Post Processing Code for LAMMPS written in Matlab®

Arun K. Subramaniyan, sarunkarthi@gmail.com

readlog.m

This function reads data from a LAMMPS log file. It is robust and can read even if different number of variables are printed in the same log file. This can happen while using the *custom* command in LAMMPS or even in standard output when different *fix* commands are used (e.g. NPT and NVE).

readdump_all.m

This function reads all timesteps from a LAMMPS dump file. Useful when the dumpfile is small. Note that the entire dumpfile is stored in one structure. Hence it is unwise to use *readdump_all.m* for very large dump files.

readdump_one.m

This function reads one specified timestep from a LAMMPS dump file. Useful when the dumpfile is huge and need to enquire some specific timestep. It is also faster than *readdump_all.m* when reading dumpfiles with large number of timesteps.

scandump.m

As the name suggests, it scans all timesteps from a LAMMPS dump file and reports the available timesteps. It is useful when the dumpfile is huge. It is much faster than *readdump_all.m* and *readdump_one.m* especially when the filesize is large.

readrdf.m

This function reads radial distribution function (rdf) output from a LAMMPS rdf file. All available timesteps can be read individually and also just the average values can be read to save time while reading large files.

readEAM.m

The EAM potential file format used by DYNAMO is in a non-standard format. This function reads the EAM potential file and presents the data in a standard (column) format.

lmp2cfg.m

AtomEye is a visualization software for molecular systems. It requires data in a special format known as CFG. This function converts all timesteps from a LAMMPS dump file to the CFG configuration. It is very useful for automatically generating a sequence of numbered files from a dumpfile with multiple timestep data.