

*Dive into
computational
physical chemistry*

*Lecture 7: Simple
MD Models with
LAMMPS*

Glen Hocky
October 18, 2024



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?

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

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

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> Theodore Hueckel¹, Glen M. Hocky¹, Jeremie Palacci² & Stefano Sacanna^{1,2,3}

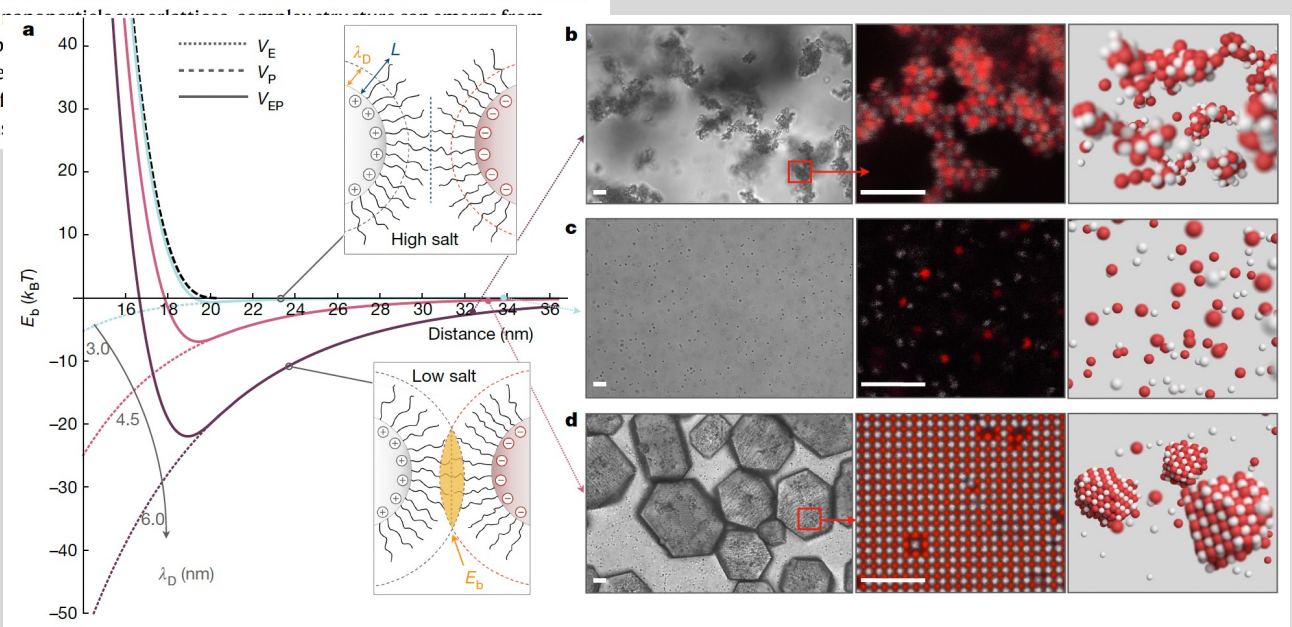
Received: 14 August 2019

Accepted: 26 February 2020

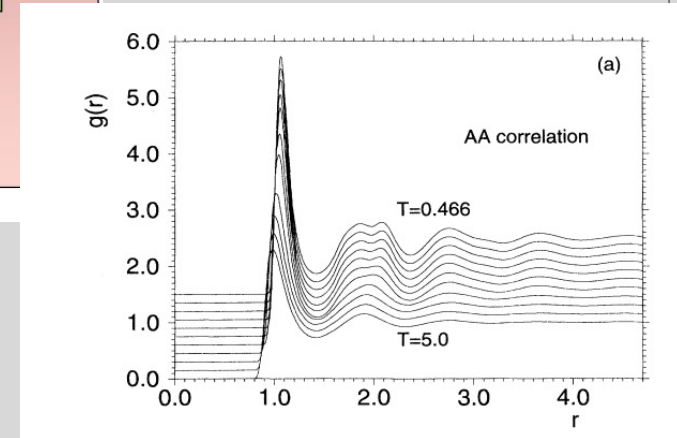
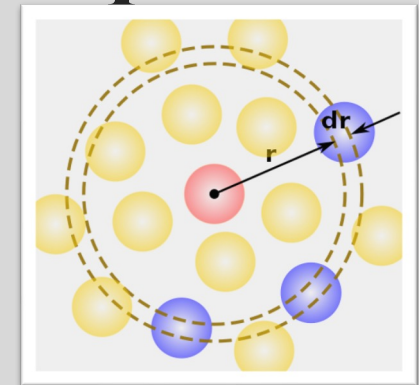
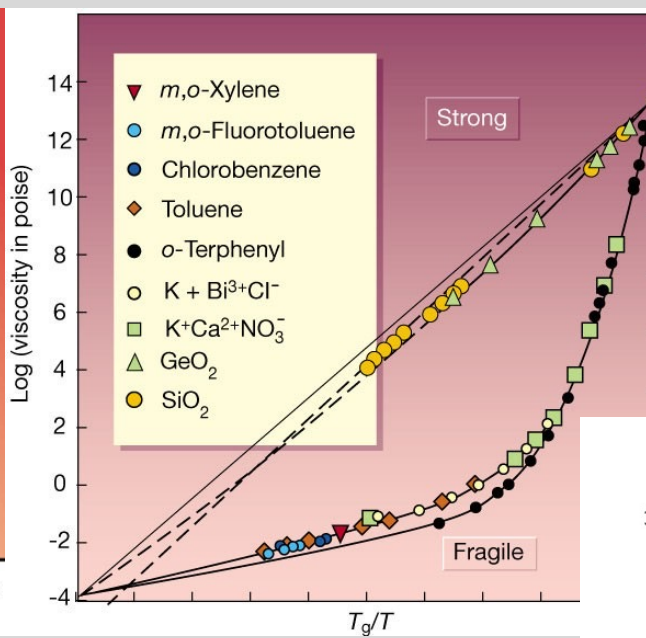
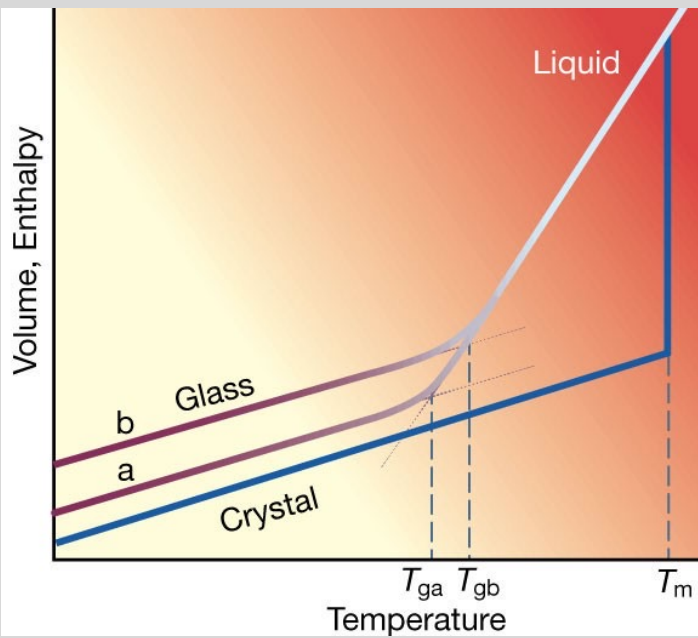
Published online: 22 April 2020

 Check for updates

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



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 ending
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

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 ...

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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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ARTICLES

<https://doi.org/10.1038/s41567-020-0842-8>

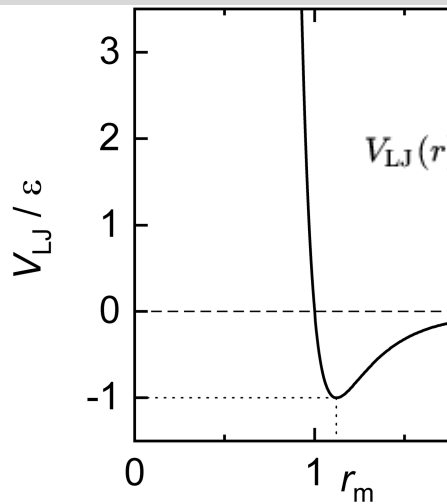
nature
physics

Check for updates

Unveiling the predictive power of static structure in glassy systems

V. Bapst^{1,3}✉, T. Keck^{1,3}, A. Grabska-Barwińska¹, C. Donner¹, E. D. Cubuk², S. S. Schoenholz², A. Obika¹, A. W. R. Nelson¹, T. Back¹, D. Hassabis¹ and P. Kohli¹

