stable_290ct2020/tools/eff/VMD-input.py
lammps-stable_290ct2020/tools/eff/bohr2ang.py
lammps-stable_290ct2020/tools/eff/cfg2lammps.py
lammps-stable_290ct2020/tools/eff/h2.out
lammps-stable_290ct2020/tools/eff/h2.vmd
lammps-stable_290ct2020/tools/eff/h2.xyz
lammps-stable_290ct2020/tools/eff/lmp2data.py
lammps-stable_290ct2020/tools/eff/lmp2radii.c
lammps-stable_290ct2020/tools/eff/lmp2radii.py
lammps-stable_290ct2020/tools/eff/lmp2radii.pyx
```

```
lammps-stable_290ct2020/tools/eff/lmp2radii_col.py
lammps-stable_290ct2020/tools/eff/lmp2xyz.py
lammps-stable_290ct2020/tools/eff/radii.vmd
lammps-stable_290ct2020/tools/eff/restart2data-pEFF.cpp
lammps-stable_290ct2020/tools/eff/setup.py
lammps-stable_290ct2020/tools/eff/structure_generators/
lammps-stable_290ct2020/tools/eff/structure_generators/Be-solid.pl
lammps-stable_290ct2020/tools/eff/structure_generators/Diamond.pl
lammps-stable_290ct2020/tools/eff/structure_generators/Li-hydride.pl
lammps-stable_290ct2020/tools/eff/structure_generators/Li-solid-angstrom.pl
lammps-stable_290ct2020/tools/eff/structure_generators/Li-solid.pl
lammps-stable_290ct2020/tools/eff/structure_generators/Uniform-electron-gas.p
l
lammps-stable_290ct2020/tools/eff/structure_generators/h2.pl
lammps-stable_290ct2020/tools/emacs/
lammps-stable_290ct2020/tools/emacs/README.md
lammps-stable_290ct2020/tools/emacs/lammps-mode.el
lammps-stable_290ct2020/tools/fep/
lammps-stable_290ct2020/tools/fep/README
lammps-stable_290ct2020/tools/fep/bar.py
lammps-stable_290ct2020/tools/fep/fdti.py
lammps-stable_290ct2020/tools/fep/fep.py
lammps-stable_290ct2020/tools/fep/nti.py
lammps-stable_290ct2020/tools/i-pi/
lammps-stable_290ct2020/tools/i-pi/.vimrc
lammps-stable_290ct2020/tools/i-pi/MANIFEST.in
lammps-stable_290ct2020/tools/i-pi/README.rst
lammps-stable_290ct2020/tools/i-pi/drivers/
lammps-stable_290ct2020/tools/i-pi/drivers/LJ.f90
lammps-stable_290ct2020/tools/i-pi/drivers/Makefile
lammps-stable_290ct2020/tools/i-pi/drivers/README
lammps-stable_290ct2020/tools/i-pi/drivers/SG.f90
lammps-stable_290ct2020/tools/i-pi/drivers/distance.f90
lammps-stable_290ct2020/tools/i-pi/drivers/driver.f90
lammps-stable_290ct2020/tools/i-pi/drivers/sockets.c
lammps-stable_290ct2020/tools/i-pi/examples/
lammps-stable_290ct2020/tools/i-pi/examples/lammps/
lammps-stable_290ct2020/tools/i-pi/examples/lammps/Makefile
lammps-stable_290ct2020/tools/i-pi/examples/lammps/README
lammps-stable_290ct2020/tools/i-pi/examples/lammps/h2o-piglet.2/
lammps-stable_290ct2020/tools/i-pi/examples/lammps/h2o-piglet.2/data.water
lammps-stable_290ct2020/tools/i-pi/examples/lammps/h2o-piglet.2/in.water
lammps-stable_290ct2020/tools/i-pi/examples/lammps/h2o-piglet.2/input.xml
lammps-stable_290ct2020/tools/i-pi/examples/lammps/h2o-piglet.2/water_298K.pd
b
lammps-stable_290ct2020/tools/i-pi/examples/lammps/h2o-piglet.4/
lammps-stable_290ct2020/tools/i-pi/examples/lammps/h2o-piglet.4/data.water
lammps-stable_290ct2020/tools/i-pi/examples/lammps/h2o-piglet.4/in.water
lammps-stable_290ct2020/tools/i-pi/examples/lammps/h2o-piglet.4/input.xml
lammps-stable_290ct2020/tools/i-pi/examples/lammps/h2o-piglet.4/water_298K.pd
b
lammps-stable_290ct2020/tools/i-pi/examples/lammps/h2o-piglet.8/
lammps-stable_290ct2020/tools/i-pi/examples/lammps/h2o-piglet.8/data.water
lammps-stable_290ct2020/tools/i-pi/examples/lammps/h2o-piglet.8/in.water
lammps-stable_290ct2020/tools/i-pi/examples/lammps/h2o-piglet.8/input.xml
lammps-stable_290ct2020/tools/i-pi/examples/lammps/h2o-piglet.8/water_298K.pd
b
lammps-stable_290ct2020/tools/i-pi/examples/lammps/h2o-pimd-rpc/
lammps-stable_290ct2020/tools/i-pi/examples/lammps/h2o-pimd-rpc/data.water_lo
ngrange
```

```
lammps-stable_290ct2020/tools/i-pi/examples/lammps/h2o-pimd-rpc/data.water_sh
orange
lammps-stable_290ct2020/tools/i-pi/examples/lammps/h2o-pimd-rpc/in.water_long
range
lammps-stable_290ct2020/tools/i-pi/examples/lammps/h2o-pimd-rpc/in.water_shor
range
lammps-stable_290ct2020/tools/i-pi/examples/lammps/h2o-pimd-rpc/input.xml
lammps-stable_290ct2020/tools/i-pi/examples/lammps/h2o-pimd-rpc/water_298K.pd
b
lammps-stable_290ct2020/tools/i-pi/examples/lammps/h2o-pimd/
lammps-stable_290ct2020/tools/i-pi/examples/lammps/h2o-pimd/data.water
lammps-stable_290ct2020/tools/i-pi/examples/lammps/h2o-pimd/in.water
lammps-stable_290ct2020/tools/i-pi/examples/lammps/h2o-pimd/input.xml
lammps-stable_290ct2020/tools/i-pi/examples/lammps/h2o-pimd/water_298K.pdb
lammps-stable_290ct2020/tools/i-pi/examples/tutorial/
lammps-stable_290ct2020/tools/i-pi/examples/tutorial/README
lammps-stable_290ct2020/tools/i-pi/examples/tutorial/tutorial-1/
lammps-stable_290ct2020/tools/i-pi/examples/tutorial/tutorial-1/our_ref.pdb
lammps-stable_290ct2020/tools/i-pi/examples/tutorial/tutorial-1/our_ref.xyz
lammps-stable_290ct2020/tools/i-pi/examples/tutorial/tutorial-1/tutorial-1.xm
l
lammps-stable_290ct2020/tools/i-pi/examples/tutorial/tutorial-2/
lammps-stable_290ct2020/tools/i-pi/examples/tutorial/tutorial-2/tutorial-1_RE
START
lammps-stable_290ct2020/tools/i-pi/examples/tutorial/tutorial-2/tutorial-2a.x
ml
lammps-stable_290ct2020/tools/i-pi/examples/tutorial/tutorial-2/tutorial-2b.x
ml
lammps-stable_290ct2020/tools/i-pi/examples/tutorial/tutorial-3/
lammps-stable_290ct2020/tools/i-pi/examples/tutorial/tutorial-3/our_ref.pdb
lammps-stable_290ct2020/tools/i-pi/examples/tutorial/tutorial-3/tutorial-3_np
t.xml
lammps-stable_290ct2020/tools/i-pi/examples/tutorial/tutorial-3/tutorial-3_nv
t.xml
lammps-stable_290ct2020/tools/i-pi/i-pi
lammps-stable_290ct2020/tools/i-pi/ipi/
lammps-stable_290ct2020/tools/i-pi/ipi/README
lammps-stable_290ct2020/tools/i-pi/ipi/__init__.py
lammps-stable_290ct2020/tools/i-pi/ipi/engine/
lammps-stable_290ct2020/tools/i-pi/ipi/engine/README
lammps-stable_290ct2020/tools/i-pi/ipi/engine/__init__.py
lammps-stable_290ct2020/tools/i-pi/ipi/engine/atoms.py
lammps-stable_290ct2020/tools/i-pi/ipi/engine/barostats.py
lammps-stable_290ct2020/tools/i-pi/ipi/engine/beads.py
lammps-stable_290ct2020/tools/i-pi/ipi/engine/cell.py
lammps-stable_290ct2020/tools/i-pi/ipi/engine/ensembles.py
lammps-stable_290ct2020/tools/i-pi/ipi/engine/forces.py
lammps-stable_290ct2020/tools/i-pi/ipi/engine/initializer.py
lammps-stable_290ct2020/tools/i-pi/ipi/engine/normalmodes.py
lammps-stable_290ct2020/tools/i-pi/ipi/engine/outputs.py
lammps-stable_290ct2020/tools/i-pi/ipi/engine/properties.py
lammps-stable_290ct2020/tools/i-pi/ipi/engine/simulation.py
lammps-stable_290ct2020/tools/i-pi/ipi/engine/thermostats.py
lammps-stable_290ct2020/tools/i-pi/ipi/inputs/
lammps-stable_290ct2020/tools/i-pi/ipi/inputs/README
lammps-stable_290ct2020/tools/i-pi/ipi/inputs/__init__.py
lammps-stable_290ct2020/tools/i-pi/ipi/inputs/atoms.py
lammps-stable_290ct2020/tools/i-pi/ipi/inputs/barostats.py
lammps-stable_290ct2020/tools/i-pi/ipi/inputs/beads.py
lammps-stable_290ct2020/tools/i-pi/ipi/inputs/cell.py
```



```
lammps-stable_290ct2020/tools/i-pi/ipi/inputs/ensembles.py
lammps-stable_290ct2020/tools/i-pi/ipi/inputs/forces.py
lammps-stable_290ct2020/tools/i-pi/ipi/inputs/initializer.py
lammps-stable_290ct2020/tools/i-pi/ipi/inputs/interface.py
lammps-stable_290ct2020/tools/i-pi/ipi/inputs/normalmodes.py
lammps-stable_290ct2020/tools/i-pi/ipi/inputs/outputs.py
lammps-stable_290ct2020/tools/i-pi/ipi/inputs/prng.py
lammps-stable_290ct2020/tools/i-pi/ipi/inputs/simulation.py
lammps-stable_290ct2020/tools/i-pi/ipi/inputs/thermostats.py
lammps-stable_290ct2020/tools/i-pi/ipi/interfaces/
lammps-stable_290ct2020/tools/i-pi/ipi/interfaces/README
lammps-stable_290ct2020/tools/i-pi/ipi/interfaces/__init__.py
lammps-stable_290ct2020/tools/i-pi/ipi/interfaces/sockets.py
lammps-stable_290ct2020/tools/i-pi/ipi/tests/
lammps-stable_290ct2020/tools/i-pi/ipi/tests/README
lammps-stable_290ct2020/tools/i-pi/ipi/tests/common.py
lammps-stable_290ct2020/tools/i-pi/ipi/tests/datest.py
lammps-stable_290ct2020/tools/i-pi/ipi/tests/test.pos_0.pdb
lammps-stable_290ct2020/tools/i-pi/ipi/tests/test.pos_0.xyz
lammps-stable_290ct2020/tools/i-pi/ipi/tests/test_contraction.py
lammps-stable_290ct2020/tools/i-pi/ipi/tests/test_io.py
lammps-stable_290ct2020/tools/i-pi/ipi/tests/test_runs.py
lammps-stable_290ct2020/tools/i-pi/ipi/utils/
lammps-stable_290ct2020/tools/i-pi/ipi/utils/README
lammps-stable_290ct2020/tools/i-pi/ipi/utils/__init__.py
lammps-stable_290ct2020/tools/i-pi/ipi/utils/depend.py
lammps-stable_290ct2020/tools/i-pi/ipi/utils/inputvalue.py
lammps-stable_290ct2020/tools/i-pi/ipi/utils/io/
lammps-stable_290ct2020/tools/i-pi/ipi/utils/io/README
lammps-stable_290ct2020/tools/i-pi/ipi/utils/io/__init__.py
lammps-stable_290ct2020/tools/i-pi/ipi/utils/io/io_binary.py
lammps-stable_290ct2020/tools/i-pi/ipi/utils/io/io_pdb.py
lammps-stable_290ct2020/tools/i-pi/ipi/utils/io/io_xml.py
lammps-stable_290ct2020/tools/i-pi/ipi/utils/io/io_xyz.py
lammps-stable_290ct2020/tools/i-pi/ipi/utils/mathtools.py
lammps-stable_290ct2020/tools/i-pi/ipi/utils/messages.py
lammps-stable_290ct2020/tools/i-pi/ipi/utils/nmtransform.py
lammps-stable_290ct2020/tools/i-pi/ipi/utils/prng.py
lammps-stable_290ct2020/tools/i-pi/ipi/utils/softexit.py
lammps-stable_290ct2020/tools/i-pi/ipi/units.py
lammps-stable_290ct2020/tools/i-pi/licenses/
lammps-stable_290ct2020/tools/i-pi/licenses/license_GPL.txt
lammps-stable_290ct2020/tools/i-pi/licenses/license_MIT.txt
lammps-stable_290ct2020/tools/i-pi/manual.pdf
lammps-stable_290ct2020/tools/ipp/
lammps-stable_290ct2020/tools/ipp/README
lammps-stable_290ct2020/tools/ipp/fill_parameters_createAtoms.input
lammps-stable_290ct2020/tools/ipp/fill_parameters_lammps.input
lammps-stable_290ct2020/tools/ipp/ipp
lammps-stable_290ct2020/tools/ipp/template_createAtoms.input
lammps-stable_290ct2020/tools/ipp/template_lammps.input
lammps-stable_290ct2020/tools/kate/
lammps-stable_290ct2020/tools/kate/README.txt
lammps-stable_290ct2020/tools/kate/lammps.xml
lammps-stable_290ct2020/tools/lammps-shell/
lammps-stable_290ct2020/tools/lammps-shell/Makefile
lammps-stable_290ct2020/tools/lammps-shell/README
lammps-stable_290ct2020/tools/lammps-shell/icons/
lammps-stable_290ct2020/tools/lammps-shell/icons/hicolor/
lammps-stable_290ct2020/tools/lammps-shell/icons/hicolor/128x128/
```

lammps-stable\_290ct2020/tools/lammps-shell/icons/hicolor/128x128/apps/  
lammps-stable\_290ct2020/tools/lammps-shell/icons/hicolor/128x128/apps/lammps.  
png  
lammps-stable\_290ct2020/tools/lammps-shell/icons/hicolor/16x16/  
lammps-stable\_290ct2020/tools/lammps-shell/icons/hicolor/16x16/apps/  
lammps-stable\_290ct2020/tools/lammps-shell/icons/hicolor/16x16/apps/lammps.pn  
g  
lammps-stable\_290ct2020/tools/lammps-shell/icons/hicolor/22x22/  
lammps-stable\_290ct2020/tools/lammps-shell/icons/hicolor/22x22/apps/  
lammps-stable\_290ct2020/tools/lammps-shell/icons/hicolor/22x22/apps/lammps.pn  
g  
lammps-stable\_290ct2020/tools/lammps-shell/icons/hicolor/32x32/  
lammps-stable\_290ct2020/tools/lammps-shell/icons/hicolor/32x32/apps/  
lammps-stable\_290ct2020/tools/lammps-shell/icons/hicolor/32x32/apps/lammps.pn  
g  
lammps-stable\_290ct2020/tools/lammps-shell/icons/hicolor/48x48/  
lammps-stable\_290ct2020/tools/lammps-shell/icons/hicolor/48x48/apps/  
lammps-stable\_290ct2020/tools/lammps-shell/icons/hicolor/48x48/apps/lammps.pn  
g  
lammps-stable\_290ct2020/tools/lammps-shell/icons/hicolor/64x64/  
lammps-stable\_290ct2020/tools/lammps-shell/icons/hicolor/64x64/apps/  
lammps-stable\_290ct2020/tools/lammps-shell/icons/hicolor/64x64/apps/lammps.pn  
g  
lammps-stable\_290ct2020/tools/lammps-shell/icons/lammps.ico  
lammps-stable\_290ct2020/tools/lammps-shell/icons/lmpfile.ico  
lammps-stable\_290ct2020/tools/lammps-shell/lammps-shell.cpp  
lammps-stable\_290ct2020/tools/lammps-shell/lammps-shell.desktop  
lammps-stable\_290ct2020/tools/lammps-shell/lmpicons.rc  
lammps-stable\_290ct2020/tools/lmp2arc/  
lammps-stable\_290ct2020/tools/lmp2arc/README  
lammps-stable\_290ct2020/tools/lmp2arc/src/  
lammps-stable\_290ct2020/tools/lmp2arc/src/Makefile  
lammps-stable\_290ct2020/tools/lmp2arc/src/ProcessPosFile01.c  
lammps-stable\_290ct2020/tools/lmp2arc/src/ProcessPosFile05.c  
lammps-stable\_290ct2020/tools/lmp2arc/src/ReadCarFile.c  
lammps-stable\_290ct2020/tools/lmp2arc/src/WriteArcFrame.c  
lammps-stable\_290ct2020/tools/lmp2arc/src/lmp2.h  
lammps-stable\_290ct2020/tools/lmp2arc/src/lmp2arc.c  
lammps-stable\_290ct2020/tools/lmp2arc/src/lmp2arc.doc  
lammps-stable\_290ct2020/tools/lmp2arc/src/unwrap\_molecules.c  
lammps-stable\_290ct2020/tools/lmp2arc/test/  
lammps-stable\_290ct2020/tools/lmp2arc/test/correct/  
lammps-stable\_290ct2020/tools/lmp2arc/test/correct/water8.arc  
lammps-stable\_290ct2020/tools/lmp2arc/test/correct/water8.arc.trueflags  
lammps-stable\_290ct2020/tools/lmp2arc/test/correct/water8.arc.unwrap  
lammps-stable\_290ct2020/tools/lmp2arc/test/water8.arc  
lammps-stable\_290ct2020/tools/lmp2arc/test/water8.arc.trueflags  
lammps-stable\_290ct2020/tools/lmp2arc/test/water8.car  
lammps-stable\_290ct2020/tools/lmp2arc/test/water8.pos  
lammps-stable\_290ct2020/tools/lmp2arc/test/water8\_unwrap.arc  
lammps-stable\_290ct2020/tools/lmp2cfg/  
lammps-stable\_290ct2020/tools/lmp2cfg/README.txt  
lammps-stable\_290ct2020/tools/lmp2cfg/examples/  
lammps-stable\_290ct2020/tools/lmp2cfg/examples/00001.cfg  
lammps-stable\_290ct2020/tools/lmp2cfg/examples/00002.cfg  
lammps-stable\_290ct2020/tools/lmp2cfg/examples/dump.atom  
lammps-stable\_290ct2020/tools/lmp2cfg/examples/lmp2cfg\_inp.txt  
lammps-stable\_290ct2020/tools/lmp2cfg/lmp2cfg.f  
lammps-stable\_290ct2020/tools/matlab/  
lammps-stable\_290ct2020/tools/matlab/README.pdf

