Crash LAMMPS in 20 Minutes

Outline:

1. Basics, facts and my experiences.

2. Run through a simple example.

Basics of LAMMPS

LAMMPS is a classical molecular dynamics software written in C++ codes. It stands for **L**arge-scale **A**tomic/**M**olecular **M**assively **P**arallel **S**imulator. It uses common integration scheme (velocity-Verlet), but also can minimize energy to desired energy tolerance (gradient descent), etc. Users write a simple text file with LAMMPS’s own syntax to run a simulation.

LAMMPS has potentials for a range of materials: metals, semiconductors, small molecules, colloids, polymers, biomolecules, granular matter, etc., by simulating discrete particles with a variety of interactions, both in 2D and 3D. Information of particles and their interactions can be saved as files for further analysis.

Basics of LAMMPS

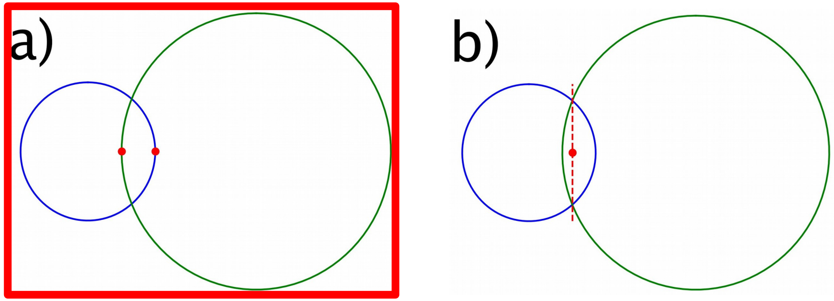
Besides running on single processors, it can be run in parallel, using a spatial-decomposition of the simulation domain and message-passing techniques to communicate between the domains. Many of its models have versions that provide accelerated performance on CPUs, GPUs, and Intel Xeon Phis.

LAMMPS is open source, and distributed by Sandia National Laboratories (DOE). All LAMMPS development is done via GitHub, which releases bug fixes and new features periodically. Its version is described by the release date, i.e. “30 April 2019”. The code is designed to be easy to modify or extend with new functionality. Users can also participate in development process.

Something You Need to Know about LAMMPS

It CANNOT simulate a continuous field such as fluid flow or deformation of an elastic body, nor electronic structures of an atom.

For granular features: contact location is on the surface of contacting spheres. a) is right, b) is wrong.



Recent release relevant for granular materials (Patch release 30 April 2019)
1. Fixes bug in calculation of relative tangential velocity for granular wall particle interactions.
2. Radius of curvature for curved regions was incorrectly used to compute wall-particle overlaps.

Performance of LAMMPS

Simulation time depends on number of particles and number of boundaries used.

My experience:
With realistic soft material (1 Gpa), one time step = 1 um, one 4GHz CPU (Intel).

~1,000 particles, 3 boundaries: ~250 simulation secs / real day
~10,000 particles (250 rigid hexapods), 2 boundaries: ~40 simulation secs / real day
~50,000 particles, 2 boundaries: ~10 simulation secs / real day

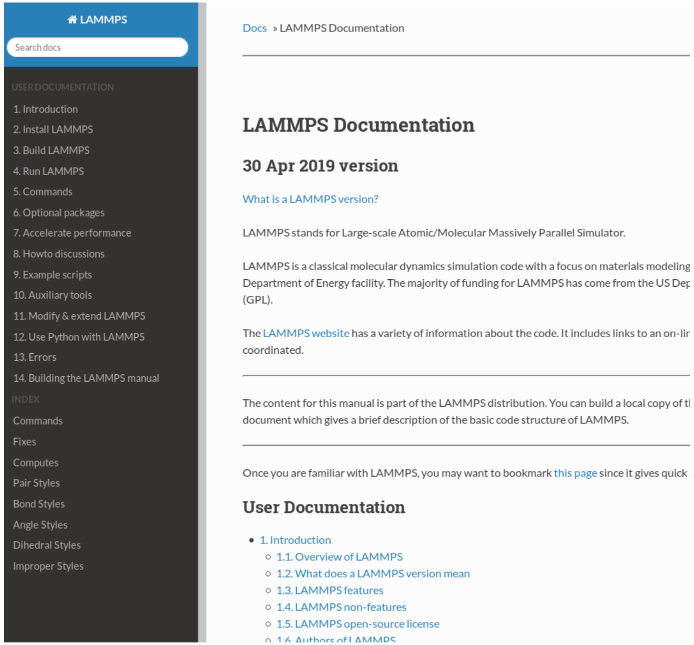
Output data files could also get huge (~1GB).

My learning experience: start playing with very simple, quick-run and relevant example codes they provided, understand them, modify and combine them into my simulation.

