Dive into computational physical chemistry

Lecture 7: Simple MD Models with LAMMPS

Glen Hocky
October 27, 2023

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

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

What are the forces?

$$\vec{F} = -\nabla U$$

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

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

Example 1 from research

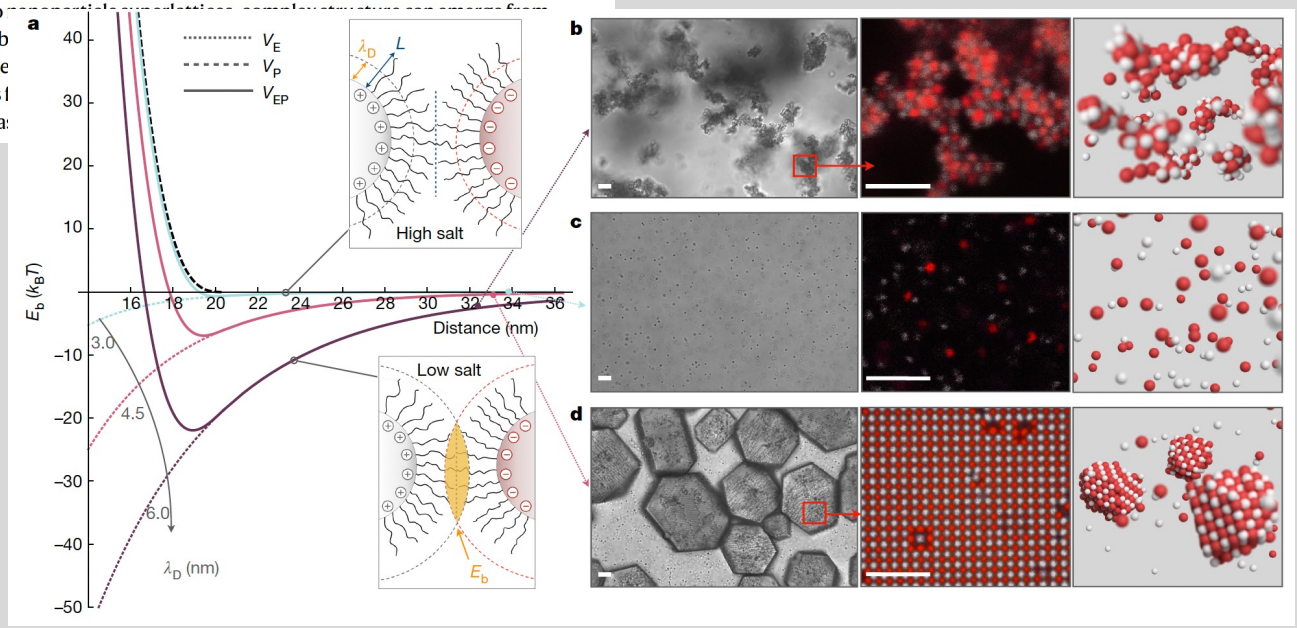
Article

Ionic solids from common colloids

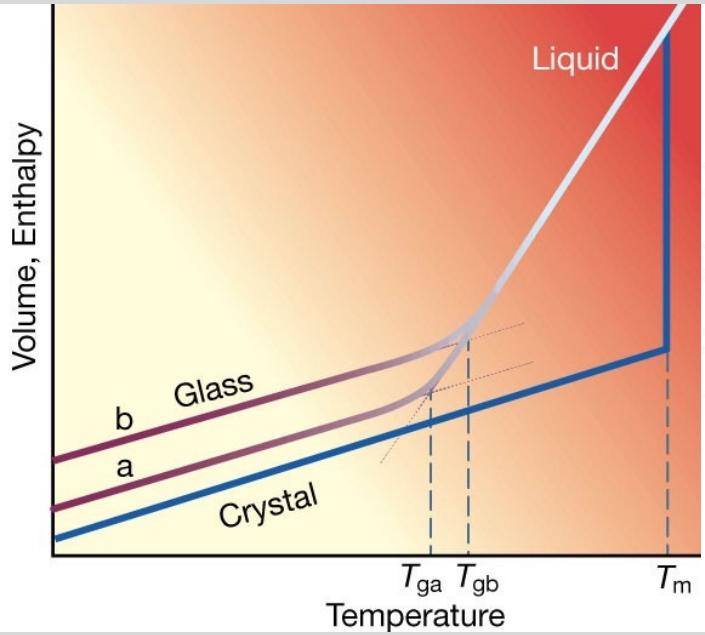
https://doi.org/10.1038/s41586-020-2205-0
Received: 14 August 2019
Accepted: 26 February 2020
Published online: 22 April 2020
Check for updates