```
lammps-stable_290ct2020/tools/matlab/lmp2cfg.m
lammps-stable_290ct2020/tools/matlab/readEAM.m
lammps-stable_290ct2020/tools/matlab/readdump_all.m
lammps-stable_290ct2020/tools/matlab/readdump_one.m
lammps-stable_290ct2020/tools/matlab/readlog.m
lammps-stable_290ct2020/tools/matlab/readrdf.m
lammps-stable_290ct2020/tools/matlab/scandump.m
lammps-stable_290ct2020/tools/mesont/
lammps-stable_290ct2020/tools/mesont/README
lammps-stable_290ct2020/tools/mesont/TMDGen/
lammps-stable_290ct2020/tools/mesont/TMDGen/Makefile
lammps-stable_290ct2020/tools/mesont/TMDGen/TMDGen.f90
lammps-stable_290ct2020/tools/mesont/TMDGen/TMDGen.xdt
lammps-stable_290ct2020/tools/mesont/TMDGen/TMDGen3D.f90
lammps-stable_290ct2020/tools/mesont/TMDGen/TMDGenData.f90
lammps-stable_290ct2020/tools/mesont/TMDGen/TMDSample.in
lammps-stable_290ct2020/tools/mesont/TMDGen/TPMGeom.f90
lammps-stable_290ct2020/tools/mesont/TMDGen/TPMLib.f90
lammps-stable_290ct2020/tools/mesont/TMDPotGen/
lammps-stable_290ct2020/tools/mesont/TMDPotGen/LinFun2.f90
lammps-stable_290ct2020/tools/mesont/TMDPotGen/Makefile
lammps-stable_290ct2020/tools/mesont/TMDPotGen/Spline1.f90
lammps-stable_290ct2020/tools/mesont/TMDPotGen/Spline2.f90
lammps-stable_290ct2020/tools/mesont/TMDPotGen/TMDPotGen.f90
lammps-stable_290ct2020/tools/mesont/TMDPotGen/TMDPotGen.xdt
lammps-stable_290ct2020/tools/mesont/TMDPotGen/TPMGeom.f90
lammps-stable_290ct2020/tools/mesont/TMDPotGen/TPMLib.f90
lammps-stable_290ct2020/tools/mesont/TMDPotGen/TubePotBase.f90
lammps-stable_290ct2020/tools/mesont/TMDPotGen/TubePotMono.f90
lammps-stable_290ct2020/tools/mesont/TMDPotGen/TubePotTrue.f90
lammps-stable_290ct2020/tools/mesont/dump2vtk.cpp
lammps-stable_290ct2020/tools/micelle2d.f
lammps-stable_290ct2020/tools/moltemplate/
lammps-stable_290ct2020/tools/moltemplate/README.txt
lammps-stable_290ct2020/tools/msi2lmp/
lammps-stable_290ct2020/tools/msi2lmp/README
lammps-stable_290ct2020/tools/msi2lmp/frc_files/
lammps-stable_290ct2020/tools/msi2lmp/frc_files/README
lammps-stable_290ct2020/tools/msi2lmp/frc_files/cff91.frc
lammps-stable_290ct2020/tools/msi2lmp/frc_files/clayff.frc
lammps-stable_290ct2020/tools/msi2lmp/frc_files/compass_published.frc
lammps-stable_290ct2020/tools/msi2lmp/frc_files/cvff.frc
lammps-stable_290ct2020/tools/msi2lmp/frc_files/cvff_aug.frc
lammps-stable_290ct2020/tools/msi2lmp/frc_files/oplsaa.frc
lammps-stable_290ct2020/tools/msi2lmp/frc_files/pcff.frc
lammps-stable_290ct2020/tools/msi2lmp/frc_files/pcff.rlb
lammps-stable_290ct2020/tools/msi2lmp/frc_files/pcff_templates.dat
lammps-stable_290ct2020/tools/msi2lmp/src/
lammps-stable_290ct2020/tools/msi2lmp/src/CheckLists.c
lammps-stable_290ct2020/tools/msi2lmp/src/Forcefield.h
lammps-stable_290ct2020/tools/msi2lmp/src/GetParameters.c
lammps-stable_290ct2020/tools/msi2lmp/src/InitializeItems.c
lammps-stable_290ct2020/tools/msi2lmp/src/MakeLists.c
lammps-stable_290ct2020/tools/msi2lmp/src/Makefile
lammps-stable_290ct2020/tools/msi2lmp/src/ReadCarFile.c
lammps-stable_290ct2020/tools/msi2lmp/src/ReadFrcFile.c
lammps-stable_290ct2020/tools/msi2lmp/src/ReadMdfFile.c
lammps-stable_290ct2020/tools/msi2lmp/src/SearchAndFill.c
lammps-stable_290ct2020/tools/msi2lmp/src/WriteDataFile.c
lammps-stable_290ct2020/tools/msi2lmp/src/msi2lmp.c
```

lammps-stable\_290ct2020/tools/msi2lmp/src/msi2lmp.h  
lammps-stable\_290ct2020/tools/msi2lmp/test/  
lammps-stable\_290ct2020/tools/msi2lmp/test/PyAC\_bulk-clayff.car  
lammps-stable\_290ct2020/tools/msi2lmp/test/PyAC\_bulk-clayff.mdf  
lammps-stable\_290ct2020/tools/msi2lmp/test/benzene-class1.car  
lammps-stable\_290ct2020/tools/msi2lmp/test/benzene-class1.mdf  
lammps-stable\_290ct2020/tools/msi2lmp/test/benzene-class2a.car  
lammps-stable\_290ct2020/tools/msi2lmp/test/benzene-class2a.mdf  
lammps-stable\_290ct2020/tools/msi2lmp/test/benzene-class2b.car  
lammps-stable\_290ct2020/tools/msi2lmp/test/benzene-class2b.mdf  
lammps-stable\_290ct2020/tools/msi2lmp/test/cnt-hexagonal-class1.car  
lammps-stable\_290ct2020/tools/msi2lmp/test/cnt-hexagonal-class1.mdf  
lammps-stable\_290ct2020/tools/msi2lmp/test/cnt-hexagonal-class2a.car  
lammps-stable\_290ct2020/tools/msi2lmp/test/cnt-hexagonal-class2a.mdf  
lammps-stable\_290ct2020/tools/msi2lmp/test/cnt-hexagonal-class2b.car  
lammps-stable\_290ct2020/tools/msi2lmp/test/cnt-hexagonal-class2b.mdf  
lammps-stable\_290ct2020/tools/msi2lmp/test/crambin-class1.car  
lammps-stable\_290ct2020/tools/msi2lmp/test/crambin-class1.mdf  
lammps-stable\_290ct2020/tools/msi2lmp/test/data-compare.pl  
lammps-stable\_290ct2020/tools/msi2lmp/test/decane-oplsaa.car  
lammps-stable\_290ct2020/tools/msi2lmp/test/decane-oplsaa.mdf  
lammps-stable\_290ct2020/tools/msi2lmp/test/ethane-class1.car  
lammps-stable\_290ct2020/tools/msi2lmp/test/ethane-class1.mdf  
lammps-stable\_290ct2020/tools/msi2lmp/test/ethane-class2a.car  
lammps-stable\_290ct2020/tools/msi2lmp/test/ethane-class2a.mdf  
lammps-stable\_290ct2020/tools/msi2lmp/test/ethane-class2b.car  
lammps-stable\_290ct2020/tools/msi2lmp/test/ethane-class2b.mdf  
lammps-stable\_290ct2020/tools/msi2lmp/test/ethane-oplsaa.car  
lammps-stable\_290ct2020/tools/msi2lmp/test/ethane-oplsaa.mdf  
lammps-stable\_290ct2020/tools/msi2lmp/test/h2-h2o-class1.car  
lammps-stable\_290ct2020/tools/msi2lmp/test/h2-h2o-class1.mdf  
lammps-stable\_290ct2020/tools/msi2lmp/test/h2-h2o-class2b.car  
lammps-stable\_290ct2020/tools/msi2lmp/test/h2-h2o-class2b.mdf  
lammps-stable\_290ct2020/tools/msi2lmp/test/hap\_crystal-class1.car  
lammps-stable\_290ct2020/tools/msi2lmp/test/hap\_crystal-class1.mdf  
lammps-stable\_290ct2020/tools/msi2lmp/test/hap\_crystal-class2b.car  
lammps-stable\_290ct2020/tools/msi2lmp/test/hap\_crystal-class2b.mdf  
lammps-stable\_290ct2020/tools/msi2lmp/test/hydrogen-class1.car  
lammps-stable\_290ct2020/tools/msi2lmp/test/hydrogen-class1.mdf  
lammps-stable\_290ct2020/tools/msi2lmp/test/hydrogen-class2a.car  
lammps-stable\_290ct2020/tools/msi2lmp/test/hydrogen-class2a.mdf  
lammps-stable\_290ct2020/tools/msi2lmp/test/in.PyAC\_bulk-clayff  
lammps-stable\_290ct2020/tools/msi2lmp/test/in.benzene-class1  
lammps-stable\_290ct2020/tools/msi2lmp/test/in.benzene-class2a  
lammps-stable\_290ct2020/tools/msi2lmp/test/in.benzene-class2b  
lammps-stable\_290ct2020/tools/msi2lmp/test/in.cnt-hexagonal-class1  
lammps-stable\_290ct2020/tools/msi2lmp/test/in.cnt-hexagonal-class2a  
lammps-stable\_290ct2020/tools/msi2lmp/test/in.cnt-hexagonal-class2b  
lammps-stable\_290ct2020/tools/msi2lmp/test/in.crambin-class1  
lammps-stable\_290ct2020/tools/msi2lmp/test/in.decane-oplsaa  
lammps-stable\_290ct2020/tools/msi2lmp/test/in.ethane-class1  
lammps-stable\_290ct2020/tools/msi2lmp/test/in.ethane-class2a  
lammps-stable\_290ct2020/tools/msi2lmp/test/in.ethane-class2b  
lammps-stable\_290ct2020/tools/msi2lmp/test/in.ethane-oplsaa  
lammps-stable\_290ct2020/tools/msi2lmp/test/in.h2-h2o-class1  
lammps-stable\_290ct2020/tools/msi2lmp/test/in.h2-h2o-class2b  
lammps-stable\_290ct2020/tools/msi2lmp/test/in.hap\_crystal-class1  
lammps-stable\_290ct2020/tools/msi2lmp/test/in.hap\_crystal-class2b  
lammps-stable\_290ct2020/tools/msi2lmp/test/in.hydrogen-class1  
lammps-stable\_290ct2020/tools/msi2lmp/test/in.hydrogen-class2a

lammps-stable\_290ct2020/tools/msi2lmp/test/in.naphthalene-class1  
lammps-stable\_290ct2020/tools/msi2lmp/test/in.naphthalene-class2a  
lammps-stable\_290ct2020/tools/msi2lmp/test/in.naphthalene-class2b  
lammps-stable\_290ct2020/tools/msi2lmp/test/in.nylon-class1  
lammps-stable\_290ct2020/tools/msi2lmp/test/in.phen3\_cff97-class1  
lammps-stable\_290ct2020/tools/msi2lmp/test/in.solv-poly-class2c  
lammps-stable\_290ct2020/tools/msi2lmp/test/in.water-class1  
lammps-stable\_290ct2020/tools/msi2lmp/test/in.water-class2b  
lammps-stable\_290ct2020/tools/msi2lmp/test/naphthalene-class1.car  
lammps-stable\_290ct2020/tools/msi2lmp/test/naphthalene-class1.mdf  
lammps-stable\_290ct2020/tools/msi2lmp/test/naphthalene-class2a.car  
lammps-stable\_290ct2020/tools/msi2lmp/test/naphthalene-class2a.mdf  
lammps-stable\_290ct2020/tools/msi2lmp/test/naphthalene-class2b.car  
lammps-stable\_290ct2020/tools/msi2lmp/test/naphthalene-class2b.mdf  
lammps-stable\_290ct2020/tools/msi2lmp/test/nylon-class1.car  
lammps-stable\_290ct2020/tools/msi2lmp/test/nylon-class1.mdf  
lammps-stable\_290ct2020/tools/msi2lmp/test/phen3\_cff97-class1.car  
lammps-stable\_290ct2020/tools/msi2lmp/test/phen3\_cff97-class1.mdf  
lammps-stable\_290ct2020/tools/msi2lmp/test/reference/  
lammps-stable\_290ct2020/tools/msi2lmp/test/reference/PyAC\_bulk-clayff.data  
lammps-stable\_290ct2020/tools/msi2lmp/test/reference/PyAC\_bulk-clayff.data2  
lammps-stable\_290ct2020/tools/msi2lmp/test/reference/benzene-class1.data  
lammps-stable\_290ct2020/tools/msi2lmp/test/reference/benzene-class1.data2  
lammps-stable\_290ct2020/tools/msi2lmp/test/reference/benzene-class1.data3  
lammps-stable\_290ct2020/tools/msi2lmp/test/reference/benzene-class2a.data  
lammps-stable\_290ct2020/tools/msi2lmp/test/reference/benzene-class2a.data2  
lammps-stable\_290ct2020/tools/msi2lmp/test/reference/benzene-class2b.data  
lammps-stable\_290ct2020/tools/msi2lmp/test/reference/benzene-class2b.data2  
lammps-stable\_290ct2020/tools/msi2lmp/test/reference/cnt-hexagonal-class1.dat  
a  
lammps-stable\_290ct2020/tools/msi2lmp/test/reference/cnt-hexagonal-class1.dat  
a2  
lammps-stable\_290ct2020/tools/msi2lmp/test/reference/cnt-hexagonal-class2a.da  
ta  
lammps-stable\_290ct2020/tools/msi2lmp/test/reference/cnt-hexagonal-class2a.da  
ta2  
lammps-stable\_290ct2020/tools/msi2lmp/test/reference/cnt-hexagonal-class2b.da  
ta  
lammps-stable\_290ct2020/tools/msi2lmp/test/reference/cnt-hexagonal-class2b.da  
ta2  
lammps-stable\_290ct2020/tools/msi2lmp/test/reference/crambin-class1.data  
lammps-stable\_290ct2020/tools/msi2lmp/test/reference/crambin-class1.data2  
lammps-stable\_290ct2020/tools/msi2lmp/test/reference/decane-oplsaa.data  
lammps-stable\_290ct2020/tools/msi2lmp/test/reference/decane-oplsaa.data2  
lammps-stable\_290ct2020/tools/msi2lmp/test/reference/ethane-class1.data  
lammps-stable\_290ct2020/tools/msi2lmp/test/reference/ethane-class1.data2  
lammps-stable\_290ct2020/tools/msi2lmp/test/reference/ethane-class2a.data  
lammps-stable\_290ct2020/tools/msi2lmp/test/reference/ethane-class2a.data2  
lammps-stable\_290ct2020/tools/msi2lmp/test/reference/ethane-class2b.data  
lammps-stable\_290ct2020/tools/msi2lmp/test/reference/ethane-class2b.data2  
lammps-stable\_290ct2020/tools/msi2lmp/test/reference/ethane-oplsaa.data  
lammps-stable\_290ct2020/tools/msi2lmp/test/reference/ethane-oplsaa.data2  
lammps-stable\_290ct2020/tools/msi2lmp/test/reference/h2-h2o-class1.data  
lammps-stable\_290ct2020/tools/msi2lmp/test/reference/h2-h2o-class1.data2  
lammps-stable\_290ct2020/tools/msi2lmp/test/reference/h2-h2o-class2b.data  
lammps-stable\_290ct2020/tools/msi2lmp/test/reference/h2-h2o-class2b.data2  
lammps-stable\_290ct2020/tools/msi2lmp/test/reference/hap\_crystal-class1.data  
lammps-stable\_290ct2020/tools/msi2lmp/test/reference/hap\_crystal-class1.data2  
lammps-stable\_290ct2020/tools/msi2lmp/test/reference/hap\_crystal-class2b.data  
lammps-stable\_290ct2020/tools/msi2lmp/test/reference/hap\_crystal-class2b.data

2

lammps-stable\_290ct2020/tools/msi2lmp/test/reference/hydrogen-class1.data  
lammps-stable\_290ct2020/tools/msi2lmp/test/reference/hydrogen-class1.data2  
lammps-stable\_290ct2020/tools/msi2lmp/test/reference/hydrogen-class2a.data  
lammps-stable\_290ct2020/tools/msi2lmp/test/reference/hydrogen-class2a.data2  
lammps-stable\_290ct2020/tools/msi2lmp/test/reference/naphthalene-class1.data  
lammps-stable\_290ct2020/tools/msi2lmp/test/reference/naphthalene-class1.data2  
lammps-stable\_290ct2020/tools/msi2lmp/test/reference/naphthalene-class2a.data  
lammps-stable\_290ct2020/tools/msi2lmp/test/reference/naphthalene-class2a.data2  
2  
lammps-stable\_290ct2020/tools/msi2lmp/test/reference/naphthalene-class2b.data  
lammps-stable\_290ct2020/tools/msi2lmp/test/reference/naphthalene-class2b.data2  
2  
lammps-stable\_290ct2020/tools/msi2lmp/test/reference/nylon-class1.data  
lammps-stable\_290ct2020/tools/msi2lmp/test/reference/nylon-class1.data2  
lammps-stable\_290ct2020/tools/msi2lmp/test/reference/phen3\_cff97-class1.data  
lammps-stable\_290ct2020/tools/msi2lmp/test/reference/phen3\_cff97-class1.data2  
lammps-stable\_290ct2020/tools/msi2lmp/test/reference/water-class1.data  
lammps-stable\_290ct2020/tools/msi2lmp/test/reference/water-class1.data2  
lammps-stable\_290ct2020/tools/msi2lmp/test/reference/water-class2b.data  
lammps-stable\_290ct2020/tools/msi2lmp/test/reference/water-class2b.data2  
lammps-stable\_290ct2020/tools/msi2lmp/test/runtests.sh  
lammps-stable\_290ct2020/tools/msi2lmp/test/water-class1.car  
lammps-stable\_290ct2020/tools/msi2lmp/test/water-class1.mdf  
lammps-stable\_290ct2020/tools/msi2lmp/test/water-class2b.car  
lammps-stable\_290ct2020/tools/msi2lmp/test/water-class2b.mdf  
lammps-stable\_290ct2020/tools/phonon/  
lammps-stable\_290ct2020/tools/phonon/Makefile  
lammps-stable\_290ct2020/tools/phonon/README  
lammps-stable\_290ct2020/tools/phonon/disp.cpp  
lammps-stable\_290ct2020/tools/phonon/dynmat.cpp  
lammps-stable\_290ct2020/tools/phonon/dynmat.h  
lammps-stable\_290ct2020/tools/phonon/global.h  
lammps-stable\_290ct2020/tools/phonon/green.cpp  
lammps-stable\_290ct2020/tools/phonon/green.h  
lammps-stable\_290ct2020/tools/phonon/interpolate.cpp  
lammps-stable\_290ct2020/tools/phonon/interpolate.h  
lammps-stable\_290ct2020/tools/phonon/kpath.cpp  
lammps-stable\_290ct2020/tools/phonon/kpath.h  
lammps-stable\_290ct2020/tools/phonon/main.cpp  
lammps-stable\_290ct2020/tools/phonon/memory.cpp  
lammps-stable\_290ct2020/tools/phonon/memory.h  
lammps-stable\_290ct2020/tools/phonon/phonon.cpp  
lammps-stable\_290ct2020/tools/phonon/phonon.h  
lammps-stable\_290ct2020/tools/phonon/phonopy.cpp  
lammps-stable\_290ct2020/tools/phonon/phonopy.h  
lammps-stable\_290ct2020/tools/phonon/qnodes.cpp  
lammps-stable\_290ct2020/tools/phonon/qnodes.h  
lammps-stable\_290ct2020/tools/phonon/timer.cpp  
lammps-stable\_290ct2020/tools/phonon/timer.h  
lammps-stable\_290ct2020/tools/phonon/version.h  
lammps-stable\_290ct2020/tools/polybond/  
lammps-stable\_290ct2020/tools/polybond/Manual.pdf  
lammps-stable\_290ct2020/tools/polybond/README  
lammps-stable\_290ct2020/tools/polybond/lmpsdata.py  
lammps-stable\_290ct2020/tools/pymol\_asphere/  
lammps-stable\_290ct2020/tools/pymol\_asphere/README  
lammps-stable\_290ct2020/tools/pymol\_asphere/doc/  
lammps-stable\_290ct2020/tools/pymol\_asphere/doc/asphere\_vis.1  
lammps-stable\_290ct2020/tools/pymol\_asphere/doc/asphere\_vis.manpage

lammps-stable\_290ct2020/tools/pymol\_asphere/doc/asphere\_vis.pdf  
lammps-stable\_290ct2020/tools/pymol\_asphere/examples/  
lammps-stable\_290ct2020/tools/pymol\_asphere/examples/README  
lammps-stable\_290ct2020/tools/pymol\_asphere/examples/colors.ellipse  
lammps-stable\_290ct2020/tools/pymol\_asphere/src/  
lammps-stable\_290ct2020/tools/pymol\_asphere/src/Makefile  
lammps-stable\_290ct2020/tools/pymol\_asphere/src/asphere\_vis.cpp  
lammps-stable\_290ct2020/tools/pymol\_asphere/src/cartesian.cpp  
lammps-stable\_290ct2020/tools/pymol\_asphere/src/cartesian.h  
lammps-stable\_290ct2020/tools/pymol\_asphere/src/colors.cpp  
lammps-stable\_290ct2020/tools/pymol\_asphere/src/colors.h  
lammps-stable\_290ct2020/tools/pymol\_asphere/src/commandline.cpp  
lammps-stable\_290ct2020/tools/pymol\_asphere/src/commandline.h  
lammps-stable\_290ct2020/tools/pymol\_asphere/src/error.cpp  
lammps-stable\_290ct2020/tools/pymol\_asphere/src/error.h  
lammps-stable\_290ct2020/tools/pymol\_asphere/src/glsurface.cpp  
lammps-stable\_290ct2020/tools/pymol\_asphere/src/glsurface.h  
lammps-stable\_290ct2020/tools/pymol\_asphere/src/m\_constants.h  
lammps-stable\_290ct2020/tools/pymol\_asphere/src/make\_manpages.sh  
lammps-stable\_290ct2020/tools/pymol\_asphere/src/misc.cpp  
lammps-stable\_290ct2020/tools/pymol\_asphere/src/misc.h  
lammps-stable\_290ct2020/tools/pymol\_asphere/src/miscm.cpp  
lammps-stable\_290ct2020/tools/pymol\_asphere/src/miscm.h  
lammps-stable\_290ct2020/tools/pymol\_asphere/src/spherical.cpp  
lammps-stable\_290ct2020/tools/pymol\_asphere/src/spherical.h  
lammps-stable\_290ct2020/tools/python/  
lammps-stable\_290ct2020/tools/python/README  
lammps-stable\_290ct2020/tools/python/dump2cfg.py  
lammps-stable\_290ct2020/tools/python/dump2pdb.py  
lammps-stable\_290ct2020/tools/python/dump2xyz.py  
lammps-stable\_290ct2020/tools/python/dumpsort.py  
lammps-stable\_290ct2020/tools/python/log2txt.py  
lammps-stable\_290ct2020/tools/python/logplot.py  
lammps-stable\_290ct2020/tools/python/neb\_combine.py  
lammps-stable\_290ct2020/tools/python/neb\_final.py  
lammps-stable\_290ct2020/tools/python/pizza/  
lammps-stable\_290ct2020/tools/python/pizza/cfg.py  
lammps-stable\_290ct2020/tools/python/pizza/dump.py  
lammps-stable\_290ct2020/tools/python/pizza/gnu.py  
lammps-stable\_290ct2020/tools/python/pizza/log.py  
lammps-stable\_290ct2020/tools/python/pizza/pdbfile.py  
lammps-stable\_290ct2020/tools/python/pizza/xyz.py  
lammps-stable\_290ct2020/tools/reax/  
lammps-stable\_290ct2020/tools/reax/Cutoff.dic  
lammps-stable\_290ct2020/tools/reax/README.txt  
lammps-stable\_290ct2020/tools/reax/reaxc\_bond.pl  
lammps-stable\_290ct2020/tools/replica/  
lammps-stable\_290ct2020/tools/replica/README.md  
lammps-stable\_290ct2020/tools/replica/example/  
lammps-stable\_290ct2020/tools/replica/example/data.peptide  
lammps-stable\_290ct2020/tools/replica/example/in.peptide  
lammps-stable\_290ct2020/tools/replica/example/parse\_ene.py  
lammps-stable\_290ct2020/tools/replica/example/run.sh  
lammps-stable\_290ct2020/tools/replica/example/runlog.05Sep19  
lammps-stable\_290ct2020/tools/replica/example/temps.txt  
lammps-stable\_290ct2020/tools/replica/reorder\_remd\_traj.py  
lammps-stable\_290ct2020/tools/singularity/  
lammps-stable\_290ct2020/tools/singularity/README.md  
lammps-stable\_290ct2020/tools/singularity/centos7.def  
lammps-stable\_290ct2020/tools/singularity/centos8.def

lammps-stable\_290ct2020/tools/singularity/fedora32\_mingw.def  
lammps-stable\_290ct2020/tools/singularity/ubuntu16.04.def  
lammps-stable\_290ct2020/tools/singularity/ubuntu18.04.def  
lammps-stable\_290ct2020/tools/singularity/ubuntu18.04\_amd\_rocm.def  
lammps-stable\_290ct2020/tools/singularity/ubuntu18.04\_gpu.def  
lammps-stable\_290ct2020/tools/singularity/ubuntu18.04\_intel\_oneapi.def  
lammps-stable\_290ct2020/tools/singularity/ubuntu18.04\_nvidia.def  
lammps-stable\_290ct2020/tools/singularity/ubuntu20.04.def  
lammps-stable\_290ct2020/tools/singularity/ubuntu20.04\_amd\_rocm.def  
lammps-stable\_290ct2020/tools/singularity/ubuntu20.04\_gpu.def  
lammps-stable\_290ct2020/tools/singularity/ubuntu20.04\_intel\_oneapi.def  
lammps-stable\_290ct2020/tools/singularity/ubuntu20.04\_nvidia.def  
lammps-stable\_290ct2020/tools/smd/  
lammps-stable\_290ct2020/tools/smd/Makefile  
lammps-stable\_290ct2020/tools/smd/dump2vtk\_tris.cpp  
lammps-stable\_290ct2020/tools/spin/  
lammps-stable\_290ct2020/tools/spin/interpolate\_gneb/  
lammps-stable\_290ct2020/tools/spin/interpolate\_gneb/README  
lammps-stable\_290ct2020/tools/spin/interpolate\_gneb/interpolate.c  
lammps-stable\_290ct2020/tools/spin/interpolate\_gneb/neb\_init.dat  
lammps-stable\_290ct2020/tools/swig/  
lammps-stable\_290ct2020/tools/swig/CMakeLists.txt  
lammps-stable\_290ct2020/tools/swig/README  
lammps-stable\_290ct2020/tools/swig/lammps.i  
lammps-stable\_290ct2020/tools/swig/lammps\_shell.i  
lammps-stable\_290ct2020/tools/swig/run\_java\_example.sh.in  
lammps-stable\_290ct2020/tools/swig/run\_lua\_example.sh.in  
lammps-stable\_290ct2020/tools/swig/run\_perl\_example.sh.in  
lammps-stable\_290ct2020/tools/swig/run\_python\_example.sh.in  
lammps-stable\_290ct2020/tools/swig/run\_ruby\_example.sh.in  
lammps-stable\_290ct2020/tools/swig/run\_tcl\_example.sh.in  
lammps-stable\_290ct2020/tools/swig/tcldummy.c  
lammps-stable\_290ct2020/tools/valgrind/  
lammps-stable\_290ct2020/tools/valgrind/GTest.supp  
lammps-stable\_290ct2020/tools/valgrind/OpenMP.supp  
lammps-stable\_290ct2020/tools/valgrind/OpenMPI.supp  
lammps-stable\_290ct2020/tools/valgrind/Python3.supp  
lammps-stable\_290ct2020/tools/valgrind/README  
lammps-stable\_290ct2020/tools/vim/  
lammps-stable\_290ct2020/tools/vim/README.txt  
lammps-stable\_290ct2020/tools/vim/filetype.vim  
lammps-stable\_290ct2020/tools/vim/lammps.vim  
lammps-stable\_290ct2020/tools/vim/mysyntax.vim  
lammps-stable\_290ct2020/tools/vim/vimrc  
lammps-stable\_290ct2020/tools/xmgrace/  
lammps-stable\_290ct2020/tools/xmgrace/README  
lammps-stable\_290ct2020/tools/xmgrace/lammpsplot.cpp  
lammps-stable\_290ct2020/tools/xmgrace/lammpsplot.pdf  
lammps-stable\_290ct2020/tools/xmgrace/logplotawk.oneliner  
lammps-stable\_290ct2020/tools/xmgrace/logplotgrep.oneliner  
lammps-stable\_290ct2020/tools/xmgrace/plotthermodata.awk  
lammps-stable\_290ct2020/unittest/  
lammps-stable\_290ct2020/unittest/.clang-format  
lammps-stable\_290ct2020/unittest/CMakeLists.txt  
lammps-stable\_290ct2020/unittest/README.md  
lammps-stable\_290ct2020/unittest/c-library/  
lammps-stable\_290ct2020/unittest/c-library/CMakeLists.txt  
lammps-stable\_290ct2020/unittest/c-library/data.fourmol  
lammps-stable\_290ct2020/unittest/c-library/in.fourmol  
lammps-stable\_290ct2020/unittest/c-library/test\_library\_commands.cpp