INSTALLATION: type *lmp* (or *lmp_serial, lmp_daily*) in your terminal and look for installation instructions, otherwise please visit the webpage https://lammps.sandia.gov/doc/Install.html

In the same folder:

1. Run *$lmp -in in.pour* it will generate a *log.lammps* file and images. Read through comments in the code and do test runs.
2. basic syntax: **command_type: command_name, parameter1, parameter2 ...**
3. documentations: https://lammps.sandia.gov/doc/Manual.html
   https://github.com/lammps/lammps



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LAMMPS Documentation

30 Apr 2019 version

What is a LAMMPS version?

LAMMPS stands for Large-scale Atomic/Molecular Massively Parallel Simulator.

LAMMPS is a classical molecular dynamics simulation code with a focus on materials modeling
Department of Energy facility. The majority of funding for LAMMPS has come from the US Dep
(GPL).

The LAMMPS website has a variety of information about the code. It includes links to an on-lir
coordinated.

The content for this manual is part of the LAMMPS distribution. You can build a local copy of tl
document which gives a brief description of the basic code structure of LAMMPS.

Once you are familiar with LAMMPS, you may want to bookmark this page since it gives quick

User Documentation

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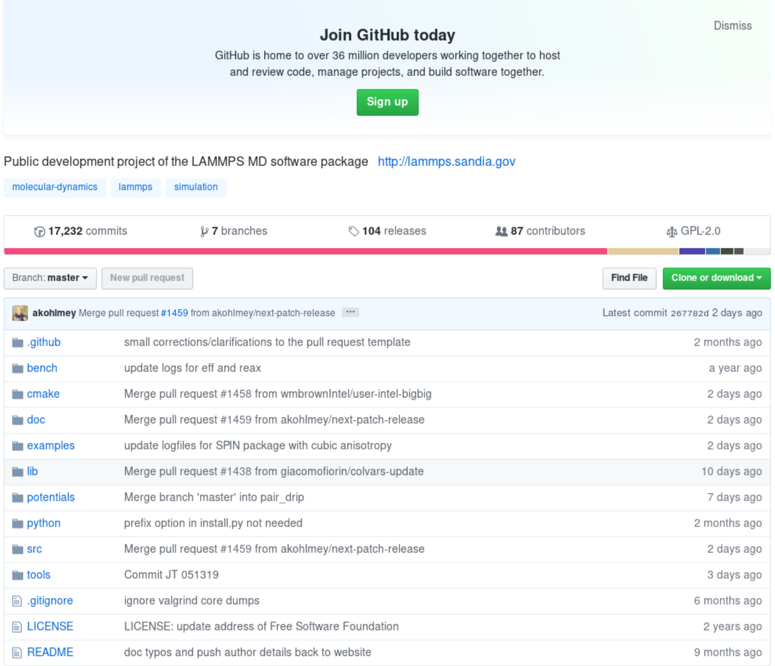

Join GitHub today

GitHub is home to over 36 million developers working together to host and review code, manage projects, and build software together.

Public development project of the LAMMPS MD software package http://lammps.sandia.gov

molecular-dynamics lammps simulation

17,232 commits | **7** branches | **104** releases | **87** contributors | GPL-2.0

akohlmey Merge pull request #1459 from akohlmey/next-patch-release ··· Latest commit 267782d 2 days ago

.github	small corrections/clarifications to the pull request template	2 months ago
bench	update logs for eff and reax	a year ago
cmake	Merge pull request #1458 from wmbrownIntel/user-intel-bigbig	2 days ago
doc	Merge pull request #1459 from akohlmey/next-patch-release	2 days ago
examples	update logfiles for SPIN package with cubic anisotropy	2 days ago
lib	Merge pull request #1438 from giacomofiorin/colvars-update	10 days ago
potentials	Merge branch 'master' into pair_drip	7 days ago
python	prefix option in install.py not needed	2 months ago
src	Merge pull request #1459 from akohlmey/next-patch-release	2 days ago
tools	Commit JT 051319	3 days ago
.gitignore	ignore valgrind core dumps	6 months ago
LICENSE	LICENSE: update address of Free Software Foundation	2 years ago
README	doc typos and push author details back to website	9 months ago

Homework !!

Some challenges to take:

1. Modify in.pour to start a chute flow after particles are poured.

    Hint: unfix the pour command ‘fix ins’ and add new ‘fix gravity’

        or look up the original pour example in LAMMPS example archive:

        https://github.com/lammps/lammps/blob/master/examples/pour/in.pour

2. Modify in.pour to add a cylindrical boundary (axis in the z direction) in the middle before pouring, so particles pack around it.

    Hint: look up command ‘fix wall/gran’ or ‘fix wall/gran/region’

3*.Following the hw2, let the cylindrical boundary to move in +x direction as a function of time.

    Hint: look up ‘region’ command and also ‘fix wall/gran/region’ command

The person who can show Yuchen
the first two simulations in action
will receive special treats.