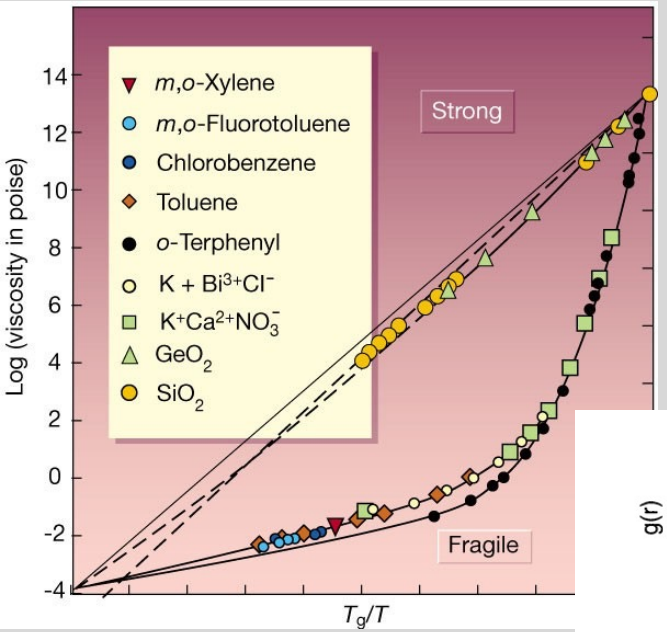
Theodore Hueckel[1], Glen M. Hocky[1], Jeremie Palacci[2] & Stefano Sacanna[1]✉

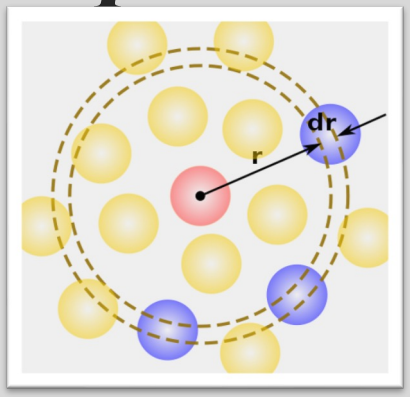
From rock salt to
simple building b
micrometre scale
forming crystals
structures such a



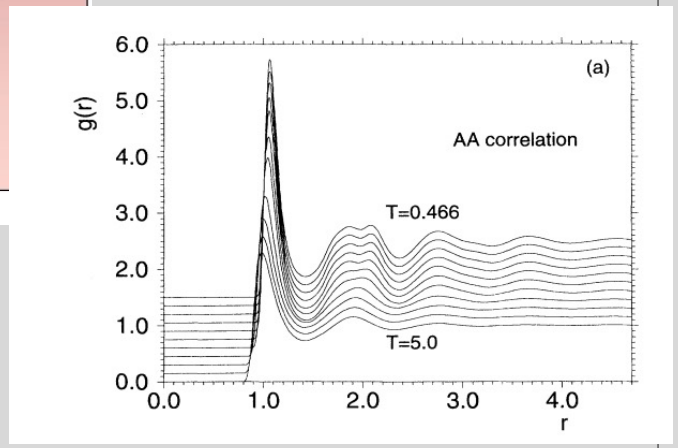
Example 2 from research – supercooled liquids







Debenedetti and Stillinger, Nature (2001)



Kob & Andresen, PRE (1995)

Example 2 from research – supercooled liquids

VOLUME 73, NUMBER 10 PHYSICAL REVIEW LETTERS 5 SEPTEMBER 1994

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

Walter Kob
Institut für Physik, Johannes Gutenberg-Universität, Staudinger Weg 7, D-55099 Mainz, Germany

Hans C. Andersen
Department of Chemistry, Stanford University, Stanford, California 94305
(Received 11 February 1994)

