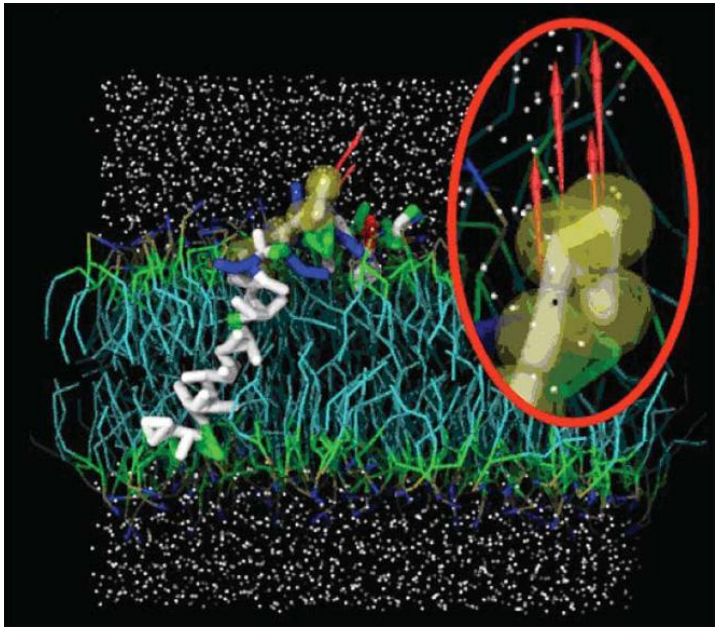
COMPUTATIONAL PHYSICS

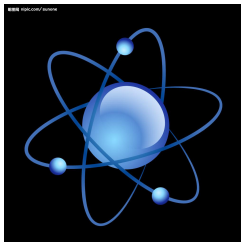
Shuai Dong



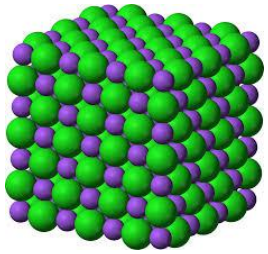
Molecular dynamics simulations

- General behavior of a classical system
- The Verlet algorithm
- Structure of atomic clusters

Many-body systems



atom



cluster

protein molecule

a drop of water

galaxy

Sun-Earth-Moon

Many-body systems

- In quantum mechanics:
- Hydrogen atom: one electron and one proton
- Analytical solutions for eigen-energies and eigen-wavefunctions.

- Helium atom: two electrons and a nucleus
- No exact analytical solution.

- A system of a large number of interacting objects is the so-called many-body system.

- Too many? Statistical mechanics!!!

General behavior of a classical system

- The molecular dynamics solves the dynamics of a classical many-body system described by the Hamiltonian.

$$\mathcal{H} = E_{\mathrm{K}} + E_{\mathrm{P}} = \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m_i} + \sum_{i>j=1}^{N} V(\mathbf{r}_{ij}) + \sum_{i=1}^{N} U_{\mathrm{ext}}(\mathbf{r}_i),$$

E_K: kinetic energy; E_P: potential energy
m_i, r_i, and p_i are the mass, position vector, and momentum of the ith particle
$V(r_{ij})$ and $U(r_i)$ are the corresponding interaction energy and external potential energy

- From Hamilton's principle, the position vector and momentum satisfy

$$\dot{\mathbf{r}}_i = \frac{\partial \mathcal{H}}{\partial \mathbf{p}_i} = \frac{\mathbf{p}_i}{m_i}, \quad \mathbf{f}_i = -\boldsymbol{\nabla}_i U_{\text{ext}}(\mathbf{r}_i) - \sum_{j \neq i} \boldsymbol{\nabla}_i V(\mathbf{r}_{ij}).$$

$$\dot{\mathbf{p}}_i = -\frac{\partial \mathcal{H}}{\partial \mathbf{q}_i} = \mathbf{f}_i, \qquad m_i \frac{d^2 \mathbf{r}_i}{dt^2} = \mathbf{f}_i,$$

for the ith particle in the system.