```
lammps-stable_290ct2020/unittest/c-library/test_library_config.cpp
lammps-stable_290ct2020/unittest/c-library/test_library_open.cpp
lammps-stable_290ct2020/unittest/c-library/test_library_properties.cpp
lammps-stable_290ct2020/unittest/c-library/test_main.cpp
lammps-stable_290ct2020/unittest/c-library/test_main.h
lammps-stable_290ct2020/unittest/commands/
lammps-stable_290ct2020/unittest/commands/CMakeLists.txt
lammps-stable_290ct2020/unittest/commands/data.fourmol
lammps-stable_290ct2020/unittest/commands/in.fourmol
lammps-stable_290ct2020/unittest/commands/test_kim_commands.cpp
lammps-stable_290ct2020/unittest/commands/test_lattice_region.cpp
lammps-stable_290ct2020/unittest/commands/test_reset_ids.cpp
lammps-stable_290ct2020/unittest/commands/test_simple_commands.cpp
lammps-stable_290ct2020/unittest/cplusplus/
lammps-stable_290ct2020/unittest/cplusplus/CMakeLists.txt
lammps-stable_290ct2020/unittest/cplusplus/test_input_class.cpp
lammps-stable_290ct2020/unittest/cplusplus/test_lammps_class.cpp
lammps-stable_290ct2020/unittest/force-styles/
lammps-stable_290ct2020/unittest/force-styles/CMakeLists.txt
lammps-stable_290ct2020/unittest/force-styles/check_tests.py
lammps-stable_290ct2020/unittest/force-styles/error_stats.cpp
lammps-stable_290ct2020/unittest/force-styles/error_stats.h
lammps-stable_290ct2020/unittest/force-styles/test_angle_style.cpp
lammps-stable_290ct2020/unittest/force-styles/test_bond_style.cpp
lammps-stable_290ct2020/unittest/force-styles/test_config.h
lammps-stable_290ct2020/unittest/force-styles/test_config_reader.cpp
lammps-stable_290ct2020/unittest/force-styles/test_config_reader.h
lammps-stable_290ct2020/unittest/force-styles/test_error_stats.cpp
lammps-stable_290ct2020/unittest/force-styles/test_fix_timestep.cpp
lammps-stable_290ct2020/unittest/force-styles/test_main.cpp
lammps-stable_290ct2020/unittest/force-styles/test_main.h
lammps-stable_290ct2020/unittest/force-styles/test_pair_style.cpp
lammps-stable_290ct2020/unittest/force-styles/tests/
lammps-stable_290ct2020/unittest/force-styles/tests/angle-charmm.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/angle-class2.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/angle-class2_p6.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/angle-cosine.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/angle-cosine_delta.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/angle-cosine_periodic.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/angle-cosine_shift.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/angle-cosine_shift_exp.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/angle-cosine_squared.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/angle-cross.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/angle-fourier.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/angle-fourier_simple.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/angle-harmonic.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/angle-hybrid.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/angle-mm3.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/angle-quartic.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/angle-table_linear.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/angle-table_spline.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/angle-zero.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/angle_table.txt
lammps-stable_290ct2020/unittest/force-styles/tests/atomic-pair-adp.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/atomic-pair-atm.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/atomic-pair-beck.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/atomic-pair-born.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/atomic-pair-colloid.yaml
```

lammps-stable\_290ct2020/unittest/force-styles/tests/atomic-pair-colloid\_multi.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/atomic-pair-colloid\_multi\_tri.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/atomic-pair-colloid\_tiled.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/atomic-pair-colloid\_tiled\_tri.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/atomic-pair-eam.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/atomic-pair-eam\_alloy.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/atomic-pair-eam\_alloy\_real.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/atomic-pair-eam\_cd.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/atomic-pair-eam\_cd\_old.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/atomic-pair-eam\_cd\_real.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/atomic-pair-eam\_fs.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/atomic-pair-eam\_fs\_real.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/atomic-pair-eam\_real.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/atomic-pair-edip.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/atomic-pair-eim.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/atomic-pair-gauss.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/atomic-pair-hybrid-eam.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/atomic-pair-hybrid-eam\_fs.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/atomic-pair-kim\_lj.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/atomic-pair-meam\_c.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/atomic-pair-meam\_spline.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/atomic-pair-meam\_sw\_spline.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/atomic-pair-momb.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/atomic-pair-polymorphic\_eam.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/atomic-pair-reax\_c.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/atomic-pair-reax\_c\_lgvdw.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/atomic-pair-reax\_c\_noeq.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/atomic-pair-table\_bitmap.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/atomic-pair-table\_linear.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/atomic-pair-table\_lookup.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/atomic-pair-table\_spline.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/atomic-pair-yukawa\_colloid.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/bond-class2.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/bond-fene.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/bond-fene\_expand.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/bond-gromos.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/bond-harmonic.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/bond-harmonic\_shift.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/bond-harmonic\_shift\_cut.yaml

```
aml
lammps-stable_290ct2020/unittest/force-styles/tests/bond-hybrid.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/bond-mm3.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/bond-morse.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/bond-nonlinear.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/bond-quartic.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/bond-table_linear.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/bond-table_spline.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/bond-zero.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/bond_table.txt
lammps-stable_290ct2020/unittest/force-styles/tests/data.airebo
lammps-stable_290ct2020/unittest/force-styles/tests/data.colloid
lammps-stable_290ct2020/unittest/force-styles/tests/data.fourmol
lammps-stable_290ct2020/unittest/force-styles/tests/data.manybody
lammps-stable_290ct2020/unittest/force-styles/tests/data.manybody-charge
lammps-stable_290ct2020/unittest/force-styles/tests/data.metal
lammps-stable_290ct2020/unittest/force-styles/tests/dump.colloid
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-addforce_const.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-addforce_variable.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-aveforce_const.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-aveforce_variable.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-drag.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-efield_constant.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-efield_region.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-efield_variable.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-heat.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-heat_region.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-lineforce.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-momentum.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-momentum_chunk.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-nph.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-npt_aniso.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-npt_iso.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-npt_tri.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-nve.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-nve_limit.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-nve_noforce.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-nvt.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-oneway.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-planeforce.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-press_berendsen_iso.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-rattle_angle.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-rattle_bond.
```

```
yaml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-restrain.yam
l
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-rigid_group.
yaml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-rigid_molecu
le.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-rigid_molecu
le_tri.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-rigid_nph.ya
ml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-rigid_nph_sm
all.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-rigid_npt.ya
ml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-rigid_npt_sm
all.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-rigid_nve_gr
oup.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-rigid_nve_mo
lecule.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-rigid_nve_si
ngle.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-rigid_nve_sm
all.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-rigid_nvt.ya
ml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-rigid_nvt_sm
all.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-rigid_singl
e.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-rigid_small.
yaml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-setforce_con
st.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-setforce_reg
ion.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-setforce_var
iable.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-shake_angle.
yaml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-shake_bond.y
aml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-smd_couple.y
aml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-smd_tether.y
aml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-spring_chun
k.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-spring_coupl
e.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-spring_rg.ya
ml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-spring_self.
yaml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-spring_tethe
r.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-temp_berends
en.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-temp_csld.ya
```

```
ml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-temp_csvr.ya
ml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-temp_rescal
e.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-wall_harmoni
c_const.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-wall_lj1043_
const.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-wall_lj126_c
onst.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-wall_lj93_co
nst.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/fix-timestep-wall_morse_c
onst.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/gen_angle_table.py
lammps-stable_290ct2020/unittest/force-styles/tests/in.airebo
lammps-stable_290ct2020/unittest/force-styles/tests/in.colloid
lammps-stable_290ct2020/unittest/force-styles/tests/in.empty
lammps-stable_290ct2020/unittest/force-styles/tests/in.fourmol
lammps-stable_290ct2020/unittest/force-styles/tests/in.manybody
lammps-stable_290ct2020/unittest/force-styles/tests/in.manybody-charge
lammps-stable_290ct2020/unittest/force-styles/tests/in.metal
lammps-stable_290ct2020/unittest/force-styles/tests/kspace-ewald.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/kspace-ewald_disp.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/kspace-ewald_nozforce.yam
l
lammps-stable_290ct2020/unittest/force-styles/tests/kspace-ewald_slab.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/kspace-ewald_tri.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/kspace-msm.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/kspace-msm_cg.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/kspace-msm_nopbc.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/kspace-pppm.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/kspace-pppm_ad.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/kspace-pppm_cg.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/kspace-pppm_cg_ad.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/kspace-pppm_cg_tiled.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/kspace-pppm_disp.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/kspace-pppm_disp_ad.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/kspace-pppm_disp_ad_only.
yaml
lammps-stable_290ct2020/unittest/force-styles/tests/kspace-pppm_disp_only.yam
l
lammps-stable_290ct2020/unittest/force-styles/tests/kspace-pppm_disp_tip4p.ya
ml
lammps-stable_290ct2020/unittest/force-styles/tests/kspace-pppm_nozforce.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/kspace-pppm_slab.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/kspace-pppm_stagger.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/kspace-pppm_stagger_tile
d.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/kspace-pppm_tiled.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/kspace-pppm_tip4p.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/kspace-pppm_tip4p_ad.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/kspace-pppm_tip4p_nozforc
e.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/kspace-pppm_tip4p_slab.ya
ml
lammps-stable_290ct2020/unittest/force-styles/tests/kspace-pppm_tri.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/manybody-pair-airebo.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/manybody-pair-airebo_00.y
```

