Dive into computational physical chemistry

Lecture 7: Simple MD Models with LAMMPS

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Recap (Lecture 3): What is a classical Molecular Dynamics (MD) Simulation?

Classical particles obey Newton’s Equations of Motion

\[ F = m \ a \]

But really 3N differential equations

\[ F_i^x = m_i \ \frac{d^2 x_i}{dt^2} \; , \; F_i^y = m_i \ \frac{d^2 y_i}{dt^2} \; , \; F_i^z = m_i \ \frac{d^2 z_i}{dt^2} \]

What are the forces?

\[ \vec{F} = -\nabla U \]

\[ \Rightarrow F_i^x = -\frac{dU(x_1,y_1,z_1,...,x_N,y_N,z_N)}{dx_i} \], etc.

Good reference: https://livecomsjournal.org/index.php/livecoms/article/view/v1i1e5957
Simulation “box”

Bunch of molecules particles are put in a box

Typically: **periodic boundary conditions** – particles interact with their closest periodic image. Note: This prevents **edge effects** but not **finite size effects**.

After simulation: have to **wrap molecules into box** for visualization and certain kinds of analysis
Going away from atomistic MD

- Many problems can be studied by developing a simplified model (sometimes “coarse-grained”) representation of a system
- Physical principles can be discovered by studying very simplified systems including
  - A “particle” on an N-d potential energy surface
  - Particles interacting with simple potentials
- Interesting part of problem is what model to choose to represent your experiments
Ionic solids from common colloids

From rock salt to simple building blocks: micrometre scale forming crystals and structures such as...

Example 1 from research
Example 2 from research – supercooled liquids

Debenedetti and Stillinger, Nature (2001)

Kob & Andreassen, PRE (1995)
Example 2 from research – supercooled liquids

Scaling Behavior in the β-Relaxation Regime of a Supercooled Lennard-Jones Mixture

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Growing Point-to-Set Length Scale Correlates with Growing Relaxation Times in Model Supercooled Liquids

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Unveiling the predictive power of static structure in glassy systems

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Example 2 from research – supercooled liquids

The system we are studying in this work is a binary mixture of classical particles. Both types of particles (A and B) have the same mass \( m \) and all particles interact by means of a Lennard-Jones potential, i.e.,

\[ V_{\alpha\beta}(r) = 4\epsilon_{\alpha\beta} \left[ \left( \frac{\sigma_{\alpha\beta}}{r} \right)^{12} - \left( \frac{\sigma_{\alpha\beta}}{r} \right)^{6} \right] \]

with \( \alpha, \beta \in \{A, B\} \).

The reason for our choice of a mixture was to prevent the crystallization of the system at low temperatures. However, as we found out in the course of our work, choosing a binary mixture is by no means sufficient to prevent crystallization, if the system is cooled slowly. In particular, we found that a model that has previously been used to investigate the glass transition [24], namely, a mixture of 80% A particles and 20% B particles with \( \epsilon_{AA} = \epsilon_{AB} = \epsilon_{BB}, \sigma_{BB} = 0.8\sigma_{AA}, \) and \( \sigma_{AB} = 0.9\sigma_{AA}, \) crystallizes at low temperatures, as evidenced by a sudden drop in the pressure. In order to obtain a model system that is less prone to crystallization, we adjusted the parameters in the Lennard-Jones potential in such a way that the resulting potential is similar to one that was proposed by Weber and Stillinger to describe amorphous Ni_{80}P_{20} [25]. Thus we chose \( \epsilon_{AA} = 1.0, \sigma_{AA} = 1.0, \)

\( \epsilon_{AB} = 1.5, \sigma_{AB} = 0.8, \epsilon_{BB} = 0.5, \) and \( \sigma_{BB} = 0.88. \) The numbers of particles of type A and B were 800 and 200, respectively. The length of the cubic box was 9.4\( \sigma_{AA} \) and

Lennard-Jones potential
- 12-6 potential
- Minimum at \( 2^{\frac{1}{6}} \sigma \)
- 0 at diameter \( \sigma \)

WCA potential
- shift up at minimum and cut off

Kob & Andersen, PRE (1995)

Berthier and Biroli, RMP (2010)
Example 3 – crystallization of hard particles

Phase Transition for a Hard Sphere System

B. J. ALDER and T. E. WAINWRIGHT
University of California Radiation Laboratory, Livermore, California
(Received August 12, 1957)

\[ U(r) = \begin{cases} 
0, & r > \sigma \\
\infty, & r \leq \sigma 
\end{cases} \quad F = U - TS \]

A 32-particle system in a cube and initially in a face-centered cubic lattice proceeded at about 300 collisions an hour on the UNIVAC. For comparison a 96-particle system in a rectangular box and initially in a hexagonal arrangement has been calculated, however only at high

Phase Transition in Elastic Disks

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(Received October 30, 1961)

A study has been made of a two-dimensional system consisting of 870 hard-disk particles. Simultaneous motions of the particles have been calculated by means of an electronic computer as described previously. The disks were again placed in a periodically repeated rectangular array. The computer program has been improved such that about 200,000 collisions per hour can be calculated by the LARC computer regardless of the number of particles in the system. This speed made it possible to follow large systems for several million collisions.
**MD simulation software**

Many MD software, some of which have specialized purposes:

- **Bio systems:** GROMACS, AMBER, NAMD, OPENMM, ...
- **General/materials:** LAMMPS, HOOMD-BLUE

**Speed:** these are all optimized to greater or lesser degrees to parallelize computation across many CPUs and/or on GPU
LAMMPS

- Large-scale Atomic/Molecular Massively Parallel Simulator
- Development led by Steve Plimpton
- Very easy to customize
- Very general in terms of types of systems
- Downside – not as fast as GROMACS, AMBER etc
- FYI – Can use with PLUMED and other types of plugins, also can be called from Python and other cool features that can be useful in research
**LAMMPS usage**

- LAMMPS provides a number of examples to get you started
- Some good tutorials exist, e.g. [https://lammpstutorials.github.io/](https://lammpstutorials.github.io/)

**Key items:**
1. Units / atom_style
2. Create box/ atoms
3. Set mass
4. Initialize velocities
5. Set pair interactions
6. Fixes – nve, nvt, npt etc
7. Computes – various properties
8. Thermo – write properties to screen
9. Dump – write positions to files
10. Minimize / run – compute forces/ execute
Today

1. Pull updates on comp-lab-class github page
   https://github.com/hockyg/comp-lab-class-2023/blob/main/Week8/Assignment.md
2. Run an example from LAMMPS
3. Use LAMMPS and VMD to determine approximately when hard disks/spheres crystallize

Next time:
1) Special lecture
2) Catch up / run & analyze KA-LJ system for supercooled liquids