- To simplify the notation,
- **R:** all the coordinates ($\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N$)
- **G:** all the accelerations ($\mathbf{f}_1/m_1, \mathbf{f}_2/m_2, \ldots, \mathbf{f}_N/m_N$).
- Rewrite Newton's equations: $\dfrac{d^2\mathbf{R}}{dt^2} = \mathbf{G}.$

- We can also apply the three-point formula to the velocity

$$\mathbf{V} = \frac{d\mathbf{R}}{dt} = \frac{1}{2\tau}(\mathbf{R}_{k+1} - \mathbf{R}_{k-1}) + O(\tau^2).$$

$$\frac{d^2\mathbf{R}}{dt^2} = \frac{1}{\tau^2}(\mathbf{R}_{k+1} - 2\mathbf{R}_k + \mathbf{R}_{k-1}) + O(\tau^2), \quad \text{with } t = k\tau.$$

- The Verlet algorithm for a classical many-body system is:

$$\mathbf{R}_{k+1} = 2\mathbf{R}_k - \mathbf{R}_{k-1} + \tau^2\mathbf{G}_k + O(\tau^4),$$

$$\mathbf{V}_k = \frac{\mathbf{R}_{k+1} - \mathbf{R}_{k-1}}{2\tau} + O(\tau^2).$$

- The Verlet algorithm can be started if the first two positions $\mathbf{R_o}$ and $\mathbf{R_1}$ of the particles are given.
- If only the initial position $\mathbf{R_o}$ and initial velocity $\mathbf{V_o}$ are given, we need to figure out $\mathbf{R_1}$ before we can start the recursion.

- A common practice is to treat the force during the first time interval $[0, \tau]$ as a constant, and then to apply the kinematic equation to obtain

$$\mathbf{R}_1 \simeq \mathbf{R}_0 + \tau \mathbf{V}_0 + \frac{\tau^2}{2}\mathbf{G}_0,$$

where $\mathbf{G_o}$ is the acceleration vector evaluated at the initial configuration $\mathbf{R_o}$.

- The position $\mathbf{R}_1$ can be improved by carrying out the Taylor expansion to higher-order terms if the accuracy in the first two points is critical.

- We can also replace $\mathbf{G}_o$ with the average $(\mathbf{G}_o+\mathbf{G}_1)/2$, with $\mathbf{G}_1$ evaluated at $\mathbf{R}_1$.This procedure can be iterated several times before starting the algorithm for the velocity $\mathbf{V}_1$ and the next position $\mathbf{R}_2$.

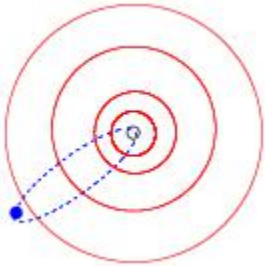
$$\mathbf{R}_{k+1} = \mathbf{R}_k + \tau \mathbf{V}_k + \frac{\tau^2}{2}\mathbf{G}_k + O(\tau^4),$$

$$\mathbf{V}_{k+1} = \mathbf{V}_k + \frac{\tau}{2}(\mathbf{G}_{k+1} + \mathbf{G}_k) + O(\tau^2).$$

Halley's comet

Edmond Halley
1656-1742
Predicted the re-appearance of comet in 1758.
Observed in Dec. 25, 1758

前613年，《春秋》“秋七月，有星孛入于北斗”。
前240年，《史记·始皇本纪》“始皇七年，彗星先出东方，见北方；五月见西方，十六日”



1910-1986-2061

- The gravitational potential: $V(r) = -G\frac{Mm}{r}$,

  where r is the distance between the comet and the Sun, M and m are the masses of the Sun and comet, respectively. G is the gravitational constant.

- Using the center-of-mass coordinate system for the two-body system, the dynamics of the comet is governed by:

$$\mu\frac{d^2\mathbf{r}}{dt^2} = \mathbf{f} = -GMm\frac{\mathbf{r}}{r^3},$$

with the reduced mass: $\mu = \frac{Mm}{M+m} \simeq m$

- We can take the farthest point (aphelion) as the starting point, and then we can easily obtain the comet's whole orbit with the Verlet algorithm.

- Two conservations: the total energy and the angular momentum.

- The motion of the comet in the xy plane:
  $x_o = r_{max} = 5.28 \times 10^{12}$ m, $v_{xo} = 0$
  $y_o = 0$, $v_{yo} = v_{min} = 9.13 \times 10^{2}$ m/s.

- Let us apply the Verlet algorithm to this problem.

Then we have

$$x^{(k+1)} = x^{(k)} + \tau v_x^{(k)} + \frac{\tau^2}{2} g_x^{(k)},$$

$$v_x^{(k+1)} = v_x^{(k)} + \frac{\tau}{2}\left[g_x^{(k+1)} + g_x^{(k)}\right],$$

$$y^{(k+1)} = y^{(k)} + \tau v_y^{(k)} + \frac{\tau^2}{2} g_y^{(k)},$$

$$v_y^{(k+1)} = v_y^{(k)} + \frac{\tau}{2}\left[g_y^{(k+1)} + g_y^{(k)}\right],$$

where the time-step index is given in parentheses as superscripts.