PRL **108,** 225506 (2012) PHYSICAL REVIEW LETTERS week endi 1 JUNE 20

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

Glen M. Hocky,[1] Thomas E. Markland,[2] and David R. Reichman[1,*]
[1]*Department of Chemistry, Columbia University, 3000 Broadway, New York, New York 10027, USA*
[2]*Department of Chemistry, Stanford University, 333 Campus Drive, Stanford, California 94305, USA*
(Received 17 January 2012; published 1 June 2012)

It has been demonstrated recently that supercooled liquids sharing simple structural features (e.g. pair distribution functions) may exhibit strikingly distinct dynamical behavior. Here we show that a more

ARTICLES
https://doi.org/10.1038/s41567-020-0842-8
nature physics
Check for updates

Unveiling the predictive power of static structure in glassy systems

V. Bapst[1,3], T. Keck[1,3], A. Grabska-Barwińska[1], C. Donner[1], E. D. Cubuk[2], S. S. Schoenholz[2], A. Obika[1], A. W. R. Nelson[1], T. Back[1], D. Hassabis[1] and P. Kohli[1]

Testing mode-coupling theory for a supercooled binary Lennard-Jones mixture I: The van Hove correlation function
W Kob, HC Andersen - Physical Review E, 1995 - APS
We report the results of a large scale computer simulation of a binary supercooled Lennard-Jones liquid. We find that at low temperatures the curves for the mean squared displacement …
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Testing mode-coupling theory for a supercooled binary Lennard-Jones mixture. II. Intermediate scattering function and dynamic susceptibility
W Kob, HC Andersen - Physical Review E, 1995 - APS
We have performed a molecular dynamics computer simulation of a supercooled binary Lennard-Jones system in order to compare the dynamical behavior of this system with the …
☆ Save 99 Cite Cited by 725 Related articles All 10 versions »

Scaling Behavior in the β-Relaxation Regime of a Supercooled Lennard-Jones Mixture
W Kob, HC Andersen - Physical review letters, 1994 - APS
We have performed molecular dynamics simulations of a supercooled atomic liquid. The self-intermediate-scattering function in the β-relaxation regime has a power-law time …
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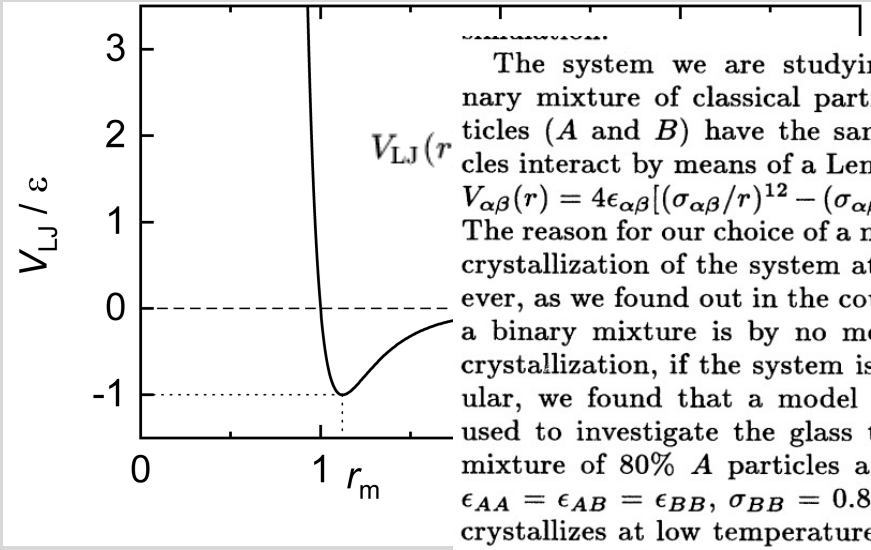
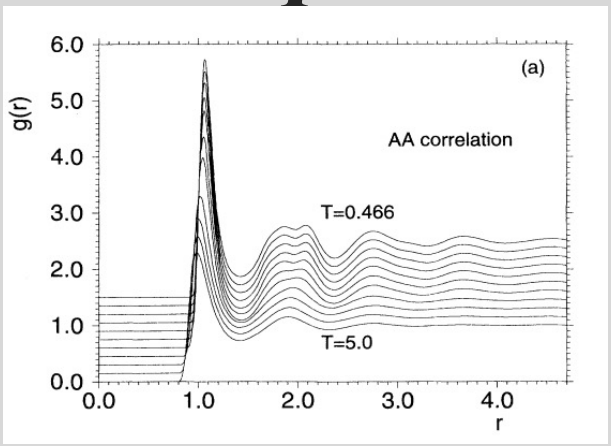
Example 2 from research – supercooled liquids