```
aml
lammps-stable_290ct2020/unittest/force-styles/tests/manybody-pair-airebo_m.ya
ml
lammps-stable_290ct2020/unittest/force-styles/tests/manybody-pair-airebo_m00.
yaml
lammps-stable_290ct2020/unittest/force-styles/tests/manybody-pair-bop.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/manybody-pair-bop_save.ya
ml
lammps-stable_290ct2020/unittest/force-styles/tests/manybody-pair-comb.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/manybody-pair-comb3.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/manybody-pair-edip_multi.
yaml
lammps-stable_290ct2020/unittest/force-styles/tests/manybody-pair-extep.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/manybody-pair-gw.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/manybody-pair-gw_zbl.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/manybody-pair-lcbop.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/manybody-pair-meam_c.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/manybody-pair-mliap_snap.
yaml
lammps-stable_290ct2020/unittest/force-styles/tests/manybody-pair-mliap_snap_
chem.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/manybody-pair-nb3b_harmon
ic.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/manybody-pair-polymorphic
_sw.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/manybody-pair-polymorphic
_tersoff.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/manybody-pair-rebo.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/manybody-pair-snap.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/manybody-pair-snap_chem.y
aml
lammps-stable_290ct2020/unittest/force-styles/tests/manybody-pair-sw-multi.ya
ml
lammps-stable_290ct2020/unittest/force-styles/tests/manybody-pair-sw.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/manybody-pair-tersoff.yam
l
lammps-stable_290ct2020/unittest/force-styles/tests/manybody-pair-tersoff_mo
d.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/manybody-pair-tersoff_mod
_c.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/manybody-pair-tersoff_tab
le.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/manybody-pair-tersoff_zb
l.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/manybody-pair-vashishta.y
aml
lammps-stable_290ct2020/unittest/force-styles/tests/manybody-pair-vashishta_t
able.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/manybody-pair_edip_multi.
yaml
lammps-stable_290ct2020/unittest/force-styles/tests/mol-pair-beck.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/mol-pair-born.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/mol-pair-born_coul_dsf.ya
ml
lammps-stable_290ct2020/unittest/force-styles/tests/mol-pair-born_coul_dsf_c
s.yaml
lammps-stable_290ct2020/unittest/force-styles/tests/mol-pair-born_coul_long.y
aml
lammps-stable_290ct2020/unittest/force-styles/tests/mol-pair-born_coul_long_c
s.yaml
```

lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-born\_coul\_msm.ya  
ml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-born\_coul\_msm\_ta  
ble.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-born\_coul\_table\_  
cs.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-born\_coul\_wolf.y  
aml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-born\_coul\_wolf\_c  
s.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-buck.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-buck\_coul\_cut.ya  
ml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-buck\_coul\_long.y  
aml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-buck\_coul\_long\_c  
s.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-buck\_coul\_msm.ya  
ml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-buck\_coul\_msm\_ta  
ble.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-buck\_coul\_table.  
yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-buck\_coul\_table\_  
cs.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-buck\_long\_coul\_l  
ong.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-buck\_long\_coul\_o  
ff.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-buck\_long\_cut\_co  
ul\_long.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-buck\_mdf.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-buck\_table\_coul\_  
long.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-buck\_table\_coul\_  
off.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-buck\_table\_coul\_  
table.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-cosine\_squared.y  
aml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-coul\_cut.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-coul\_cut\_soft.ya  
ml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-coul\_debye.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-coul\_diel.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-coul\_dsf.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-coul\_long.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-coul\_long\_cs.yam  
l  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-coul\_long\_soft.y  
aml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-coul\_msm.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-coul\_msm\_table.y  
aml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-coul\_shield.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-coul\_slater\_cut.  
yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-coul\_slater\_lon  
g.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-coul\_streitz\_lon

g.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-coul\_streitz\_wol  
f.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-coul\_table.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-coul\_table\_cs.ya  
ml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-coul\_wolf.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-coul\_wolf\_cs.yam  
l  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-dpd.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-dpd\_tstat.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-e3b.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-gauss.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-gauss\_cut.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-hybrid-overlay.y  
aml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-hybrid.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lennard\_mdf.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj96\_cut.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_charmm\_coul\_c  
harmm.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_charmm\_coul\_c  
harmm\_implicit.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_charmm\_coul\_l  
ong.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_charmm\_coul\_l  
ong\_soft.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_charmm\_coul\_m  
sm.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_charmm\_coul\_m  
sm\_table.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_charmm\_coul\_t  
able.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_charmmfsw\_cou  
l\_charmmfsw.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_charmmfsw\_cou  
l\_long.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_charmmfsw\_cou  
l\_table.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_class2.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_class2\_coul\_c  
ut.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_class2\_coul\_c  
ut\_soft.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_class2\_coul\_l  
ong.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_class2\_coul\_l  
ong\_cs.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_class2\_coul\_l  
ong\_soft.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_class2\_coul\_t  
able.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_class2\_coul\_t  
able\_cs.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_class2\_soft.y  
aml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_cubic.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_cut.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_cut\_coul\_cut.  
yaml



lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_cut\_coul\_cut\_soft.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_cut\_coul\_debye.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_cut\_coul\_dsf.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_cut\_coul\_long.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_cut\_coul\_long\_cs.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_cut\_coul\_long\_soft.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_cut\_coul\_msm.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_cut\_coul\_msm\_table.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_cut\_coul\_table.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_cut\_coul\_table\_cs.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_cut\_coul\_wolf.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_cut\_soft.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_cut\_tip4p\_cut.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_cut\_tip4p\_long.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_cut\_tip4p\_long\_soft.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_cut\_tip4p\_table.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_expand.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_expand\_coul\_long.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_expand\_coul\_table.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_gromacs.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_gromacs\_coul\_gromacs.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_long\_coul\_long.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_long\_coul\_off.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_long\_cut\_coul\_long.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_long\_cut\_tip4p\_long.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_long\_tip4p\_long.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_mdf.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_sdk.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_sdk\_coul\_long.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_sdk\_coul\_msm.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_sdk\_coul\_msm\_table.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_sdk\_coul\_table.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_smooth.yaml

lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_smooth\_linear.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_table\_coul\_long.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_table\_coul\_of.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_table\_coul\_table.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_table\_tip4p\_long.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-lj\_table\_tip4p\_table.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-mie\_cut.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-morse.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-morse\_smooth\_linear.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-morse\_soft.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-nm\_cut.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-nm\_cut\_coul\_cut.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-nm\_cut\_coul\_long.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-nm\_cut\_coul\_table.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-python\_hybrid.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-python\_lj.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-soft.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-table.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-tip4p\_cut.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-tip4p\_long.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-tip4p\_long\_soft.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-tip4p\_table.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-ufm.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-yukawa.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-zbl.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/mol-pair-zero.yaml  
lammps-stable\_290ct2020/unittest/force-styles/tests/pair\_table\_beck.txt  
lammps-stable\_290ct2020/unittest/force-styles/tests/pair\_table\_bitmap.txt  
lammps-stable\_290ct2020/unittest/force-styles/tests/pair\_table\_lj\_cut.txt  
lammps-stable\_290ct2020/unittest/force-styles/tests/py\_pot.py  
lammps-stable\_290ct2020/unittest/force-styles/yaml\_reader.h  
lammps-stable\_290ct2020/unittest/force-styles/yaml\_writer.cpp  
lammps-stable\_290ct2020/unittest/force-styles/yaml\_writer.h  
lammps-stable\_290ct2020/unittest/formats/  
lammps-stable\_290ct2020/unittest/formats/CMakeLists.txt  
lammps-stable\_290ct2020/unittest/formats/test\_atom\_styles.cpp  
lammps-stable\_290ct2020/unittest/formats/test\_dump\_atom.cpp  
lammps-stable\_290ct2020/unittest/formats/test\_dump\_atom\_gz.cpp  
lammps-stable\_290ct2020/unittest/formats/test\_dump\_atom\_zstd.cpp  
lammps-stable\_290ct2020/unittest/formats/test\_dump\_cfg.cpp  
lammps-stable\_290ct2020/unittest/formats/test\_dump\_cfg\_gz.cpp  
lammps-stable\_290ct2020/unittest/formats/test\_dump\_cfg\_zstd.cpp  
lammps-stable\_290ct2020/unittest/formats/test\_dump\_custom.cpp  
lammps-stable\_290ct2020/unittest/formats/test\_dump\_custom\_gz.cpp  
lammps-stable\_290ct2020/unittest/formats/test\_dump\_custom\_zstd.cpp  
lammps-stable\_290ct2020/unittest/formats/test\_dump\_local\_gz.cpp  
lammps-stable\_290ct2020/unittest/formats/test\_dump\_local\_zstd.cpp  
lammps-stable\_290ct2020/unittest/formats/test\_dump\_xyz\_gz.cpp

```
lammps-stable_290ct2020/unittest/formats/test_dump_xyz_zstd.cpp
lammps-stable_290ct2020/unittest/formats/test_eim_potential_file_reader.cpp
lammps-stable_290ct2020/unittest/formats/test_file_operations.cpp
lammps-stable_290ct2020/unittest/formats/test_pair_unit_convert.cpp
lammps-stable_290ct2020/unittest/formats/test_potential_file_reader.cpp
lammps-stable_290ct2020/unittest/fortran/
lammps-stable_290ct2020/unittest/fortran/CMakeLists.txt
lammps-stable_290ct2020/unittest/fortran/mpi_stubs.f90
lammps-stable_290ct2020/unittest/fortran/test_fortran_commands.f90
lammps-stable_290ct2020/unittest/fortran/test_fortran_create.f90
lammps-stable_290ct2020/unittest/fortran/wrap_commands.cpp
lammps-stable_290ct2020/unittest/fortran/wrap_create.cpp
lammps-stable_290ct2020/unittest/python/
lammps-stable_290ct2020/unittest/python/CMakeLists.txt
lammps-stable_290ct2020/unittest/python/func.py
lammps-stable_290ct2020/unittest/python/python-capabilities.py
lammps-stable_290ct2020/unittest/python/python-commands.py
lammps-stable_290ct2020/unittest/python/python-numpy.py
lammps-stable_290ct2020/unittest/python/python-open.py
lammps-stable_290ct2020/unittest/python/python-pylammps.py
lammps-stable_290ct2020/unittest/python/test_python_package.cpp
lammps-stable_290ct2020/unittest/testing/
lammps-stable_290ct2020/unittest/testing/core.h
lammps-stable_290ct2020/unittest/testing/systems/
lammps-stable_290ct2020/unittest/testing/systems/melt.h
lammps-stable_290ct2020/unittest/testing/utils.h
lammps-stable_290ct2020/unittest/tools/
lammps-stable_290ct2020/unittest/tools/CMakeLists.txt
lammps-stable_290ct2020/unittest/tools/test_lammps_shell.py
lammps-stable_290ct2020/unittest/utils/
lammps-stable_290ct2020/unittest/utils/CMakeLists.txt
lammps-stable_290ct2020/unittest/utils/test_fmtlib.cpp
lammps-stable_290ct2020/unittest/utils/test_math_eigen_impl.cpp
lammps-stable_290ct2020/unittest/utils/test_mempool.cpp
lammps-stable_290ct2020/unittest/utils/test_tokenizer.cpp
lammps-stable_290ct2020/unittest/utils/test_utils.cpp
aenet-lammps-2021May04/
aenet-lammps-2021May04/ANN/
aenet-lammps-2021May04/ANN/Fe/
aenet-lammps-2021May04/ANN/Fe/Fe.10tw-10tw.ann
aenet-lammps-2021May04/ANN/Fe/in.aenet_mm
aenet-lammps-2021May04/ANN/Fe/in.aenet_nve
aenet-lammps-2021May04/ANN/Fe/log.lammps.g++_mm
aenet-lammps-2021May04/ANN/Fe/log.lammps.icc_mm
aenet-lammps-2021May04/ANN/TiO2/
aenet-lammps-2021May04/ANN/TiO2/O.15t-15t.nn
aenet-lammps-2021May04/ANN/TiO2/Ti.15t-15t.nn
aenet-lammps-2021May04/ANN/TiO2/TiO2.lmp
aenet-lammps-2021May04/ANN/TiO2/in.aenet_nve
aenet-lammps-2021May04/ANN/TiO2/log.lammps.g++
aenet-lammps-2021May04/ANN/TiO2/readme.txt
aenet-lammps-2021May04/README.md
aenet-lammps-2021May04/USER-AENET/
aenet-lammps-2021May04/USER-AENET/Install.sh
aenet-lammps-2021May04/USER-AENET/pair_aenet.cpp
aenet-lammps-2021May04/USER-AENET/pair_aenet.h
aenet-lammps-2021May04/aenet/
aenet-lammps-2021May04/aenet/Makefile.lammps.empty
aenet-lammps-2021May04/aenet/Makefile.lammps.gfortran
aenet-lammps-2021May04/aenet/Makefile.lammps.ifort
```

```
aenet-lammps-2021May04/aenet/aenet-2.0.3_lammps.patch
aenet-lammps-2021May04/aenet/aenet-2.0.4_lammps.patch
```

### 3. Clone aenet package to lib/aenet/

In [3]:

```
%cd lammps-stable_290ct2020/lib/aenet/
!git clone https://github.com/atomisticnet/aenet

/data/home/na2782/Programs/test/lammps-stable_290ct2020/lib/aenet
Cloning into 'aenet'...
remote: Enumerating objects: 969, done.
remote: Counting objects: 100% (26/26), done.
remote: Compressing objects: 100% (17/17), done.
remote: Total 969 (delta 12), reused 15 (delta 9), pack-reused 943
Receiving objects: 100% (969/969), 28.10 MiB | 38.07 MiB/s, done.
Resolving deltas: 100% (654/654), done.
Checking out files: 100% (569/569), done.
```

### 4. Compiling aenet as LAMMPS library

Patch and compile aenet library. Please check the below two files are created:

1. libaenet.a: library of aenet
2. Makefile.lammps: linker of aenet and lammps

In [4]:

```
!patch -u -p1 -d aenet/ < aenet-2.0.4_lammps.patch
%cd aenet/src/
!make -f makefiles/Makefile.gfortran_serial lib
%cd ../../

patching file src/Makefile.inc
patching file src/ext/feedforward.f90
patching file src/ext/sfbasis.f90
patching file src/makefiles/Makefile.gfortran_serial
patching file src/makefiles/Makefile.ifort_serial
/data/home/na2782/Programs/test/lammps-stable_290ct2020/lib/aenet/aenet/src
gfortran -c -O3 -pedantic ext/io.f90 -o io.o
ext/io.f90:239:0:

    out = out // ' '

Warning: '__builtin_memset': specified size 18446744073709551615 exceeds maximum object size 9223372036854775807 [-Wstringop-overflow=]
gfortran -c -O3 -pedantic aeio.f90 -o aeio.o
gfortran -c -O3 -pedantic ext/chebyshev.f90 -o chebyshev.o
gfortran -c -O3 -pedantic constants.f90 -o constants.o
gfortran -c -O3 -pedantic ext/xsflib.f90 -o xsflib.o
gfortran -c -O3 -pedantic geometry.f90 -o geometry.o
gfortran -c -O3 -pedantic ext/sortlib.f90 -o sortlib.o
gfortran -c -O3 -pedantic ext/lclist.f90 -o lclist.o
gfortran -c -O3 -pedantic ext/feedforward.f90 -o feedforward.o
gfortran -c -O3 -pedantic ext/sfbasis.f90 -o sfbasis.o
gfortran -c -O3 -pedantic ext/symmfunc.f90 -o symmfunc.o
```

```

gfortran -c -O3 -pedantic sfsetup.f90 -o sfsetup.o
gfortran -c -O3 -pedantic trainset.f90 -o trainset.o
gfortran -c -O3 -pedantic potential.f90 -o potential.o
gfortran -c -O3 -pedantic ext/timing.f90 -o timing.o
gfortran -c -O3 -pedantic aenet.f90 -o aenet.o
gfortran -c -O3 -pedantic input.f90 -o input.o
gfortran -c -O3 -pedantic parallel.F90 -o parallel.o
gfortran -c -O3 -pedantic random.f90 -o random.o
gfortran -c -O3 -pedantic optimize.f90 -o optimize.o
ar -crUusv ../../libaenet.a aenet.o aeio.o chebyshev.o constants.o feedforward.o geometry.o input.o io.o lclist.o optimize.o parallel.o potential.o random.o sfbasis.o sfsetup.o sortlib.o symmfunc.o timing.o trainset.o xsflib.o
a - aenet.o
a - aeio.o
a - chebyshev.o
a - constants.o
a - feedforward.o
a - geometry.o
a - input.o
a - io.o
a - lclist.o
a - optimize.o
a - parallel.o
a - potential.o
a - random.o
a - sfbasis.o
a - sfsetup.o
a - sortlib.o
a - symmfunc.o
a - timing.o
a - trainset.o
a - xsflib.o
gfortran -c -O3 -pedantic -fPIC -o aenet_pic.o aenet.f90
gfortran -c -O3 -pedantic -fPIC -o aeio_pic.o aeio.f90
gfortran -c -O3 -pedantic -fPIC -o chebyshev_pic.o ext/chebyshev.f90
gfortran -c -O3 -pedantic -fPIC -o constants_pic.o constants.f90
gfortran -c -O3 -pedantic -fPIC -o feedforward_pic.o ext/feedforward.f90
gfortran -c -O3 -pedantic -fPIC -o geometry_pic.o geometry.f90
gfortran -c -O3 -pedantic -fPIC -o input_pic.o input.f90
gfortran -c -O3 -pedantic -fPIC -o io_pic.o ext/io.f90
ext/io.f90:239:0:

```

```

out = out // ' '

```

**Warning:** '\_\_\_builtin\_memset': specified size 18446744073709551615 exceeds maximum object size 9223372036854775807 [-Wstringop-overflow=]

```

gfortran -c -O3 -pedantic -fPIC -o lclist_pic.o ext/lclist.f90
gfortran -c -O3 -pedantic -fPIC -o optimize_pic.o optimize.f90
gfortran -c -O3 -pedantic -fPIC -o parallel_pic.o parallel.F90
gfortran -c -O3 -pedantic -fPIC -o potential_pic.o potential.f90
gfortran -c -O3 -pedantic -fPIC -o random_pic.o random.f90
gfortran -c -O3 -pedantic -fPIC -o sfbasis_pic.o ext/sfbasis.f90
gfortran -c -O3 -pedantic -fPIC -o sfsetup_pic.o sfsetup.f90
gfortran -c -O3 -pedantic -fPIC -o sortlib_pic.o ext/sortlib.f90
gfortran -c -O3 -pedantic -fPIC -o symmfunc_pic.o ext/symmfunc.f90
gfortran -c -O3 -pedantic -fPIC -o timing_pic.o ext/timing.f90
gfortran -c -O3 -pedantic -fPIC -o trainset_pic.o trainset.f90
gfortran -c -O3 -pedantic -fPIC -o xsflib_pic.o ext/xsflib.f90
gcc -shared aenet_pic.o aeio_pic.o chebyshev_pic.o constants_pic.o feedforward_pic.o geometry_pic.o input_pic.o io_pic.o lclist_pic.o optimize_pic.o paral

```