- The acceleration components are given by

$$g_x = -\kappa \frac{x}{r^3},$$

$$g_y = -\kappa \frac{y}{r^3},$$

with $r^2 = x^2 + y^2$ and $\kappa = GM$.

- We can use more specific units in the numerical calculations, for example, 76 years as the time unit and the semimajor axis of the orbital a = 2.68×10^{12} m as the length unit. Then we have $r_{max} = 1.97$, $v_{min} = 0.816$, and $\kappa = 39.5$.

Code example

- 7.1.Halley.cpp

Structure of atomic clusters

- To determine the structure and dynamics of a cluster consisting N atoms that interact with each other through the Lennard-Jones potential

$$V(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right],$$

where r is the distance between the two atoms, and ε and σ are the system dependent parameters.

- The force exerted on the ith atom is:

$$\mathbf{f}_i = \frac{48\varepsilon}{\sigma^2} \sum_{j \neq i}^{N} (\mathbf{r}_i - \mathbf{r}_j) \left[\left(\frac{\sigma}{r_{ij}} \right)^{14} - \frac{1}{2} \left(\frac{\sigma}{r_{ij}} \right)^{8} \right].$$

- The Verlet algorithm:

$$\mathbf{r}_i^{(k+1)} = \mathbf{r}_i^{(k)} + \tau \mathbf{v}_i^{(k)} + \frac{\tau^2}{2} \mathbf{g}_i^{(k)},$$

$$\mathbf{v}_i^{(k+1)} = \mathbf{v}_i^{(k)} + \frac{\tau}{2} \left[\mathbf{g}_i^{(k+1)} + \mathbf{g}_i^{(k)} \right].$$

We can then simulate the structure and dynamics of the cluster starting from a given initial position and velocity for each particle.

N bodies= N x 1 body???

4 August 1972, Volume 177, Number 4047

SCIENCE

Philip Warren Anderson (1923-2020)
Nobel Prize in Physics (1977)

More Is Different

Broken symmetry and the nature of the hierarchical structure of science.

P. W. Anderson

less relevance they seem to have to the very real problems of the rest of science, much less to those of society.

The constructionist hypothesis breaks down when confronted with the twin difficulties of scale and complexity. The behavior of large and complex aggregates of elementary particles, it turns out, is not to be understood in terms of a simple extrapolation of the properties of a few particles. Instead, at each level of complexity entirely new properties appear, and the understanding of the new behaviors requires re-

Phase transition
-from solid to liquid

Total energy: $$E = \sum_{i=1}^{N} \frac{m_i v_i^2}{2} + \sum_{i>j=1}^{N} V(r_{ij}),$$

Average kinetic energy: $\langle E_K \rangle = 3/2 N k_B T$

For each simulation, we can calculate the $\langle E_k \rangle$ (thus temperature).

We can tune the temperature to see what will happen.

Examples-animations

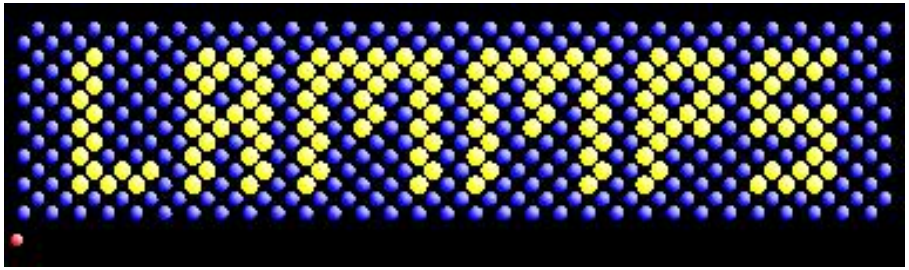
- Solid-Liquid-Gas
- Growth of a cluster
- Growth dynamics at the droplet-nanowire interface

A powerful tool

LAMMPS:
Large-scale Atomic/Molecular Massively Parallel Simulator
by Sandia National Labortories, USA

http://lammps.sandia.gov/

Free software, distributed under the terms of the GNU General Public License.



Homework

- Use the molecular dynamics simulation to simulate the one-dimensional lattice vibration and analyze its spectrum.