Classical MD simulations in PACE

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1 Preparations for classical MD simulations in LAMMPS

1. LAMMPS executable
2. Input scripts (in.file), force field parameters file and structure data (option)

1.1 LAMMPS executable

There are three options to access LMMAPS:

1. LAMMPS from Pace: module load gcc; module load lammps
2. Install LAMMPS in your local account: https://lammps.sandia.gov/doc/Install.html
3. My executable: lmp_mpi in the executable folder (copy it to your local account, and change the path in the lmp.pbs)

1.2 Input scripts

LAMMPS executes by reading commands from a input script (in.file), e.g., in.lmp. A LAMMPS input script typically has 4 parts: Initialization; Atom definition; Settings; Run a simulation. Details are available in https://lammps.sandia.gov/doc/.

1.2.1 Initialization

Set parameters that need to be defined before atoms are created or read-in from a file. The relevant commands are units, dimension, newton, processors, boundary, atom_style, atom_modify.

1.2.2 Atom definition

There are 3 ways to define atoms in LAMMPS. Read them in from a data or restart file via the read_data or read_restart commands. These files can contain

molecular topology information. Or create atoms on a lattice (with no molecular topology).

If read_data is selected, the corresponding **structure data** should be provided with a specific format.

1.2.3 Settings

Once atoms and molecular topology are defined, a variety of settings can be specified: force field coefficients, simulation parameters, output options, etc.

1. **Force field coefficients** are set by these commands (they can also be set in the read-in files): For example, Al_jnp.eam, Si.sw, and parameters.data (polymers). More force fields are available in the potentials folder.
2. Various simulation parameters are set by these commands
3. Fixes impose a variety of boundary conditions, time integration, and diagnostic options. The fix command comes in many flavors.
4. Output options are set by the thermo, dump, and restart commands.

1.2.4 Run a simulation

A molecular dynamics simulation is run using the run command. Energy minimization (molecular statics) is performed using the minimize command. A parallel tempering (replica-exchange) simulation can be run using the temper command.

2 Basics of running LAMMPS

LAMMPS is run from the command line, reading commands from a file via the -in command line flag, or from standard input. Using the "in.file" variant is recommended: e.g., mpirun $\sim$ /bin/lmp $-$ mpi $<$ in.lmp $>$ log. For pace, we use a specific lmp.pbs script in executable.

3 Supporting information for MD simulations

3.1 Force field parameters and structures data for polymers from medeA

Because the complex structures of polymers, we will use medeA software to build the initial structures for this step- in medeA we will follow the steps given below-

1. Go to **Builders** $\rightarrow$ **Polymers** $\rightarrow$ **Repeat unit** $\rightarrow$ **Add** $\rightarrow$ **ethers** $\rightarrow$ **ethylene oxide** $\rightarrow$ **Degree of Polymerization- set to the number of units needed**

2. Right Click to create **Create a periodic copy** OR Go to **Edit** → **Edit in molecular builder** → **Cell** → Adjust cell size and then **Create a periodic copy**

3. Next set the force fields by clicking on **Forcefields** → **read** → oplsaa+.frc → open

4. **Jobcontrol** → **New** → **LAMMPS** → **Initialize** → **Minimize** → OK

5. **Run**

6. **Jobcontrol** → **View and Control jobs** → **Jobs** → **Job ID**→ **Stage 1** → **get parameters.data and structure.data**

7. Move to MD simulations in LAMMPS (PACE) (Section 1.1), see examples (peo)

3.2 Benchmark

1. NVE run of Al (example/Al)

2. Generation of disorder slabs for polymers (example/peo)