Pre & post processing tools for LAMMPS

While trying to generate the data file, we bumped into some tools that might help us in before and before the simulations using LAMMPS. The 36 tools given can be found in the public LAMMPS repository in GitHub, under the folder name “tools”.

Each tool is associated with a different function. It will assist you either in creating LAMMPS input files, or process LAMMPS output data.

Moreover, there will be sub-directories in each file. Be sure to read the README file for information on how to build and use the tools given.

For more instructions of how to use the tools and their functions are documented here: https://lammps.sandia.gov/doc/Tools.html

Here is a quick list on what the names and brief functions of the included tools:

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amber2lmp              python scripts for using AMBER to setup LAMMPS input
binary2txt             convert a LAMMPS dump file from binary to ASCII text
ch2lmp                 convert CHARMM files to LAMMPS input
chain                  create a data file of bead-spring chains
cmake                  tools and scripts for use with CMake
coding_standard        python scripts to detect and fix some LAMMPS conventions
colvars                post-process output of the fix colvars command
createatoms            generate lattices of atoms within a geometry
drude                  create Drude core/electron atom pairs in a data file
eam_database           one tool to generate EAM alloy potential files
eam_generate           2nd tool to generate EAM alloy potential files
eff                    scripts for working with the eFF (electron force field)
emacs                  add-ons to EMACS editor for editing LAMMPS input scripts
fep                    scripts for free-energy perturbation with USER-FEP pkg
i-pi                   Python wrapper for performing path-integral MD (PIMD)
ipp                    input pre-processor Perl tool for creating input scripts
kate                   add-ons to Kate editor for editing LAMMPS input scripts
lmp2arc                convert LAMMPS output to Accelrys Insight format
lmp2cfg                convert LAMMPS output to CFG files for AtomEye viz
matlab                 MatLab scripts for post-processing LAMMPS output
mesont                 Tools for use with the USER-MESONT package
micelle2d              create a data file of small lipid chains in solvent
moltemplate            Instructions for installing the Moltemplate builder program
msi2lmp                use Accelrys Insight code to setup LAMMPS input
phonon                 post-process output of the fix phonon command
polybond               Python tool for programmable polymer bonding
pymol_asphere          convert LAMMPS output of ellipsoids to PyMol format
python                 Python scripts for post-processing LAMMPS output
reax                   Tools for analyzing output of ReaxFF simulations
replica                tool to reorder LAMMPS replica trajectories according to temperature
singularity            Singularity container descriptions suitable for LAMMPS development
smd                    convert Smooth Mach Dynamics triangles to VTK
spin                   perform a cubic polynomial interpolation of a GNEB MEP
valgrind               suppression files for use with valgrind's memcheck tool
vim                    add-ons to VIM editor for editing LAMMPS input scripts
xmgrace                a collection of scripts to generate xmgrace plots
```

Again, to clone, or download the said resources to your computer:

Go to https://github.com/lammps/lammps → Copy the URL under the green “Code” button, i.e. [https://github.com/lammps/lammps.git]→ Open Git Bash and enter this command:

$ git clone https://github.com/lammps/lammps.git (ignore the dollar sign as it has already been done for you).