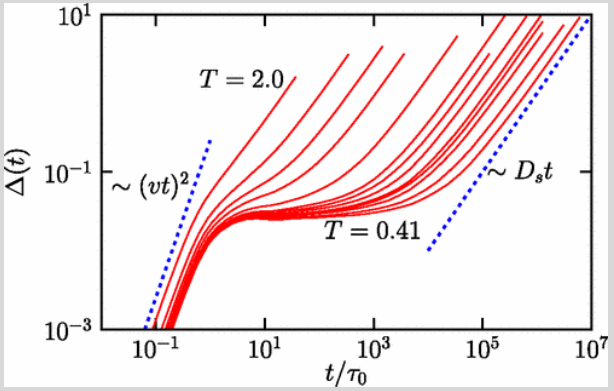
The system we are studying in this work is a binary mixture of classical particles. Both types of particles (A and B) have the same mass m and all particles interact by means of a Lennard-Jones potential, i.e., $V_{\alpha\beta}(r) = 4\epsilon_{\alpha\beta}[(\sigma_{\alpha\beta}/r)^{12} - (\sigma_{\alpha\beta}/r)^{6}]$ 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 σ

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)

$$U(r) = \begin{cases} 0, r > \sigma \\ \infty, r \leq \sigma \end{cases} \qquad F = U - TS$$

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

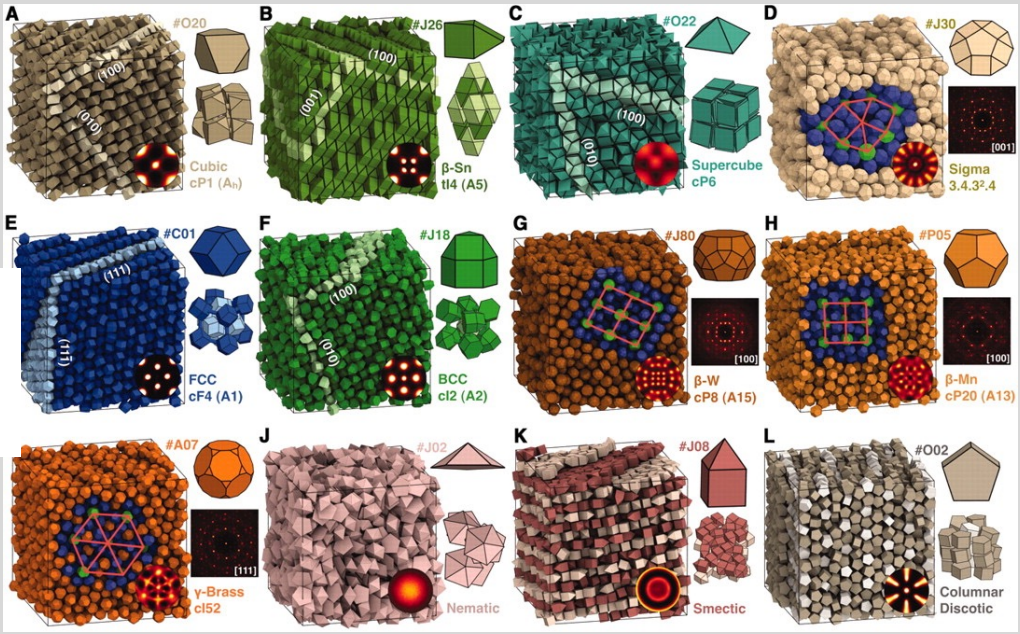
Phase Transition in Elastic Disks*

B. J. Alder and T. E. Wainwright
University of California, Lawrence Radiation Laboratory, Livermore, California
(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.[1] 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.