```
lcl_pic.o potential_pic.o random_pic.o sfbasis_pic.o sfsetup_pic.o sortlib_pi
c.o symmfunc_pic.o timing_pic.o trainset_pic.o xsflib_pic.o -lgfortran -o lib
aenet.so
```

## 5. Compiling LAMMPS with aenet library

If you use intel compiler, replace mpi to icc\_openmpi. Other compile option of LAMMPS, please see LAMMPS manual.

In [5]:

```
%cd ../../src/
!make yes-user-aenet
!make mpi
```

```
/data/home/na2782/Programs/test/lammps-stable_290ct2020/src
Installing package user-aenet
Gathering installed package information (may take a little while)
make[1]: Entering directory '/data/home/na2782/Programs/test/lammps-stable_29
0ct2020/src'
Gathering git version information
make[1]: Leaving directory '/data/home/na2782/Programs/test/lammps-stable_290
ct2020/src'
Compiling LAMMPS for machine mpi
make[1]: Entering directory '/data/home/na2782/Programs/test/lammps-stable_29
0ct2020/src/Obj_mpi'
cc -O -o fastdep.exe ../DEPEND/fastdep.c
make[1]: Leaving directory '/data/home/na2782/Programs/test/lammps-stable_290
ct2020/src/Obj_mpi'
make[1]: Entering directory '/data/home/na2782/Programs/test/lammps-stable_29
0ct2020/src/Obj_mpi'
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../main.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../ntopo_bond_all.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../fix_drag.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../region_sphere.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../compute_deprecated.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../compute_rdf.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../pair_lj_cut_coul_dsf.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../npair_full_multi.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../write_dump.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../compute_pressure.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../dump_movie.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../nstencil_half_multi_2d_newton_tri.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../fix_nvt_sllod.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
```

```

PI_SKIP_MPICXX=1      -c ../fix_tmd.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../input.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../compute_property_local.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../fix_wall.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../compute_dipole_chunk.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../compute_angle_local.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../region_plane.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../kpace_deprecated.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../fix_nph_sphere.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../fix_lineforce.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../ntopo_bond_partial.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../run.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../min_fire.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../imbalance.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../create_box.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../npair_half_nsq_newtoff_ghost.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../compute_com.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../compute_ke.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../pair_lj_expand.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../npair_half_size_bin_newtoff.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../library.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../compute_gyration_chunk.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../pair_hybrid.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../pair_lj_gromacs_coul_gromacs.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../comm_brick.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../fix_spring_self.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../fix_nve_noforce.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../angle_hybrid.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../compute_angle.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../atom_vec_line.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM

```

```

PI_SKIP_MPICXX=1      -c ../respa.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../nstencil_half_ghost_bin_2d_newtoff.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../reader.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../fix_dummy.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../pair_born_coul_wolf.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../compute_pe_atom.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../fix_wall_lj1043.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../pair_beck.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../pair_zbl.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../velocity.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../npair_skip_size_off2on.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../min_hftn.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../compute_pair_local.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../npair_half_size_nsq_newtoff.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../compute_temp_sphere.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../npair_half_size_bin_newton.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../compute_heat_flux.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../compute_temp_region.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../angle_zero.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../irregular.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../fix_numdiff.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../npair_half_nsq_newtoff.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../nstencil_half_bin_2d_newtoff.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../ntopo_improper_template.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../npair_full_nsq_ghost.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../nstencil_half_bin_2d_newton.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../read_restart.cpp
../read_restart.cpp: In member function 'void LAMMPS_NS::ReadRestart::check_e
of_magic()':
../read_restart.cpp:1198:10: warning: ignoring return value of 'size_t fread
(void*, size_t, size_t, FILE*)', declared with attribute warn_unused_result
[-Wunused-result]
    fread(str,sizeof(char),n,fp);
    ~~~~~^~~~~~

```



```
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../lattice.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../pair_dpd.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../fix_store.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../compute_group_group.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../nstencil_full_ghost_bin_3d.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../dump_custom.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../nstencil_half_ghost_bin_3d_newtoff.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../npair_halffull_newtoff.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../min_quickmin.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../compute_centro_atom.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../pair_lj_gromacs.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../compute_reduce_region.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../thermo.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../pair_buck_coul_cut.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../improper_zero.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../compute_contact_atom.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../pair_morse.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../pair.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../region_intersect.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../compute_hexorder_atom.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../fix_langevin.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../compute_angmom_chunk.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../fix_nvt.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../compute_aggregate_atom.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../body.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../npair_full_bin.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../output.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../nstencil_half_bin_2d_newton_tri.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../fix_plane_force.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../fix_ave_correlate.cpp
```

```
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../compute_msd_chunk.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../compute_cna_atom.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../neigh_request.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../compute_slice.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../domain.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../lmpython.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../compute_msd.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../region.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../pair_table.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../math_extra.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../imbalance_group.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../nstencil_full_bin_2d.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../fix_enforce2d.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../compute_temp_deform.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../lammps.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../pair_uvm.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../nstencil_full_bin_3d.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../npair_half_respa_bin_newton.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../npair_full_nsq.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../ntopo_improper_partial.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../pair_lj_cut_coul_cut.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../nstencil_full_multi_3d.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../fix_spring_chunk.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../compute_vcm_chunk.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../nstencil_full_ghost_bin_2d.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../fix_deprecated.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../table_file_reader.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../region_union.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../fix_temp_rescale.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../fix_gravity.cpp
```

```

mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../compute_pe.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../comm_tiled.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../fix_vector.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../dump_deprecated.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../replicate.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../read_dump.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../npair_skip_size.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../molecule.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../fix_temp_csvr.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../npair_half_multi_newtoff.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../min_cg.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../npair_full_bin_atomonly.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../procmap.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../compute_cluster_atom.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../fix_deform.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../pair_born_coul_dsf.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../imbalance_neigh.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../variable.cpp
../variable.cpp: In member function 'int LAMMPS_NS::Variable::next(int, char*
*)':
../variable.cpp:712:14: warning: ignoring return value of 'size_t fread(void
*, size_t, size_t, FILE*)', declared with attribute warn_unused_result [-Wunu
sed-result]
    fread(buf,1,64,fp);
    ~~~~~^~~~~~
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../compute_omega_chunk.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../ntopo_improper_all.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../pair_lj_cut_coul_debye.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../npair_half_full_newton.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../compute_erotate_sphere.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../npair_skip.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../pair_buck.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1 -c ../fix_external.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM

```

```

PI_SKIP_MPICXX=1      -c ../math_special.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../delete_bonds.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../force.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../finish.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../compute_fragment_atom.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../pair_coul_wolf.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../npair_skip_respa.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../fix_ave_histo.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../bond.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../fix_store_state.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../improper.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../npair_half_bin_newtoff.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../compute_com_chunk.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../compute_temp_chunk.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../math_eigen.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../nstencil_half_multi_2d_newtoff.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../hashlittle.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../pair_deprecated.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../min_linesearch.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../angle_deprecated.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../write_coeff.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../pair_born.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../neigh_list.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../pair_lj96_cut.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../verlet.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../pair_lj_smooth_linear.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../atom.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../fix_press_berendsen.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../pair_aenet.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../nstencil_half_multi_2d_newton.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM

```

```
PI_SKIP_MPICXX=1      -c ../fix_wall_harmonic.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../compute_global_atom.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../compute_chunk_atom.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../min.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../fix_print.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../displace_atoms.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../nstencil_half_bin_3d_newtoff.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../imbalance_time.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../npair_skip_size_off2on_oneside.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../pair_mie_cut.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../imbalance_store.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../fix_wall_reflect.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../fix_indent.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../npair_half_respa_nsq_newtoff.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../compute_stress_atom.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../reader_native.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../fix_respa.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../compute_gyration.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../special.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../fix_spring.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../fix_viscous.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../dump_image.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../compute_erotate_sphere_atom.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../rerun.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../compute_pair.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../rcb.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../balance.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../compute_temp.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../info.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../error.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
```

```
PI_SKIP_MPICXX=1      -c ../fix_nh.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../nbin_standard.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../fix_temp_csld.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../fix_property_atom.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../delete_atoms.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../ntopo_dihedral_partial.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../fix.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../ntopo_angle_template.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../pair_lj_cubic.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../compute_displace_atom.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../npair.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../compute_dihedral.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../pair_lj_cut.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../npair_half_bin_newton.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../dump.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../pair_yukawa.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../region_cone.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../npair_half_size_bin_newton_tri.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../pair_coul_dsf.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../fmtlib_format.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../nstencil_half_multi_3d_newtoff.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../compute_bond_local.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../npair_half_respa_bin_newton_tri.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../image.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../tokenizer.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../minimize.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../compute_improper_local.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../fix_dt_reset.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../dihedral_deprecated.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../ntopo_dihedral_all.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
```

```
PI_SKIP_MPICXX=1      -c ../pair_coul_streitz.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../npair_half_size_nsq_newton.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../fix_addforce.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../atom_vec_hybrid.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../random_park.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../compute_vacf.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../citeme.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../npair_half_bin_newton_tri.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../fix_npt_sphere.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../dump_local.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../atom_vec_tri.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../create_bonds.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../write_data.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../compute_centroid_stress_atom.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../my_pool_chunk.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../compute_bond.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../fix_ave_histo_weight.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../pair_dpd_tstat.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../fix_momentum.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../fix_store_force.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../region_block.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../compute_torque_chunk.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../bond_deprecated.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../ntopo_bond_template.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../nstencil_half_multi_3d_newton.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../angle.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../compute_inertia_chunk.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../compute_temp_profile.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../compute_property_chunk.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../nstencil_half_bin_3d_newton_tri.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
```

```
PI_SKIP_MPICXX=1      -c ../compute_coord_atom.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../fix_group.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../fix_npt.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../compute_improper.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../pair_hybrid_overlay.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../compute_ke_atom.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../npair_copy.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../fix_read_restart.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../my_page.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../fix_ave_time.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../compute_property_atom.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../pair_coul_debye.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../compute_chunk_spread_atom.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../universe.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../random_mars.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../nstencil.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../fix_minimize.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../improper_hybrid.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../compute.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../dihedral.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../atom_vec_sphere.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../write_restart.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../dump_dcd.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../change_box.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../set.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../ntopo_angle_partial.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../kspace.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../region_prism.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../nstencil_half_bin_3d_newton.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../atom_vec_body.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
```



```
PI_SKIP_MPICXX=1      -c ../fix_nvt_sphere.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../min_sd.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../atom_vec_charge.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../npair_full_bin_ghost.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../pair_lj_smooth.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../integrate.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../compute_temp_com.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../atom_vec_ellipsoid.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../nstencil_full_multi_2d.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../compute_adf.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../region_cylinder.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../pair_coul_cut.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../comm.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../npair_half_respa_nsq_newton.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../fix_adapt.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../ntopo_dihedral_template.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../fix_nph.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../group.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../dump_xyz.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../fmtlib_os.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../reset_mol_ids.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../fix_balance.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../compute_temp_ramp.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../bond_hybrid.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../fix_heat.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../improper_deprecated.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../npair_half_multi_newton.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../update.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../fix_nve_limit.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../compute_temp_partial.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
```

```
PI_SKIP_MPICXX=1      -c ../atom_vec_atomic.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../fix_temp_berendsen.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../min_fire_old.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../ntopo_angle_all.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../fix_restrain.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../imbalance_var.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../dihedral_hybrid.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../reset_atom_ids.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../fix_controller.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../dump_atom.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../atom_vec.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../compute_orientorder_atom.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../fix_ave_chunk.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../bond_zero.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../deprecated.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../potential_file_reader.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../npair_half_bin_atomonly_newton.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../memory.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../fix_aveforce.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../text_file_reader.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../fix_spring_rg.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../dump_cfg.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../timer.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../fix_ave_atom.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../neighbor.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../fix_wall_region.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../pair_gauss.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../dihedral_zero.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../nbin.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../pair_soft.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
```

```

PI_SKIP_MPICXX=1      -c ../npair_half_multi_newton_tri.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../fix_halt.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../fix_wall_morse.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../fix_wall_lj126.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../utils.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../fix_move.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../fix_nve_sphere.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../reader_xyz.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../npair_half_nsq_newton.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../compute_reduce_chunk.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../compute_reduce.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../fix_neigh_history.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../npair_half_respa_bin_newtoff.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../modify.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../region_deprecated.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../read_data.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../pair_lj_cut_coul_wolf.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../pair_zero.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../create_atoms.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../nstencil_half_multi_3d_newton_tri.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../npair_half_bin_newtoff_ghost.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../fix_setforce.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../ntopo.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../atom_map.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../fix_box_relax.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../fix_nve.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../fix_nh_sphere.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../fix_recenter.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../fix_wall_lj93.cpp
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -DMPICH_SKIP_MPICXX -DOM
PI_SKIP_MPICXX=1      -c ../compute_dihedral_local.cpp
ar -rc ../liblammps_mpi.a ntopo_bond_all.o fix_drag.o region_sphere.o compute

```

\_deprecated.o compute\_rdf.o pair\_lj\_cut\_coul\_dsf.o npair\_full\_multi.o write\_dump.o compute\_pressure.o dump\_movie.o nstencil\_half\_multi\_2d\_newton\_tri.o fix\_nvt\_sllod.o fix\_tmd.o input.o compute\_property\_local.o fix\_wall.o compute\_dipole\_chunk.o compute\_angle\_local.o region\_plane.o kspace\_deprecated.o fix\_nph\_sphere.o fix\_lineforce.o ntopo\_bond\_partial.o run.o min\_fire.o imbalance.o create\_box.o npair\_half\_nsq\_newtoff\_ghost.o compute\_com.o compute\_ke.o pair\_lj\_expand.o npair\_half\_size\_bin\_newtoff.o library.o compute\_gyration\_chunk.o pair\_hybrid.o pair\_lj\_gromacs\_coul\_gromacs.o comm\_brick.o fix\_spring\_self.o fix\_nve\_noforce.o angle\_hybrid.o compute\_angle.o atom\_vec\_line.o respa.o nstencil\_half\_ghost\_bin\_2d\_newtoff.o reader.o fix\_dummy.o pair\_born\_coul\_wolf.o compute\_pe\_atom.o fix\_wall\_lj1043.o pair\_beck.o pair\_zbl.o velocity.o npair\_skip\_size\_off2on.o min\_hftn.o compute\_pair\_local.o npair\_half\_size\_nsq\_newtoff.o compute\_temp\_sphere.o npair\_half\_size\_bin\_newton.o compute\_heat\_flux.o compute\_temp\_region.o angle\_zero.o irregular.o fix\_numdiff.o npair\_half\_nsq\_newtoff.o nstencil\_half\_bin\_2d\_newtoff.o ntopo\_improper\_template.o npair\_full\_nsq\_ghost.o nstencil\_half\_bin\_2d\_newton.o read\_restart.o lattice.o pair\_dpd.o fix\_store.o compute\_group\_group.o nstencil\_full\_ghost\_bin\_3d.o dump\_custom.o nstencil\_half\_ghost\_bin\_3d\_newtoff.o npair\_half\_full\_newtoff.o min\_quickmin.o compute\_centro\_atom.o pair\_lj\_gromacs.o compute\_reduce\_region.o thermo.o pair\_buck\_coul\_cut.o improper\_zero.o compute\_contact\_atom.o pair\_morse.o pair.o region\_intersect.o compute\_hexorder\_atom.o fix\_langevin.o compute\_angmom\_chunk.o fix\_nvt.o compute\_aggregate\_atom.o body.o npair\_full\_bin.o output.o nstencil\_half\_bin\_2d\_newton\_tri.o fix\_planeforce.o fix\_ave\_correlate.o compute\_msd\_chunk.o compute\_cna\_atom.o neigh\_request.o compute\_slice.o domain.o lmpython.o compute\_msd.o region.o pair\_table.o math\_extra.o imbalance\_group.o nstencil\_full\_bin\_2d.o fix\_enforce2d.o compute\_temp\_deform.o lammmps.o pair\_uhm.o nstencil\_full\_bin\_3d.o npair\_half\_respa\_bin\_newton.o npair\_full\_nsq.o ntopo\_improper\_partial.o pair\_lj\_cut\_coul\_cut.o nstencil\_full\_multi\_3d.o fix\_spring\_chunk.o compute\_vcm\_chunk.o nstencil\_full\_ghost\_bin\_2d.o fix\_deprecated.o table\_file\_reader.o region\_union.o fix\_temp\_rescale.o fix\_gravity.o compute\_pe.o comm\_tiled.o fix\_vector.o dump\_deprecated.o replicate.o read\_dump.o npair\_skip\_size.o molecule.o fix\_temp\_csvr.o npair\_half\_multi\_newtoff.o min\_cg.o npair\_full\_bin\_atomonly.o procmmap.o compute\_cluster\_atom.o fix\_deform.o pair\_born\_coul\_dsf.o imbalance\_neigh.o variable.o compute\_omega\_chunk.o ntopo\_improper\_all.o pair\_lj\_cut\_coul\_debye.o npair\_half\_full\_newton.o compute\_erotate\_sphere.o npair\_skip.o pair\_buck.o fix\_external.o math\_special.o delete\_bonds.o force.o finishing.o compute\_fragment\_atom.o pair\_coul\_wolf.o npair\_skip\_respa.o fix\_ave\_histo.o bond.o fix\_store\_state.o improper.o npair\_half\_bin\_newtoff.o compute\_com\_chunk.o compute\_temp\_chunk.o math\_eigen.o nstencil\_half\_multi\_2d\_newtoff.o hashlittle.o pair\_deprecated.o min\_linesearch.o angle\_deprecated.o write\_coeff.o pair\_born.o neigh\_list.o pair\_lj96\_cut.o verlet.o pair\_lj\_smooth\_linear.o atom.o fix\_press\_berendsen.o pair\_aenet.o nstencil\_half\_multi\_2d\_newton.o fix\_wall\_harmonic.o compute\_global\_atom.o compute\_chunk\_atom.o min.o fix\_print.o displace\_atoms.o nstencil\_half\_bin\_3d\_newtoff.o imbalance\_time.o npair\_skip\_size\_off2on\_oneside.o pair\_mie\_cut.o imbalance\_store.o fix\_wall\_reflect.o fix\_indent.o npair\_half\_respa\_nsq\_newtoff.o compute\_stress\_atom.o reader\_native.o fix\_respa.o compute\_gyration.o special.o fix\_spring.o fix\_visous.o dump\_image.o compute\_erotate\_sphere\_atom.o rerun.o compute\_pair.o rcb.o balance.o compute\_temp.o info.o error.o fix\_nh.o nbins\_standard.o fix\_temp\_csld.o fix\_property\_atom.o delete\_atoms.o ntopo\_dihedral\_partial.o fix.o ntopo\_angle\_template.o pair\_lj\_cubic.o compute\_displace\_atom.o npair.o compute\_dihedral.o pair\_lj\_cut.o npair\_half\_bin\_newton.o dump.o pair\_yukawa.o region\_cone.o npair\_half\_size\_bin\_newton\_tri.o pair\_coul\_dsf.o fmtlib\_format.o nstencil\_half\_multi\_3d\_newtoff.o compute\_bond\_local.o npair\_half\_respa\_bin\_newton\_tri.o image.o tokenizer.o minimize.o compute\_improper\_local.o fix\_dt\_reset.o dihedral\_deprecated.o ntopo\_dihedral\_all.o pair\_coul\_streitz.o npair\_half\_size\_nsq\_newton.o fix\_addforce.o atom\_vec\_hybrid.o random\_park.o compute\_vacf.o cite.o npair\_half\_bin\_newton\_tri.o fix\_npt\_sphere.o dump\_local.o atom\_vec\_tri.o create\_bonds.o write\_data.o compute\_centroid\_stress\_atom.o my\_pool\_chunk.o compute\_bond.o fix\_ave\_histo\_weight.o pair\_dpd\_tstat.o fix\_momentum.o fix\_store\_force.o regi