Example 2 from research – supercooled liquids



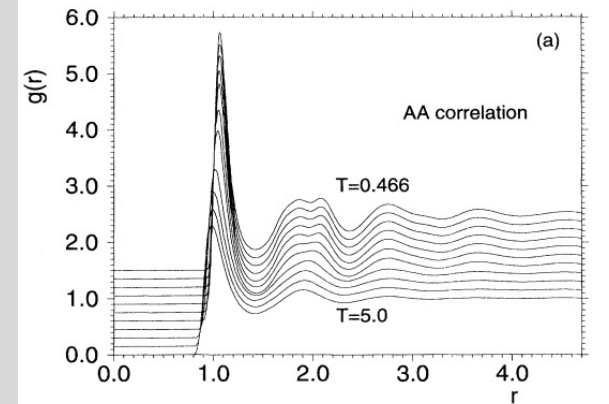
The system we are studying in this work is a binary mixture of classical particles. Both types of particles (A and B) have the same mass m and all particles interact by means of a Lennard-Jones potential, i.e., $V_{\alpha\beta}(r) = 4\epsilon_{\alpha\beta}[(\sigma_{\alpha\beta}/r)^{12} - (\sigma_{\alpha\beta}/r)^6]$ 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 $\text{Ni}_{80}\text{P}_{20}$ [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

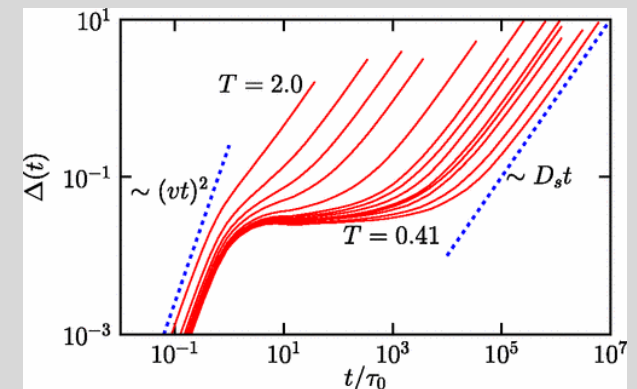
- 12-6 potential
- Minimum at $2^{1/6}\sigma$
- 0 at diameter σ

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)

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

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*

B. J. ALDER AND T. E. WAINWRIGHT

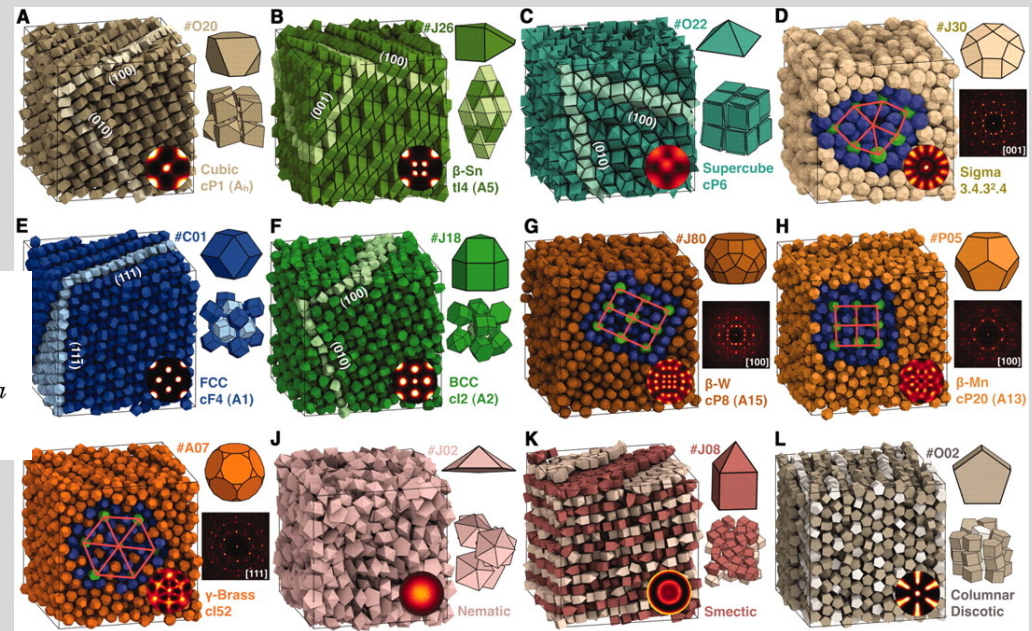
University of California, Lawrence Radiation Laboratory, Livermore, California

(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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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://lammptutorials.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

```
# 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-2024/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) Halloween + run & analyze KA-LJ system for supercooled liquids