Predictive Self-Assembly of Polyhedra into Complex Structures

Pablo F. Damasceno,[1*] Michael Engel,[2*] Sharon C. Glotzer[1,2,3†]



MD simulation software

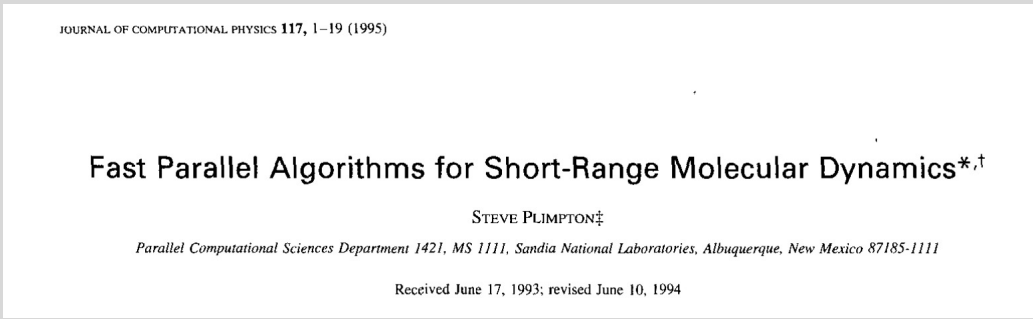
Many MD software, some of which have specialized purposes:

- ~~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



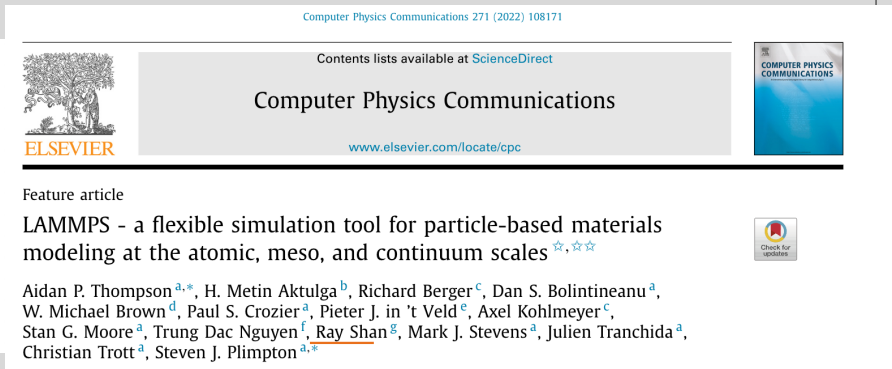
JOURNAL OF COMPUTATIONAL PHYSICS **117,** 1–19 (1995)

Fast Parallel Algorithms for Short-Range Molecular Dynamics*,†

STEVE PLIMPTON‡

Parallel Computational Sciences Department 1421, MS 1111, Sandia National Laboratories, Albuquerque, New Mexico 87185-1111

Received June 17, 1993; revised June 10, 1994



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www.elsevier.com/locate/cpc

Feature article

LAMMPS - a flexible simulation tool for particle-based materials modeling at the atomic, meso, and continuum scales ☆, ☆☆

Aidan P. Thompson [a,*], H. Metin Aktulga [b], Richard Berger [c], Dan S. Bolintineanu [a], W. Michael Brown [d], Paul S. Crozier [a], Pieter J. in 't Veld [e], Axel Kohlmeyer [c], Stan G. Moore [a], Trung Dac Nguyen [f], Ray Shan [g], Mark J. Stevens [a], Julien Tranchida [a], Christian Trott [a], Steven J. Plimpton [a,*]

LAMMPS usage

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

Key items:

1. Units / atom_style
2. Create box/ atoms
3. Set mass
4. Initialize velicities
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

```
# 3d Lennard-Jones melt

units           lj
atom_style      atomic

lattice         fcc 0.8442
region          box block 0 10 0 10 0 10
create_box      1 box
create_atoms    1 box
mass            1 1.0

velocity        all create 3.0 87287 loop geom

pair_style      lj/cut 2.5
pair_coeff      1 1 1.0 1.0 2.5

neighbor        0.3 bin
neigh_modify    every 20 delay 0 check no

fix             1 all nve

dump            id all atom 50 dump.melt

#dump           2 all image 25 image.*.jpg type type &
#               axes yes 0.8 0.02 view 60 -30
#dump_modify    2 pad 3

#dump           3 all movie 25 movie.mpg type type &
#               axes yes 0.8 0.02 view 60 -30
#dump_modify    3 pad 3

thermo          50
run             25000
```

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