```

on_block.o compute_torque_chunk.o bond_deprecated.o ntopo_bond_template.o nstencil_half_multi_3d_newton.o angle.o compute_inertia_chunk.o compute_temp_profile.o compute_property_chunk.o nstencil_half_bin_3d_newton_tri.o compute_coord_atom.o fix_group.o fix_npt.o compute_improper.o pair_hybrid_overlay.o compute_ke_atom.o npair_copy.o fix_read_restart.o my_page.o fix_ave_time.o compute_property_atom.o pair_coul_debye.o compute_chunk_spread_atom.o universe.o random_mars.o nstencil.o fix_minimize.o improper_hybrid.o compute.o dihedral.o atom_vec_sphere.o write_restart.o dump_dcd.o change_box.o set.o ntopo_angle_partial.o kspace.o region_prism.o nstencil_half_bin_3d_newton.o atom_vec_body.o fix_nvt_sphere.o min_sd.o atom_vec_charge.o npair_full_bin_ghost.o pair_lj_smooth.o integrate.o compute_temp_com.o atom_vec_ellipsoid.o nstencil_full_multi_2d.o compute_adf.o region_cylinder.o pair_coul_cut.o comm.o npair_half_respa_nsq_newton.o fix_adapt.o ntopo_dihedral_template.o fix_nph.o group.o dump_xyz.o fmtlib_os.o reset_mol_ids.o fix_balance.o compute_temp_ramp.o bond_hybrid.o fix_heat.o improper_deprecated.o npair_half_multi_newton.o update.o fix_nve_limit.o compute_temp_partial.o atom_vec_atomic.o fix_temp_berendsen.o min_fire_old.o ntopo_angle_all.o fix_restrain.o imbalance_var.o dihedral_hybrid.o reset_atom_ids.o fix_controller.o dump_atom.o atom_vec.o compute_orient_order_atom.o fix_ave_chunk.o bond_zero.o deprecated.o potential_file_reader.o npair_half_bin_atomonly_newton.o memory.o fix_aveforce.o text_file_reader.o fix_spring_rg.o dump_cfg.o timer.o fix_ave_atom.o neighbor.o fix_wall_region.o pair_gauss.o dihedral_zero.o nbins.o pair_soft.o npair_half_multi_newton_tri.o fix_halt.o fix_wall_morse.o fix_wall_lj126.o utils.o fix_move.o fix_nve_sphere.o reader_xyz.o npair_half_nsq_newton.o compute_reduce_chunk.o compute_reduce.o fix_neigh_history.o npair_half_respa_bin_newtoff.o modify.o region_deprecated.o read_data.o pair_lj_cut_coul_wolf.o pair_zero.o create_atoms.o nstencil_half_multi_3d_newton_tri.o npair_half_bin_newtoff_ghost.o fix_setforce.o ntopo.o atom_map.o fix_box_relax.o fix_nve.o fix_nh_sphere.o fix_recenter.o fix_wall_lj93.o compute_dihedral_local.o
mpicxx -g -O3 main.o -L../lib/aenet -L. -llammps_mpi -laenet -lgfortran -o ../lmp_mpi
size ../lmp_mpi
      text      data      bss      dec      hex filename
5750146 136972    24040 5911158  5a3276 ../lmp_mpi
make[1]: Leaving directory '/data/home/na2782/Programs/test/lammps-stable_290ct2020/src'

```

## 6. How to run LAMMPS with ANN potential

In ANN/Fe/ directory parameter file and example input file for LAMMPS

1. Fe.10tw-10tw.ann: parameter file of ANN potential for BCC iron
2. in.aenet\_mm: example input file for LAMMPS, lattice optimization of BCC iron
3. in.aenet\_nve: example input file for LAMMPS, run nve MD of BCC iron

To check the LAMMPS work properly, for example, in ANN/Fe/ directory

In [6]:

```
%cd ../../aenet-lammps-2021May04/ANN/Fe/
!../../../lammps-stable_290ct2020/src/lmp_mpi -i in.aenet_mm
```

```
/data/home/na2782/Programs/test/aenet-lammps-2021May04/ANN/Fe
```

```
[[42214,1],0]: A high-performance Open MPI point-to-point messaging module
was unable to find any relevant network interfaces:
```

```
Module: OpenFabrics (openib)
```

Host: nernst

Another transport will be used instead, although this may result in lower performance.

NOTE: You can disable this warning by setting the MCA parameter `btl_base_warn_component_unused` to 0.

-----  
LAMMPS (29 Oct 2020)

Lattice spacing in x,y,z = 2.9000000 2.9000000 2.9000000

Created orthogonal box = (0.0000000 0.0000000 0.0000000) to (2.9000000 2.9000000 2.9000000)

1 by 1 by 1 MPI processor grid

Created 2 atoms

create\_atoms CPU = 0.001 seconds

WARNING: Using 'neigh\_modify every 1 delay 0 check yes' setting during minimization (../min.cpp:187)

Neighbor list info ...

update every 1 steps, delay 0 steps, check yes

max neighbors/atom: 2000, page size: 100000

master list distance cutoff = 8.5

ghost atom cutoff = 8.5

binsize = 4.25, bins = 1 1 1

1 neighbor lists, perpetual/occasional/extra = 1 0 0

(1) pair aenet, perpetual

attributes: full, newton on

pair build: full/bin/atomonly

stencil: full/bin/3d

bin: standard

Setting up cg style minimization ...

Unit style : metal

Current step : 0

WARNING: Energy due to 1 extra global DOFs will be included in minimizer energies

Per MPI rank memory allocation (min/avg/max) = 4.115 | 4.115 | 4.115 Mbytes

Step PotEng Lx Volume Press

0	-8959.7099	2.9	24.389	-105938.5
10	-8959.7147	2.8971	24.315906	-103326.24
20	-8959.7193	2.8942	24.242958	-100412.17
30	-8959.7238	2.8913	24.170157	-97221.184
40	-8959.7281	2.8884	24.097501	-93775.55
50	-8959.7323	2.8855	24.024991	-90094.834
60	-8959.7363	2.8826	23.952627	-86195.977
70	-8959.7401	2.8797	23.880408	-82093.435
80	-8959.7437	2.8768	23.808334	-77799.38
90	-8959.7471	2.8739	23.736406	-73323.964
100	-8959.7502	2.871	23.664622	-68675.612
110	-8959.7532	2.8681	23.592984	-63861.338
120	-8959.756	2.8652	23.52149	-58887.053
130	-8959.7585	2.8623	23.450141	-53757.85
140	-8959.7607	2.8594	23.378936	-48478.252
150	-8959.7628	2.8565	23.307875	-43052.408
160	-8959.7645	2.8536	23.236959	-37484.224
170	-8959.7661	2.8507	23.166186	-31777.453
180	-8959.7673	2.8478	23.095558	-25935.73
190	-8959.7684	2.8449	23.025073	-19962.606
200	-8959.7691	2.842	22.954732	-13861.598
210	-8959.7696	2.8391	22.884534	-7636.3009
220	-8959.7698	2.8362	22.814479	-1290.6199
224	-8959.7698	2.8356167	22.800405	1.4322684e-08

Loop time of 1.59487 on 1 procs for 224 steps with 2 atoms

99.5% CPU use with 1 MPI tasks x no OpenMP threads

Minimization stats:

```

Stopping criterion = energy tolerance
Energy initial, next-to-last, final =
  -8959.70990256322  -8959.7697747731  -8959.7697747731
Force two-norm initial, final = 4.8379204 6.2536218e-13
Force max component initial, final = 4.8379204 6.2535747e-13
Final line search alpha, max atom move = 1.0000000 6.2535747e-13
Iterations, force evaluations = 224 226

```

MPI task timing breakdown:

Section	min time	avg time	max time	[%varavg]	%total
Pair	1.5896	1.5896	1.5896	0.0	99.67
Neigh	0	0	0	0.0	0.00
Comm	0.0013152	0.0013152	0.0013152	0.0	0.08
Output	0.00049199	0.00049199	0.00049199	0.0	0.03
Modify	0	0	0	0.0	0.00
Other		0.003445			0.22

```

Nlocal:      2.00000 ave      2 max      2 min
Histogram: 1 0 0 0 0 0 0 0 0 0
Nghost:      557.000 ave     557 max     557 min
Histogram: 1 0 0 0 0 0 0 0 0 0
Neighs:      0.00000 ave      0 max      0 min
Histogram: 1 0 0 0 0 0 0 0 0 0
FullNghs:    360.000 ave    360 max    360 min
Histogram: 1 0 0 0 0 0 0 0 0 0

```

```

Total # of neighbors = 360
Ave neighs/atom = 180.00000
Neighbor list builds = 0
Dangerous builds = 0
Total wall time: 0.00001

```

## 7. Checking the result

After job done, please check lattice constant (lx) in log.lammps and log.lammps.g++\_mm

In in.aenet\_mm the following two lines activate the ANN potential:

```

pair_style aenet
pair_coeff v01 Fe 10tw-10tw.ann Fe

```

In pair\_coeff line, **v01** means to use our (Mori and Ozaki) original version. If you chose **v00**, you can use parameter file from original aenet package. The Fe between v01 and 10tw-10tw.ann set element(s). The term:10tw-10tw.ann is **file mask** for name of parameter file, in this case, file name is set as Fe.10tw-10tw.ann. Please see TiO2 directory for binary system.

In [7]:

```
!../../../../lammps-stable_29Oct2020/src/lmp_mpi -i in.aenet_nve
```

[[42764,1],0]: A high-performance Open MPI point-to-point messaging module was unable to find any relevant network interfaces:

Module: OpenFabrics (openib)  
Host: nernst

Another transport will be used instead, although this may result in lower performance.

NOTE: You can disable this warning by setting the MCA parameter btl\_base\_warn\_component\_unused to 0.

LAMMPS (29 Oct 2020)

Lattice spacing in x,y,z = 2.8351700 2.8351700 2.8351700

Created orthogonal box = (0.0000000 0.0000000 0.0000000) to (5.6703400 5.6703400 5.6703400)

1 by 1 by 1 MPI processor grid

Created 16 atoms

create\_atoms CPU = 0.001 seconds

Neighbor list info ...

update every 1 steps, delay 10 steps, check yes

max neighbors/atom: 2000, page size: 100000

master list distance cutoff = 8.5

ghost atom cutoff = 8.5

binsize = 4.25, bins = 2 2 2

1 neighbor lists, perpetual/occasional/extra = 1 0 0

(1) pair aenet, perpetual

attributes: full, newton on

pair build: full/bin/atomonly

stencil: full/bin/3d

bin: standard

Setting up Verlet run ...

Unit style : metal

Current step : 0

Time step : 0.0005

Per MPI rank memory allocation (min/avg/max) = 2.978 | 2.978 | 2.978 Mbytes

Step TotEng PotEng KinEng Temp Volume Press

0	-71677.189	-71678.158	0.96945109	500	182.31706
6670.9254					
10	-71677.189	-71678.1	0.91161606	470.17125	182.31706
7715.0904					
20	-71677.189	-71677.943	0.75408921	388.92587	182.31706
10665.073					
30	-71677.189	-71677.728	0.53983482	278.42293	182.31706
14968.621					
40	-71677.189	-71677.515	0.32653966	168.41472	182.31706
19868.298					
50	-71677.189	-71677.358	0.16961277	87.478767	182.31706
24303.319					
60	-71677.189	-71677.293	0.10429417	53.790321	182.31706
27258.551					
70	-71677.189	-71677.325	0.13591825	70.100625	182.31706
28334.979					
80	-71677.189	-71677.43	0.24136594	124.48588	182.31706
27668.029					



90	-71677.189	-71677.569	0.37989281	195.93191	182.31706
25731.553					
100	-71677.189	-71677.697	0.50795472	261.98058	182.31706
23181.611					
110	-71677.189	-71677.781	0.59269718	305.687	182.31706
20480.448					
120	-71677.189	-71677.809	0.62046982	320.0109	182.31706
18063.096					
130	-71677.189	-71677.787	0.59848546	308.67233	182.31706
16079.609					
140	-71677.189	-71677.739	0.54992202	283.62546	182.31706
14688.463					
150	-71677.189	-71677.693	0.50420309	260.04565	182.31706
13965.046					
160	-71677.189	-71677.675	0.48601671	250.66593	182.31706
13794.264					
170	-71677.189	-71677.694	0.50577733	260.85758	182.31706
13931.802					
180	-71677.189	-71677.744	0.55489704	286.19136	182.31706
14184.148					
190	-71677.189	-71677.798	0.60895976	314.07451	182.31706
14553.047					
200	-71677.189	-71677.827	0.63831519	329.21475	182.31706
15218.661					
210	-71677.189	-71677.81	0.62110994	320.34104	182.31706
16374.669					
220	-71677.189	-71677.741	0.55280192	285.11078	182.31706
18041.155					
230	-71677.189	-71677.637	0.44875124	231.44604	182.31706
19986.025					
240	-71677.189	-71677.528	0.33933318	175.01305	182.31706
21798.211					
250	-71677.189	-71677.448	0.25921556	133.69192	182.31706
23065.36					
260	-71677.189	-71677.423	0.23466393	121.02928	182.31706
23604.377					
270	-71677.189	-71677.463	0.27395415	141.29343	182.31706
23454.72					
280	-71677.189	-71677.553	0.36468518	188.08849	182.31706
22719.519					
290	-71677.189	-71677.667	0.47848223	246.77998	182.31706
21565.483					
300	-71677.189	-71677.769	0.58064494	299.47098	182.31706
20173.955					
310	-71677.189	-71677.83	0.64156891	330.89287	182.31706
18704.587					
320	-71677.189	-71677.835	0.64681835	333.6003	182.31706
17347.648					
330	-71677.189	-71677.791	0.6023888	310.68551	182.31706
16261.3					
340	-71677.189	-71677.721	0.53265965	274.72229	182.31706
15455.196					
350	-71677.189	-71677.659	0.47068065	242.75626	182.31706
14790.172					
360	-71677.189	-71677.633	0.44395621	228.97298	182.31706
14143.858					
370	-71677.189	-71677.651	0.46247601	238.52467	182.31706
13602.38					
380	-71677.189	-71677.704	0.51534186	265.79054	182.31706
13480.975					

390	-71677.189	-71677.765	0.57669618	297.43439	182.31706
14130.127					
400	-71677.189	-71677.805	0.61637562	317.89929	182.31706
15689.76					
410	-71677.189	-71677.799	0.61059897	314.91994	182.31706
17998.129					
420	-71677.189	-71677.739	0.55031991	283.83067	182.31706
20676.493					
430	-71677.189	-71677.634	0.44556021	229.80025	182.31706
23268.915					
440	-71677.189	-71677.513	0.32404021	167.12561	182.31706
25290.501					
450	-71677.189	-71677.412	0.22368172	115.36514	182.31706
26318.238					
460	-71677.189	-71677.369	0.18063202	93.162009	182.31706
26127.803					
470	-71677.189	-71677.405	0.21624169	111.5279	182.31706
24686.815					
480	-71677.189	-71677.517	0.32804518	169.1912	182.31706
22129.76					
490	-71677.189	-71677.678	0.48890839	252.15733	182.31706
18858.773					
500	-71677.189	-71677.844	0.65506149	337.85175	182.31706
15352.805					
510	-71677.189	-71677.969	0.78006015	402.32053	182.31706
12217.067					
520	-71677.189	-71678.018	0.82932638	427.72987	182.31706
10079.229					
530	-71677.189	-71677.979	0.79048927	407.69941	182.31706
9467.7326					
540	-71677.189	-71677.865	0.67664926	348.98576	182.31706
10619.786					
550	-71677.189	-71677.711	0.52226437	269.36087	182.31706
13280.019					
560	-71677.189	-71677.562	0.37311635	192.43692	182.31706
16687.525					
570	-71677.189	-71677.461	0.27221868	140.39836	182.31706
19893.842					
580	-71677.189	-71677.434	0.24508859	126.40585	182.31706
22219.564					
590	-71677.189	-71677.479	0.29071097	149.93586	182.31706
23469.944					
600	-71677.189	-71677.572	0.38347567	197.77979	182.31706
23834.304					
610	-71677.189	-71677.674	0.48493517	250.10812	182.31706
23631.211					
620	-71677.189	-71677.748	0.55884957	288.2299	182.31706
23041.614					
630	-71677.189	-71677.772	0.58331442	300.84778	182.31706
22132.317					
640	-71677.189	-71677.745	0.55683091	287.18876	182.31706
20981.144					
650	-71677.189	-71677.686	0.49727371	256.47179	182.31706
19749.709					
660	-71677.189	-71677.623	0.43423229	223.95781	182.31706
18606.071					
670	-71677.189	-71677.586	0.39725133	204.88467	182.31706
17596.71					
680	-71677.189	-71677.593	0.40417339	208.45476	182.31706
16635.496					

690	-71677.189	-71677.643	0.45414726	234.22907	182.31706
15650.671					
700	-71677.189	-71677.717	0.52832809	272.48827	182.31706
14747.973					
710	-71677.189	-71677.787	0.59789833	308.36952	182.31706
14215.291					
720	-71677.189	-71677.824	0.63567672	327.85394	182.31706
14338.285					
730	-71677.189	-71677.815	0.62650639	323.12429	182.31706
15176.464					
740	-71677.189	-71677.761	0.57278281	295.41604	182.31706
16493.825					
750	-71677.189	-71677.682	0.49330363	254.4242	182.31706
17902.556					
760	-71677.189	-71677.604	0.41577002	214.43579	182.31706
19094.421					
770	-71677.189	-71677.555	0.3660598	188.79746	182.31706
19972.427					
780	-71677.189	-71677.548	0.35897296	185.14238	182.31706
20610.352					
790	-71677.189	-71677.582	0.39372984	203.06844	182.31706
21121.651					
800	-71677.189	-71677.643	0.45482389	234.57805	182.31706
21563.879					
810	-71677.189	-71677.706	0.51735883	266.83081	182.31706
21860.672					
820	-71677.189	-71677.744	0.55561286	286.56054	182.31706
21949.966					
830	-71677.189	-71677.741	0.55248306	284.94633	182.31706
21824.621					
840	-71677.189	-71677.695	0.50654524	261.25363	182.31706
21468.514					
850	-71677.189	-71677.623	0.43396779	223.82139	182.31706
20846.167					
860	-71677.189	-71677.553	0.36408535	187.77912	182.31706
19881.907					
870	-71677.189	-71677.518	0.32943583	169.90843	182.31706
18477.515					
880	-71677.189	-71677.542	0.35302711	182.07577	182.31706
16567.712					
890	-71677.189	-71677.626	0.43765285	225.72199	182.31706
14316.072					
900	-71677.189	-71677.751	0.5624572	290.09055	182.31706
12179.834					
910	-71677.189	-71677.878	0.68900842	355.36007	182.31706
10849.12					
920	-71677.189	-71677.963	0.77415896	399.27696	182.31706
10921.902					
930	-71677.189	-71677.973	0.78437183	404.5443	182.31706
12597.292					
940	-71677.189	-71677.896	0.70720105	364.74303	182.31706
15599.668					
950	-71677.189	-71677.746	0.5571012	287.32816	182.31706
19294.148					
960	-71677.189	-71677.562	0.37353885	192.65482	182.31706
22874.808					
970	-71677.189	-71677.399	0.21063257	108.63497	182.31706
25684.945					
980	-71677.189	-71677.308	0.1195979	61.68331	182.31706
27088.2					

990	-71677.189	-71677.318	0.12985646	66.974222	182.31706
26919.406					
1000	-71677.189	-71677.426	0.23744594	122.46412	182.31706
25276.802					
1010	-71677.189	-71677.595	0.40679325	209.80597	182.31706
22501.177					
1020	-71677.189	-71677.773	0.58474671	301.5865	182.31706
19091.163					
1030	-71677.189	-71677.908	0.71954775	371.11091	182.31706
15663.456					
1040	-71677.189	-71677.965	0.77672952	400.60274	182.31706
12923.905					
1050	-71677.189	-71677.936	0.7477907	385.67738	182.31706
11487.084					
1060	-71677.189	-71677.839	0.6505755	335.53807	182.31706
11650.789					
1070	-71677.189	-71677.711	0.52243693	269.44986	182.31706
13171.256					
1080	-71677.189	-71677.597	0.40808353	210.47144	182.31706
15316.89					
1090	-71677.189	-71677.533	0.3443127	177.58127	182.31706
17304.235					
1100	-71677.189	-71677.535	0.34656391	178.74234	182.31706
18689.905					
1110	-71677.189	-71677.593	0.40423517	208.48662	182.31706
19505.386					
1120	-71677.189	-71677.676	0.48719769	251.27503	182.31706
20060.097					
1130	-71677.189	-71677.748	0.55902826	288.32206	182.31706
20569.24					
1140	-71677.189	-71677.779	0.59053123	304.5699	182.31706
21092.264					
1150	-71677.189	-71677.758	0.56928071	293.60981	182.31706
21588.253					
1160	-71677.189	-71677.692	0.50298757	259.41875	182.31706
21903.586					
1170	-71677.189	-71677.605	0.41598636	214.54737	182.31706
22014.878					
1180	-71677.189	-71677.529	0.34023645	175.47891	182.31706
21917.723					
1190	-71677.189	-71677.493	0.30431693	156.95321	182.31706
21558.085					
1200	-71677.189	-71677.512	0.32379561	166.99946	182.31706
20825.78					
1210	-71677.189	-71677.584	0.39540158	203.93065	182.31706
19589.258					
1220	-71677.189	-71677.686	0.4974117	256.54296	182.31706
17890.375					
1230	-71677.189	-71677.786	0.59696294	307.88708	182.31706
16052.126					
1240	-71677.189	-71677.851	0.66207494	341.46898	182.31706
14542.305					
1250	-71677.189	-71677.862	0.67328578	347.25103	182.31706
13739.111					
1260	-71677.189	-71677.819	0.63023068	325.04511	182.31706
13754.405					
1270	-71677.189	-71677.74	0.55124755	284.30911	182.31706
14424.461					
1280	-71677.189	-71677.655	0.46642993	240.56393	182.31706
15451.712					

1290	-71677.189	-71677.595	0.40627392	209.53812	182.31706
16591.828					
1300	-71677.189	-71677.579	0.38997729	201.13304	182.31706
17769.234					
1310	-71677.189	-71677.607	0.41821836	215.69853	182.31706
18979.756					
1320	-71677.189	-71677.662	0.47339468	244.15604	182.31706
20186.855					
1330	-71677.189	-71677.716	0.52709292	271.85122	182.31706
21332.297					
1340	-71677.189	-71677.74	0.55152645	284.45295	182.31706
22348.837					
1350	-71677.189	-71677.719	0.53066304	273.69253	182.31706
23224.89					
1360	-71677.189	-71677.656	0.46713776	240.929	182.31706
23844.222					
1370	-71677.189	-71677.571	0.38255102	197.3029	182.31706
24088.28					
1380	-71677.189	-71677.499	0.31045007	160.11642	182.31706
23583.382					
1390	-71677.189	-71677.472	0.28387433	146.40983	182.31706
22076.5					
1400	-71677.189	-71677.51	0.32178999	165.96505	182.31706
19556.743					
1410	-71677.189	-71677.609	0.42037819	216.81248	182.31706
16453.254					
1420	-71677.189	-71677.742	0.55372295	285.58581	182.31706
13408.585					
1430	-71677.189	-71677.872	0.68318143	352.35477	182.31706
11120.973					
1440	-71677.189	-71677.959	0.76992202	397.09173	182.31706
10134.905					
1450	-71677.189	-71677.975	0.78642298	405.6022	182.31706
10668.166					
1460	-71677.189	-71677.913	0.72475408	373.7961	182.31706
12620.331					
1470	-71677.189	-71677.788	0.59982007	309.36067	182.31706
15629.425					
1480	-71677.189	-71677.635	0.44599408	230.02403	182.31706
19102.14					
1490	-71677.189	-71677.496	0.30695755	158.31513	182.31706
22311.081					
1500	-71677.189	-71677.41	0.22170243	114.34431	182.31706
24734.289					
1510	-71677.189	-71677.4	0.21137254	109.01661	182.31706
26035.764					
1520	-71677.189	-71677.461	0.2726196	140.60514	182.31706
26119.441					
1530	-71677.189	-71677.569	0.3800447	196.01025	182.31706
25129.569					
1540	-71677.189	-71677.685	0.49641004	256.02635	182.31706
23278.41					
1550	-71677.189	-71677.774	0.58573238	302.09486	182.31706
20907.756					
1560	-71677.189	-71677.813	0.62440891	322.0425	182.31706
18484.429					
1570	-71677.189	-71677.796	0.60744343	313.29246	182.31706
16423.213					
1580	-71677.189	-71677.737	0.54865681	282.97292	182.31706
15091.984					

1590	-71677.189	-71677.664	0.47567824	245.3338	182.31706
14582.652					
1600	-71677.189	-71677.61	0.42112545	217.19789	182.31706
14633.134					
1610	-71677.189	-71677.599	0.41084805	211.89726	182.31706
14836.95					
1620	-71677.189	-71677.641	0.45237736	233.31624	182.31706
14980.07					
1630	-71677.189	-71677.719	0.53012517	273.41512	182.31706
15181.311					
1640	-71677.189	-71677.8	0.61164965	315.46184	182.31706
15726.246					
1650	-71677.189	-71677.85	0.66179109	341.32258	182.31706
16771.922					
1660	-71677.189	-71677.846	0.65688463	338.79205	182.31706
18209.657					
1670	-71677.189	-71677.782	0.59325945	305.97699	182.31706
19786.081					
1680	-71677.189	-71677.677	0.48814022	251.76114	182.31706
21286.766					
1690	-71677.189	-71677.562	0.37346549	192.61698	182.31706
22571.762					
1700	-71677.189	-71677.474	0.28493627	146.95753	182.31706
23508.739					
1710	-71677.189	-71677.438	0.24980449	128.83811	182.31706
23854.283					
1720	-71677.189	-71677.466	0.27728175	143.00967	182.31706
23377.996					
1730	-71677.189	-71677.544	0.35551493	183.35888	182.31706
22075.325					
1740	-71677.189	-71677.645	0.4565494	235.46799	182.31706
20204.368					
1750	-71677.189	-71677.736	0.5472362	282.24023	182.31706
18244.647					
1760	-71677.189	-71677.79	0.60138422	310.16739	182.31706
16598.28					
1770	-71677.189	-71677.797	0.60871348	313.9475	182.31706
15443.44					
1780	-71677.189	-71677.766	0.57748641	297.84195	182.31706
14719.085					
1790	-71677.189	-71677.719	0.53017342	273.44	182.31706
14235.628					
1800	-71677.189	-71677.682	0.49360183	254.578	182.31706
13876.372					
1810	-71677.189	-71677.676	0.4873928	251.37565	182.31706
13717.027					
1820	-71677.189	-71677.704	0.51569419	265.97226	182.31706
13975.994					
1830	-71677.189	-71677.754	0.56560078	291.71187	182.31706
14850.045					
1840	-71677.189	-71677.801	0.61226139	315.77735	182.31706
16372.529					
1850	-71677.189	-71677.817	0.62825427	324.02577	182.31706
18393.902					
1860	-71677.189	-71677.783	0.59412474	306.42327	182.31706
20661.612					
1870	-71677.189	-71677.695	0.50679339	261.38162	182.31706
22910.068					
1880	-71677.189	-71677.571	0.38278303	197.42256	182.31706
24839.592					

1890	-71677.189	-71677.443	0.25485841	131.4447	182.31706
26102.752					
1900	-71677.189	-71677.351	0.16278795	83.958824	182.31706
26303.977					
1910	-71677.189	-71677.329	0.14077375	72.604875	182.31706
25202.819					
1920	-71677.189	-71677.394	0.20521392	105.84026	182.31706
22726.678					
1930	-71677.189	-71677.536	0.34726296	179.10288	182.31706
19179.619					
1940	-71677.189	-71677.722	0.53362869	275.22208	182.31706
15218.665					
1950	-71677.189	-71677.905	0.71584537	369.20138	182.31706
11664.734					
1960	-71677.189	-71678.034	0.84504043	435.83448	182.31706
9215.5729					
1970	-71677.189	-71678.075	0.88655141	457.24401	182.31706
8389.1119					
1980	-71677.189	-71678.019	0.83025832	428.21052	182.31706
9346.236					
1990	-71677.189	-71677.883	0.69391799	357.89221	182.31706
11857.532					
2000	-71677.189	-71677.707	0.51834824	267.3411	182.31706
15330.92					
2010	-71677.189	-71677.544	0.35498845	183.08734	182.31706
18967.215					
2020	-71677.189	-71677.437	0.24866521	128.25052	182.31706
22034.506					
2030	-71677.189	-71677.411	0.22191096	114.45186	182.31706
24147.558					
2040	-71677.189	-71677.457	0.26827733	138.36558	182.31706
25113.399					
2050	-71677.189	-71677.547	0.35798411	184.63237	182.31706
25038.436					
2060	-71677.189	-71677.64	0.45180084	233.0189	182.31706
24215.413					
2070	-71677.189	-71677.704	0.51581931	266.03679	182.31706
22994.098					
2080	-71677.189	-71677.721	0.53219081	274.48049	182.31706
21634.57					
2090	-71677.189	-71677.692	0.50379665	259.83603	182.31706
20298.791					
2100	-71677.189	-71677.641	0.45193738	233.08932	182.31706
19043.136					
2110	-71677.189	-71677.596	0.40781866	210.33483	182.31706
17762.899					
2120	-71677.189	-71677.589	0.40009732	206.3525	182.31706
16359.468					
2130	-71677.189	-71677.631	0.44283951	228.39703	182.31706
14848.726					
2140	-71677.189	-71677.718	0.52893717	272.8024	182.31706
13436.016					
2150	-71677.189	-71677.821	0.63208092	325.99939	182.31706
12474.164					
2160	-71677.189	-71677.905	0.71641497	369.49516	182.31706
12293.046					
2170	-71677.189	-71677.938	0.74958881	386.60476	182.31706
13040.595					
2180	-71677.189	-71677.903	0.71428186	368.395	182.31706
14658.083					

2190	-71677.189	-71677.803	0.61445429	316.90835	182.31706
16940.278					
2200	-71677.189	-71677.663	0.47432095	244.63377	182.31706
19578.184					
2210	-71677.189	-71677.519	0.33069364	170.55716	182.31706
22192.126					
2220	-71677.189	-71677.41	0.22178881	114.38886	182.31706
24396.108					
2230	-71677.189	-71677.365	0.17595804	90.751373	182.31706
25736.421					
2240	-71677.189	-71677.392	0.20328478	104.8453	182.31706
25930.54					
2250	-71677.189	-71677.481	0.29280292	151.0148	182.31706
24992.773					
2260	-71677.189	-71677.605	0.4162045	214.65988	182.31706
23169.44					
2270	-71677.189	-71677.726	0.5373265	277.12925	182.31706
20902.986					
2280	-71677.189	-71677.813	0.62405371	321.85931	182.31706
18578.561					
2290	-71677.189	-71677.847	0.65844171	339.59512	182.31706
16503.455					
2300	-71677.189	-71677.83	0.6413413	330.77548	182.31706
14864.259					
2310	-71677.189	-71677.779	0.59071413	304.66422	182.31706
13701.014					
2320	-71677.189	-71677.723	0.53395277	275.38923	182.31706
13079.135					
2330	-71677.189	-71677.686	0.49687624	256.26679	182.31706
13003.074					
2340	-71677.189	-71677.682	0.49352873	254.5403	182.31706
13388.488					
2350	-71677.189	-71677.709	0.52070898	268.55867	182.31706
14128.182					
2360	-71677.189	-71677.748	0.55945506	288.54218	182.31706
15192.891					
2370	-71677.189	-71677.772	0.58306772	300.72055	182.31706
16657.102					
2380	-71677.189	-71677.757	0.56854861	293.23223	182.31706
18660.281					
2390	-71677.189	-71677.696	0.50689414	261.43358	182.31706
21152.816					
2400	-71677.189	-71677.597	0.40818135	210.52189	182.31706
23813.307					
2410	-71677.189	-71677.488	0.2998465	154.64757	182.31706
25910.506					
2420	-71677.189	-71677.407	0.21831583	112.59765	182.31706
26893.703					
2430	-71677.189	-71677.385	0.1961438	101.1623	182.31706
26431.645					
2440	-71677.189	-71677.438	0.24898584	128.41588	182.31706
24565.371					
2450	-71677.189	-71677.557	0.36844706	190.0287	182.31706
21845.621					
2460	-71677.189	-71677.713	0.52405495	270.28437	182.31706
18801.215					
2470	-71677.189	-71677.862	0.67332335	347.27041	182.31706
15862.565					
2480	-71677.189	-71677.964	0.775399	399.91652	182.31706
13292.774					



2490	-71677.189	-71677.992	0.80329686	414.305	182.31706
11478.166					
2500	-71677.189	-71677.94	0.75178243	387.73613	182.31706
10851.46					
2510	-71677.189	-71677.827	0.63871103	329.4189	182.31706
11660.95					
2520	-71677.189	-71677.688	0.49948164	257.61054	182.31706
13693.062					
2530	-71677.189	-71677.565	0.37593907	193.89275	182.31706
16342.53					
2540	-71677.189	-71677.491	0.30239835	155.96369	182.31706
18907.095					
2550	-71677.189	-71677.482	0.29362971	151.44122	182.31706
20829.597					
2560	-71677.189	-71677.53	0.34102376	175.88498	182.31706
22026.97					
2570	-71677.189	-71677.607	0.41823044	215.70477	182.31706
22717.371					
2580	-71677.189	-71677.681	0.49240554	253.961	182.31706
23029.637					
2590	-71677.189	-71677.725	0.53620321	276.5499	182.31706
23001.645					
2600	-71677.189	-71677.725	0.53645537	276.67996	182.31706
22720.613					
2610	-71677.189	-71677.686	0.49783154	256.75949	182.31706
22109.1					
2620	-71677.189	-71677.629	0.4404715	227.17572	182.31706
21253.122					
2630	-71677.189	-71677.581	0.39241546	202.39054	182.31706
20222.392					
2640	-71677.189	-71677.568	0.37927139	195.61141	182.31706
18993.65					
2650	-71677.189	-71677.603	0.41388624	213.46422	182.31706
17500.839					
2660	-71677.189	-71677.679	0.48990633	252.67202	182.31706
15796.655					
2670	-71677.189	-71677.772	0.58299475	300.68291	182.31706
14170.138					
2680	-71677.189	-71677.849	0.66001051	340.40423	182.31706
13071.666					
2690	-71677.189	-71677.881	0.6919081	356.8556	182.31706
12873.505					
2700	-71677.189	-71677.853	0.66468396	342.8146	182.31706
13668.084					
2710	-71677.189	-71677.773	0.58460271	301.51222	182.31706
15249.214					
2720	-71677.189	-71677.665	0.47628417	245.64631	182.31706
17229.575					
2730	-71677.189	-71677.563	0.37411421	192.95157	182.31706
19185.666					
2740	-71677.189	-71677.498	0.30980893	159.78575	182.31706
20782.324					
2750	-71677.189	-71677.49	0.30106961	155.27839	182.31706
21849.152					
2760	-71677.189	-71677.535	0.34601186	178.45762	182.31706
22393.853					
2770	-71677.189	-71677.614	0.42505073	219.22237	182.31706
22455.301					
2780	-71677.189	-71677.697	0.50860726	262.31714	182.31706
22145.989					

2790	-71677.189	-71677.756	0.56736886	292.62377	182.31706
21630.275					
2800	-71677.189	-71677.771	0.58206631	300.20406	182.31706
21010.636					
2810	-71677.189	-71677.739	0.55031365	283.82744	182.31706
20329.95					
2820	-71677.189	-71677.677	0.48800444	251.69111	182.31706
19551.982					
2830	-71677.189	-71677.612	0.42378821	218.57122	182.31706
18587.717					
2840	-71677.189	-71677.576	0.38772711	199.9725	182.31706
17368.94					
2850	-71677.189	-71677.587	0.39872659	205.64554	182.31706
15926.833					
2860	-71677.189	-71677.645	0.45674813	235.57049	182.31706
14451.159					
2870	-71677.189	-71677.732	0.54313266	280.12381	182.31706
13286.716					
2880	-71677.189	-71677.816	0.62779767	323.79028	182.31706
12826.502					
2890	-71677.189	-71677.868	0.67963611	350.52625	182.31706
13347.074					
2900	-71677.189	-71677.865	0.67675754	349.04161	182.31706
14880.425					
2910	-71677.189	-71677.803	0.6140196	316.68416	182.31706
17175.298					
2920	-71677.189	-71677.694	0.50577623	260.85701	182.31706
19761.52					
2930	-71677.189	-71677.571	0.38254565	197.30013	182.31706
22113.908					
2940	-71677.189	-71677.47	0.28181378	145.34709	182.31706
23848.596					
2950	-71677.189	-71677.424	0.23537197	121.39446	182.31706
24659.186					
2960	-71677.189	-71677.447	0.25803771	133.08444	182.31706
24518.744					
2970	-71677.189	-71677.531	0.34214406	176.46278	182.31706
23558.942					
2980	-71677.189	-71677.649	0.46013879	237.31924	182.31706
21895.727					
2990	-71677.189	-71677.763	0.57432281	296.21031	182.31706
19725.092					
3000	-71677.189	-71677.838	0.64976598	335.12056	182.31706
17448.586					
3010	-71677.189	-71677.854	0.66569384	343.33544	182.31706
15571.341					
3020	-71677.189	-71677.811	0.62189042	320.74358	182.31706
14477.472					
3030	-71677.189	-71677.727	0.5384503	277.70885	182.31706
14303.54					
3040	-71677.189	-71677.638	0.44917088	231.66247	182.31706
14820.396					
3050	-71677.189	-71677.579	0.38990936	201.098	182.31706
15558.636					
3060	-71677.189	-71677.573	0.38460327	198.36136	182.31706
16124.84					
3070	-71677.189	-71677.623	0.43473212	224.21561	182.31706
16456.703					
3080	-71677.189	-71677.707	0.51847688	267.40745	182.31706
16811.969					

3090	-71677.189	-71677.789	0.6003058	309.61118	182.31706
17512.717					
3100	-71677.189	-71677.834	0.64531829	332.82664	182.31706
18670.66					
3110	-71677.189	-71677.82	0.63181265	325.86103	182.31706
20128.861					
3120	-71677.189	-71677.747	0.55863689	288.1202	182.31706
21631.668					
3130	-71677.189	-71677.635	0.44593387	229.99297	182.31706
22934.034					
3140	-71677.189	-71677.518	0.32892618	169.64558	182.31706
23808.7					
3150	-71677.189	-71677.435	0.24635336	127.05817	182.31706
24073.54					
3160	-71677.189	-71677.416	0.22719193	117.17555	182.31706
23538.936					
3170	-71677.189	-71677.469	0.2803253	144.57939	182.31706
22050.511					
3180	-71677.189	-71677.58	0.3912631	201.7962	182.31706
19744.814					
3190	-71677.189	-71677.716	0.5272181	271.91578	182.31706
17069.581					
3200	-71677.189	-71677.837	0.64847541	334.45494	182.31706
14549.103					
3210	-71677.189	-71677.91	0.72133132	372.0308	182.31706
12766.845					
3220	-71677.189	-71677.917	0.72809856	375.52104	182.31706
12102.144					
3230	-71677.189	-71677.86	0.67162011	346.39195	182.31706
12608.122					
3240	-71677.189	-71677.762	0.57348537	295.77839	182.31706
14027.549					
3250	-71677.189	-71677.655	0.46659858	240.65091	182.31706
15915.442					
3260	-71677.189	-71677.573	0.38428165	198.19548	182.31706
17811.3					
3270	-71677.189	-71677.538	0.34928526	180.14589	182.31706
19390.439					
3280	-71677.189	-71677.555	0.36635855	188.95154	182.31706
20531.397					
3290	-71677.189	-71677.61	0.421225	217.24923	182.31706
21306.833					
3300	-71677.189	-71677.675	0.48656175	250.94703	182.31706
21779.102					
3310	-71677.189	-71677.722	0.5328315	274.81092	182.31706
22043.679					
3320	-71677.189	-71677.728	0.53964206	278.32351	182.31706
22123.649					
3330	-71677.189	-71677.692	0.50339394	259.62833	182.31706
21994.158					
3340	-71677.189	-71677.627	0.43864474	226.23356	182.31706
21629.465					
3350	-71677.189	-71677.562	0.37288336	192.31675	182.31706
20957.342					
3360	-71677.189	-71677.525	0.33630643	173.45199	182.31706
19962.013					
3370	-71677.189	-71677.539	0.34999231	180.51055	182.31706
18598.491					
3380	-71677.189	-71677.606	0.41701834	215.07962	182.31706
16882.481					

3390	-71677.189	-71677.709	0.52036178	268.37959	182.31706
14998.562					
3400	-71677.189	-71677.817	0.62852448	324.16513	182.31706
13328.344					
3410	-71677.189	-71677.895	0.70636531	364.31199	182.31706
12338.35					
3420	-71677.189	-71677.916	0.7270157	374.96255	182.31706
12398.186					
3430	-71677.189	-71677.87	0.68118904	351.32718	182.31706
13611.373					
3440	-71677.189	-71677.77	0.58125069	299.7834	182.31706
15722.571					
3450	-71677.189	-71677.647	0.45824369	236.34183	182.31706
18194.879					
3460	-71677.189	-71677.54	0.3513935	181.23323	182.31706
20471.94					
3470	-71677.189	-71677.482	0.29304879	151.1416	182.31706
22239.134					
3480	-71677.189	-71677.485	0.29610162	152.71612	182.31706
23368.205					
3490	-71677.189	-71677.539	0.35061474	180.83158	182.31706
23869.981					
3500	-71677.189	-71677.619	0.43042158	221.99242	182.31706
23759.435					
3510	-71677.189	-71677.693	0.50458894	260.24466	182.31706
23076.177					
3520	-71677.189	-71677.737	0.54844383	282.86308	182.31706
21912.944					
3530	-71677.189	-71677.74	0.55090025	284.12999	182.31706
20484.532					
3540	-71677.189	-71677.706	0.51709761	266.69608	182.31706
19085.58					
3550	-71677.189	-71677.655	0.4661555	240.42239	182.31706
17840.281					
3560	-71677.189	-71677.613	0.42447242	218.9241	182.31706
16696.785					
3570	-71677.189	-71677.604	0.41565878	214.37842	182.31706
15549.163					
3580	-71677.189	-71677.639	0.45031871	232.25448	182.31706
14361.948					
3590	-71677.189	-71677.709	0.52062422	268.51495	182.31706
13443.42					
3600	-71677.189	-71677.791	0.60270986	310.85109	182.31706
13230.259					
3610	-71677.189	-71677.855	0.66584188	343.4118	182.31706
13931.871					
3620	-71677.189	-71677.872	0.68381175	352.67986	182.31706
15468.417					
3630	-71677.189	-71677.833	0.64424909	332.27519	182.31706
17564.612					
3640	-71677.189	-71677.742	0.55320419	285.31826	182.31706
19875.269					
3650	-71677.189	-71677.622	0.43362993	223.64714	182.31706
22079.17					
3660	-71677.189	-71677.507	0.31872273	164.38309	182.31706
23915.734					
3670	-71677.189	-71677.431	0.2420749	124.85153	182.31706
25092.96					
3680	-71677.189	-71677.416	0.2271065	117.13149	182.31706
25300.184					

3690	-71677.189	-71677.467	0.27869252	143.73728	182.31706
24373.592					
3700	-71677.189	-71677.569	0.38049827	196.24418	182.31706
22445.818					
3710	-71677.189	-71677.689	0.50037687	258.07226	182.31706
19886.399					
3720	-71677.189	-71677.791	0.6019513	310.45986	182.31706
17305.412					
3730	-71677.189	-71677.846	0.65737724	339.04611	182.31706
15250.293					
3740	-71677.189	-71677.845	0.65614577	338.41097	182.31706
13998.67					
3750	-71677.189	-71677.796	0.60728869	313.21265	182.31706
13545.896					
3760	-71677.189	-71677.724	0.53500815	275.93354	182.31706
13721.537					
3770	-71677.189	-71677.658	0.4694921	242.14326	182.31706
14304.094					
3780	-71677.189	-71677.624	0.4358332	224.78349	182.31706
15092.495					
3790	-71677.189	-71677.633	0.44467103	229.34165	182.31706
15963.673					
3800	-71677.189	-71677.677	0.48814653	251.76439	182.31706
16910.838					
3810	-71677.189	-71677.732	0.54320451	280.16087	182.31706
17982.876					
3820	-71677.189	-71677.77	0.58112713	299.71968	182.31706
19251.836					
3830	-71677.189	-71677.768	0.57923239	298.74245	182.31706
20703.145					
3840	-71677.189	-71677.719	0.53004898	273.37583	182.31706
22223.602					
3850	-71677.189	-71677.633	0.44478136	229.39855	182.31706
23604.212					
3860	-71677.189	-71677.538	0.34975556	180.38845	182.31706
24484.691					
3870	-71677.189	-71677.466	0.27741656	143.07919	182.31706
24627.468					
3880	-71677.189	-71677.443	0.25473809	131.38264	182.31706
23842.933					
3890	-71677.189	-71677.482	0.29322502	151.2325	182.31706
22117.217					
3900	-71677.189	-71677.574	0.38504348	198.5884	182.31706
19660.625					
3910	-71677.189	-71677.694	0.50579593	260.86717	182.31706
16893.985					
3920	-71677.189	-71677.811	0.62223623	320.92193	182.31706
14442.246					
3930	-71677.189	-71677.891	0.70249179	362.3142	182.31706
12702.138					
3940	-71677.189	-71677.915	0.72593123	374.40322	182.31706
11907.745					
3950	-71677.189	-71677.878	0.68933269	355.52732	182.31706
12153.133					
3960	-71677.189	-71677.796	0.60779478	313.47367	182.31706
13342.944					
3970	-71677.189	-71677.698	0.5097003	262.88088	182.31706
15124.033					
3980	-71677.189	-71677.615	0.42683963	220.14501	182.31706
17135.256					

3990	-71677.189	-71677.571	0.38268788	197.37348	182.31706
19140.201					
4000	-71677.189	-71677.572	0.38374187	197.91709	182.31706
20910.045					
4010	-71677.189	-71677.607	0.41804887	215.61112	182.31706
22248.627					
4020	-71677.189	-71677.65	0.46163131	238.08902	182.31706
23106.567					
4030	-71677.189	-71677.678	0.48909042	252.25121	182.31706
23515.856					
4040	-71677.189	-71677.672	0.48375811	249.50104	182.31706
23566.721					
4050	-71677.189	-71677.633	0.44397962	228.98506	182.31706
23333.03					
4060	-71677.189	-71677.573	0.38396471	198.03202	182.31706
22859.895					
4070	-71677.189	-71677.518	0.32954438	169.96442	182.31706
21944.577					
4080	-71677.189	-71677.498	0.30981619	159.78949	182.31706
20401.75					
4090	-71677.189	-71677.535	0.34600517	178.45416	182.31706
18166.867					
4100	-71677.189	-71677.63	0.44102077	227.45901	182.31706
15440.001					
4110	-71677.189	-71677.764	0.57495146	296.53454	182.31706
12738.194					
4120	-71677.189	-71677.899	0.71016026	366.26926	182.31706
10763.224					
4130	-71677.189	-71677.993	0.80418949	414.76538	182.31706
10093.191					
4140	-71677.189	-71678.013	0.82446108	425.22056	182.31706
10927.099					
4150	-71677.189	-71677.948	0.75931838	391.62284	182.31706
13088.127					
4160	-71677.189	-71677.811	0.62238494	320.99863	182.31706
16182.246					
4170	-71677.189	-71677.638	0.44897861	231.56331	182.31706
19691.999					
4180	-71677.189	-71677.474	0.28554974	147.27393	182.31706
22988.246					
4190	-71677.189	-71677.364	0.17542572	90.476827	182.31706
25468.952					
4200	-71677.189	-71677.334	0.14521767	74.896851	182.31706
26592.408					
4210	-71677.189	-71677.386	0.19692082	101.56305	182.31706
26211.346					
4220	-71677.189	-71677.497	0.30885071	159.29154	182.31706
24485.444					
4230	-71677.189	-71677.633	0.44448903	229.24779	182.31706
21997.16					
4240	-71677.189	-71677.754	0.5650241	291.41444	182.31706
19373.628					
4250	-71677.189	-71677.83	0.64103445	330.61722	182.31706
17084.205					
4260	-71677.189	-71677.849	0.66022368	340.51418	182.31706
15380.576					
4270	-71677.189	-71677.818	0.62936435	324.5983	182.31706
14288.541					
4280	-71677.189	-71677.759	0.57025623	294.11294	182.31706
13784.848					

4290	-71677.189	-71677.7	0.51102137	263.56222	182.31706
13805.16					
4300	-71677.189	-71677.664	0.47573909	245.36518	182.31706
14231.781					
4310	-71677.189	-71677.665	0.47591975	245.45836	182.31706
14902.845					
4320	-71677.189	-71677.695	0.50671223	261.33976	182.31706
15676.671					
4330	-71677.189	-71677.738	0.54926492	283.28655	182.31706
16505.894					
4340	-71677.189	-71677.767	0.57850203	298.36577	182.31706
17450.723					
4350	-71677.189	-71677.762	0.57337616	295.72207	182.31706
18605.194					
4360	-71677.189	-71677.714	0.52559194	271.07708	182.31706
19984.832					
4370	-71677.189	-71677.632	0.44354323	228.75998	182.31706
21452.748					
4380	-71677.189	-71677.539	0.35024153	180.63909	182.31706
22826.198					
4390	-71677.189	-71677.464	0.27568061	142.18387	182.31706
23702.964					
4400	-71677.189	-71677.435	0.24644734	127.10664	182.31706
23850.42					
4410	-71677.189	-71677.465	0.27613841	142.41998	182.31706
23203.327					
4420	-71677.189	-71677.549	0.36007311	185.70979	182.31706
21811.124					
4430	-71677.189	-71677.665	0.47643696	245.72512	182.31706
19819.34					
4440	-71677.189	-71677.782	0.59317759	305.93477	182.31706
17605.472					
4450	-71677.189	-71677.867	0.67841766	349.89783	182.31706
15405.302					
4460	-71677.189	-71677.899	0.71071881	366.55733	182.31706
13604.979					
4470	-71677.189	-71677.874	0.68563483	353.62013	182.31706
12578.763					
4480	-71677.189	-71677.805	0.61681677	318.12682	182.31706
12503.438					
4490	-71677.189	-71677.72	0.53094306	273.83695	182.31706
13268.214					
4500	-71677.189	-71677.646	0.45756036	235.9894	182.31706
14563.396					
4510	-71677.189	-71677.606	0.4175026	215.32938	182.31706
16085.658					
4520	-71677.189	-71677.604	0.41528979	214.18811	182.31706
17711.162					
4530	-71677.189	-71677.628	0.43918343	226.51139	182.31706
19420.533					
4540	-71677.189	-71677.657	0.46800821	241.37794	182.31706
21164.763					
4550	-71677.189	-71677.67	0.48097991	248.06817	182.31706
22859.073					
4560	-71677.189	-71677.655	0.46618826	240.43929	182.31706
24259.92					
4570	-71677.189	-71677.614	0.42519761	219.29812	182.31706
25055.773					
4580	-71677.189	-71677.562	0.37295861	192.35556	182.31706
25033.913					

4590	-71677.189	-71677.521	0.33264859	171.56543	182.31706
24105.006					
4600	-71677.189	-71677.516	0.32704644	168.67609	182.31706
22329.999					
4610	-71677.189	-71677.558	0.36909298	190.36184	182.31706
19932.137					
4620	-71677.189	-71677.644	0.45567549	235.01727	182.31706
17233.6					
4630	-71677.189	-71677.756	0.56725005	292.56249	182.31706
14626.249					
4640	-71677.189	-71677.862	0.67347931	347.35085	182.31706
12551.69					
4650	-71677.189	-71677.931	0.74275506	383.08022	182.31706
11393.181					
4660	-71677.189	-71677.941	0.75229198	387.99894	182.31706
11414.551					
4670	-71677.189	-71677.884	0.69560681	358.76323	182.31706
12699.39					
4680	-71677.189	-71677.774	0.58515709	301.79815	182.31706
15113.502					
4690	-71677.189	-71677.638	0.44939116	231.77609	182.31706
18197.132					
4700	-71677.189	-71677.513	0.32480964	167.52245	182.31706
21190.69					
4710	-71677.189	-71677.434	0.24517435	126.45009	182.31706
23413.021					
4720	-71677.189	-71677.42	0.23097349	119.12591	182.31706
24522.929					
4730	-71677.189	-71677.471	0.28257766	145.74106	182.31706
24451.422					
4740	-71677.189	-71677.569	0.38038059	196.18349	182.31706
23552.303					
4750	-71677.189	-71677.681	0.49196576	253.73418	182.31706
22240.736					
4760	-71677.189	-71677.772	0.58311475	300.7448	182.31706
20844.806					
4770	-71677.189	-71677.817	0.62875154	324.28224	182.31706
19499.431					
4780	-71677.189	-71677.809	0.62034407	319.94604	182.31706
18347.29					
4790	-71677.189	-71677.757	0.56801013	292.95451	182.31706
17432.561					
4800	-71677.189	-71677.685	0.49642193	256.03248	182.31706
16857.124					
4810	-71677.189	-71677.624	0.43552469	224.62437	182.31706
16649.395					
4820	-71677.189	-71677.598	0.40930068	211.09919	182.31706
16579.241					
4830	-71677.189	-71677.615	0.42671464	220.08054	182.31706
16369.069					
4840	-71677.189	-71677.667	0.47869633	246.8904	182.31706
15955.487					
4850	-71677.189	-71677.731	0.54232589	279.70771	182.31706
15587.849					
4860	-71677.189	-71677.779	0.59031818	304.46001	182.31706
15565.655					
4870	-71677.189	-71677.79	0.60172908	310.34525	182.31706
16153.58					
4880	-71677.189	-71677.758	0.56953072	293.73876	182.31706
17380.543					



```

      4890      -71677.189      -71677.692      0.50314828      259.50163      182.31706
18934.09
      4900      -71677.189      -71677.614      0.42524315      219.32161      182.31706
20425.746
      4910      -71677.189      -71677.552      0.36329028      187.36906      182.31706
21551.831
      4920      -71677.189      -71677.527      0.33881805      174.74737      182.31706
22161.157
      4930      -71677.189      -71677.548      0.35907175      185.19333      182.31706
22297.635
      4940      -71677.189      -71677.604      0.41492599      214.00048      182.31706
22053.538
      4950      -71677.189      -71677.674      0.4851707      250.22959      182.31706
21471.496
      4960      -71677.189      -71677.733      0.54478585      280.97645      182.31706
20571.606
      4970      -71677.189      -71677.763      0.57401648      296.05232      182.31706
19445.42
      4980      -71677.189      -71677.754      0.56513874      291.47357      182.31706
18307.155
      4990      -71677.189      -71677.714      0.52505272      270.79897      182.31706
17303.839
      5000      -71677.189      -71677.661      0.47285642      243.87843      182.31706
16438.676

```

Loop time of 290.315 on 1 procs for 5000 steps with 16 atoms

Performance: 0.744 ns/day, 32.257 hours/ns, 17.223 timesteps/s  
98.0% CPU use with 1 MPI tasks x no OpenMP threads

MPI task timing breakdown:

Section	min time	avg time	max time	%varavg	%total
Pair	290.25	290.25	290.25	0.0	99.98
Neigh	0	0	0	0.0	0.00
Comm	0.035198	0.035198	0.035198	0.0	0.01
Output	0.018024	0.018024	0.018024	0.0	0.01
Modify	0.0049432	0.0049432	0.0049432	0.0	0.00
Other		0.009049			0.00

```

Nlocal:          16.0000 ave          16 max          16 min
Histogram: 1 0 0 0 0 0 0 0 0 0
Nghost:          839.000 ave          839 max          839 min
Histogram: 1 0 0 0 0 0 0 0 0 0
Neighs:          0.00000 ave           0 max           0 min
Histogram: 1 0 0 0 0 0 0 0 0 0
FullNghs:        3648.00 ave          3648 max          3648 min
Histogram: 1 0 0 0 0 0 0 0 0 0

```

```

Total # of neighbors = 3648
Ave neighs/atom = 228.00000
Neighbor list builds = 0
Dangerous builds = 0
Total wall time: 0:04:50

```

In [ ]: