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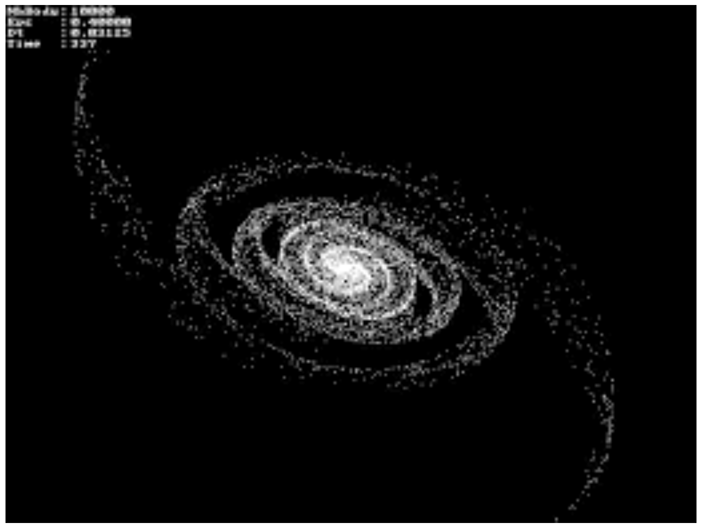
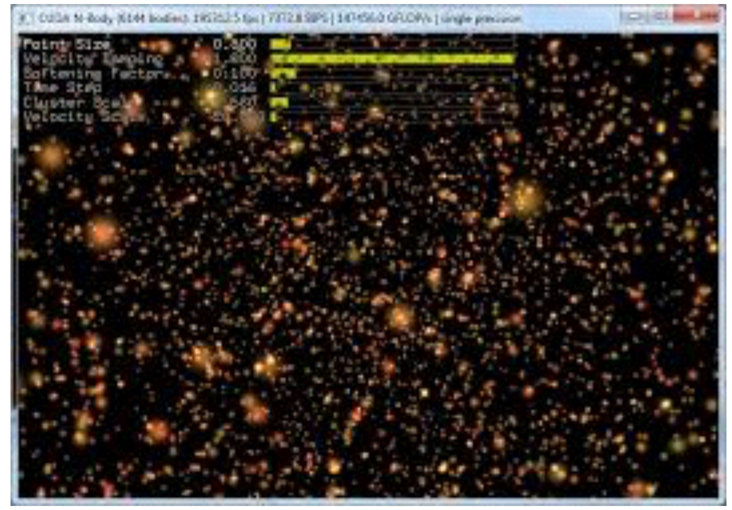
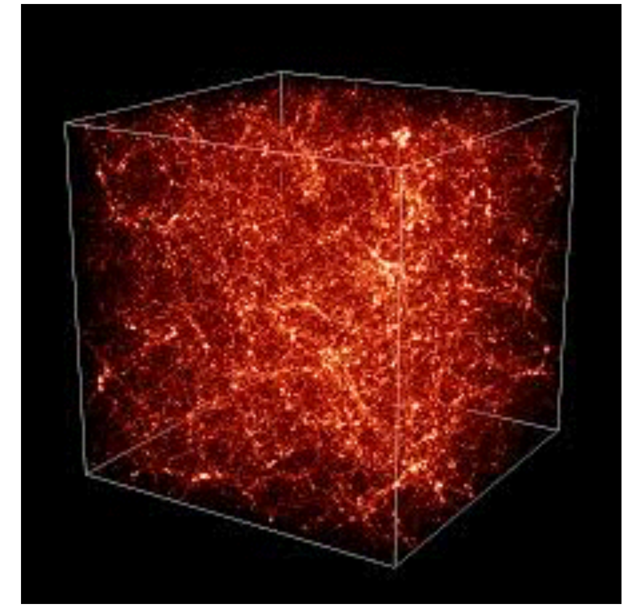
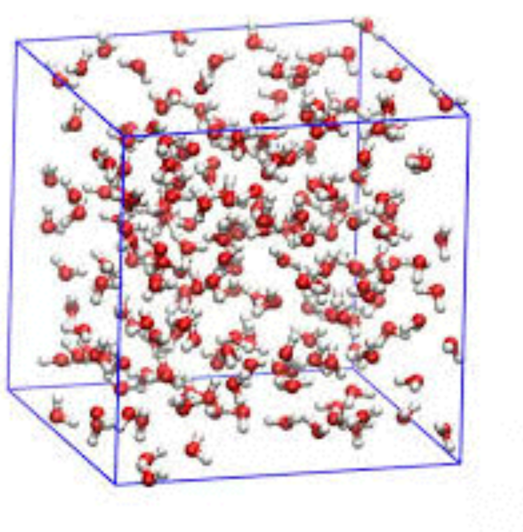
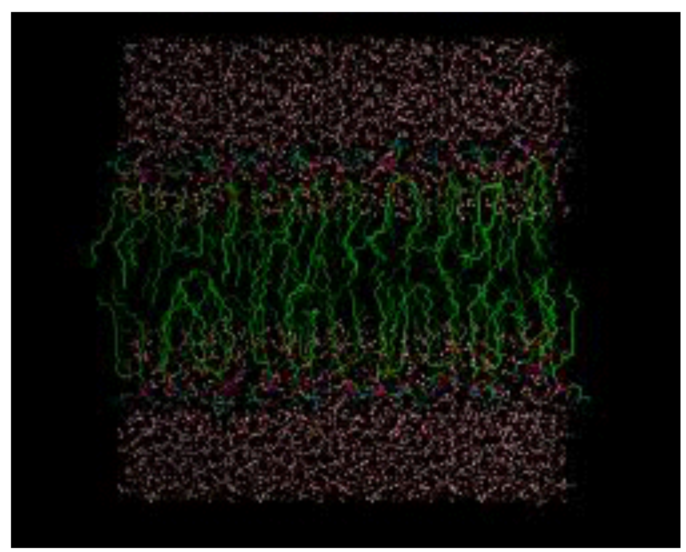
N-body dynamics

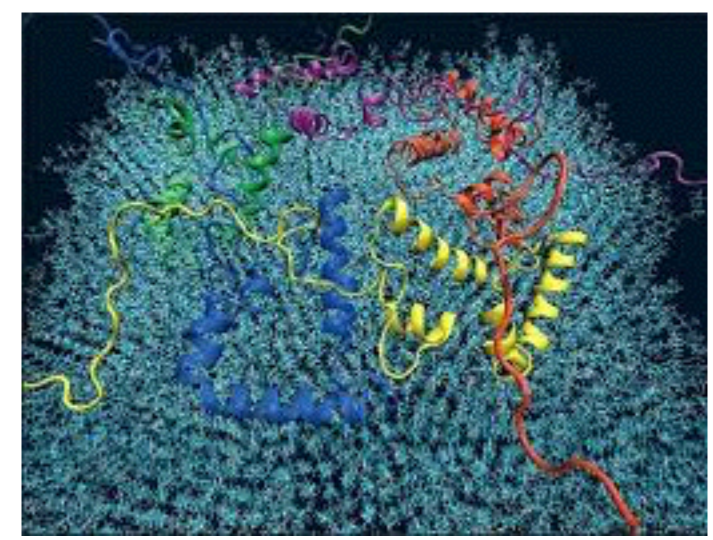




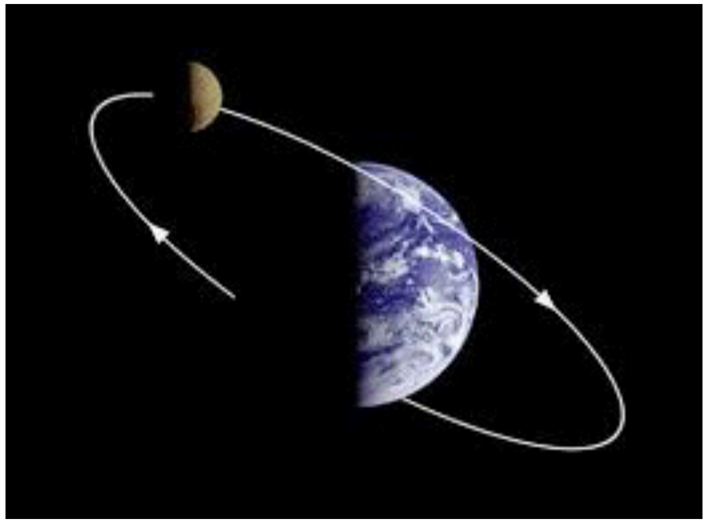


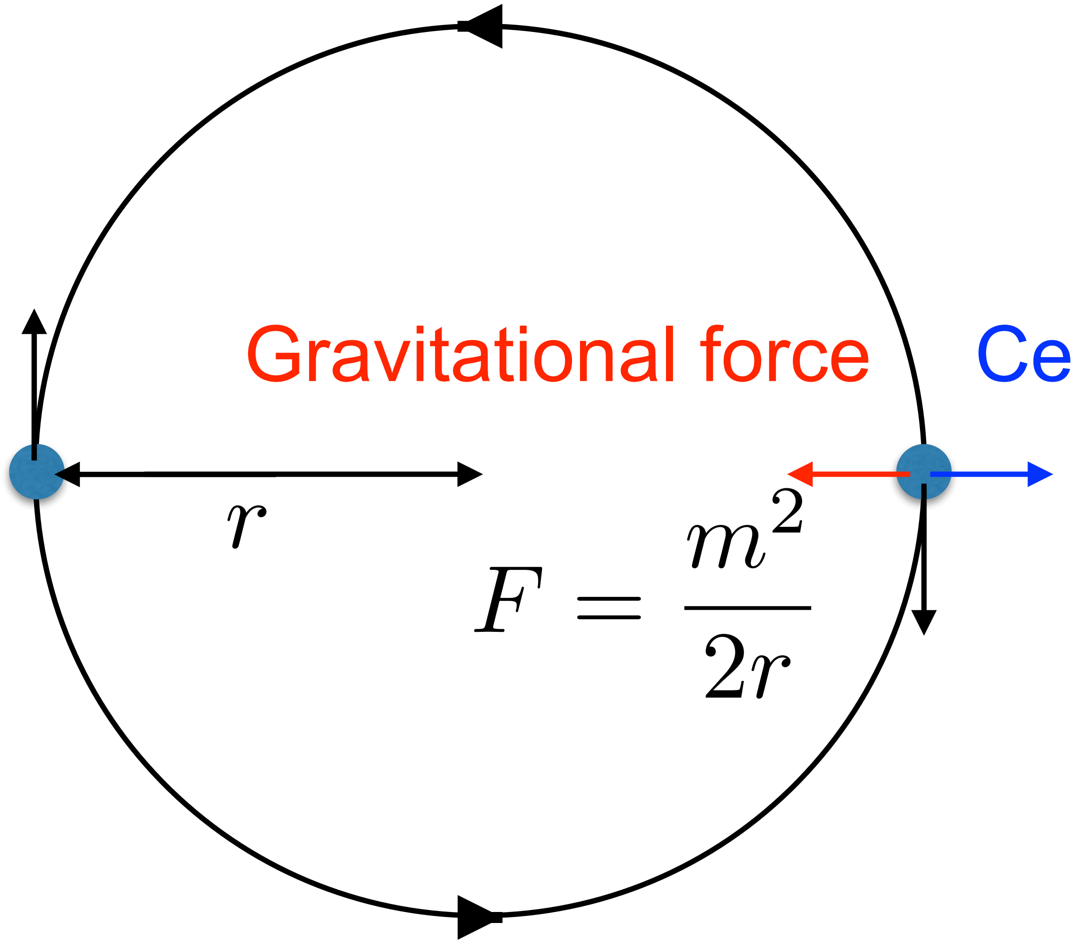






2-Body dynamics





$$v = \sqrt{\frac{m}{2}}$$

$$F = \frac{m^2}{2r}$$

$$F = mr\omega^2$$

$$v = r\omega$$

Symplectic integrators

$$\dot{p} = -\frac{\partial H}{\partial q} \quad p : \mathrm{momentum}$$

$$\dot{q} = \frac{\partial H}{\partial p} \qquad q : \mathrm{position}$$

Conserves the symplectic two-form $dp \wedge dq$

Volume-preserving

Canonical transformation

Verlet integration

$$x(t+\Delta t) = x(t) + \frac{dx}{dt}(t)\Delta t + \frac{d^2x}{dt^2}(t)\frac{\Delta t^2}{2} + \frac{d^3x}{dt^3}(t)\frac{\Delta t^3}{6} + \mathcal{O}(\Delta t^4)$$

$$x(t-\Delta t) = x(t) - \frac{dx}{dt}(t)\Delta t + \frac{d^2x}{dt^2}(t)\frac{\Delta t^2}{2} - \frac{d^3x}{dt^3}(t)\frac{\Delta t^3}{6} + \mathcal{O}(\Delta t^4)$$

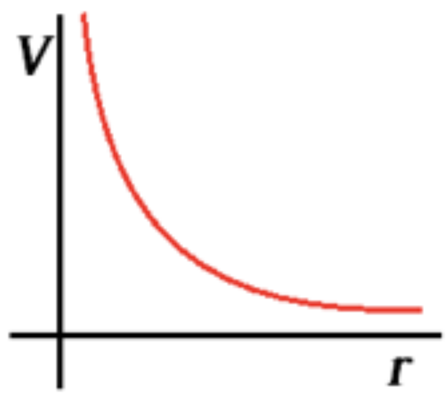
$$\downarrow$$

$$x(t+\Delta t) = 2x(t) - x(t-\Delta t) + \frac{d^2x}{dt^2}(t)\Delta t^2 + \mathcal{O}(\Delta t^4)$$

$$x(1) = x(0) + \frac{dx}{dt}(0)\Delta t + \frac{d^2x}{dt^2}(0)\frac{\Delta t^2}{2}$$

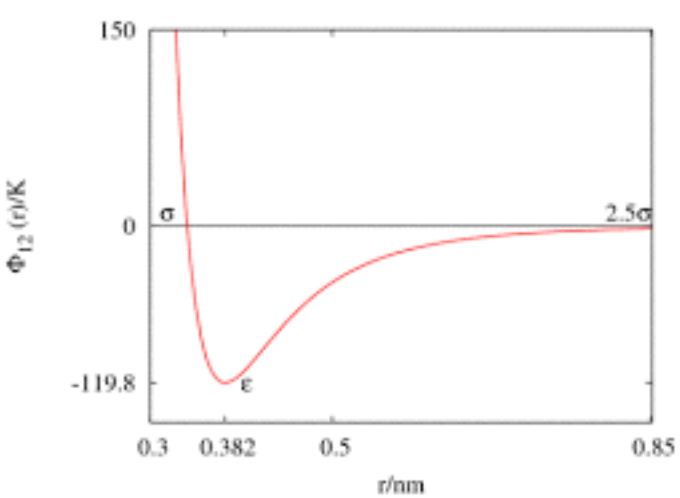
Gravitational potential

$$V(x) = \sum_{i=1}^{N} -\frac{Gm_i}{|\mathbf{x} - \mathbf{x}_i|}$$



Electrostatic potential

$$V(x) = \sum_{i=1}^{N} -\frac{1}{4\pi\epsilon_0}\frac{q_i}{|\mathbf{x} - \mathbf{x}_i|}$$



Lennard-Jones potential

$$V(x) = \sum_{i=1}^{N} 4\epsilon \left[\left(\frac{\sigma}{|\mathbf{x} - \mathbf{x}_i|} \right)^{12} - \left(\frac{\sigma}{|\mathbf{x} - \mathbf{x}_i|} \right)^{6} \right]$$

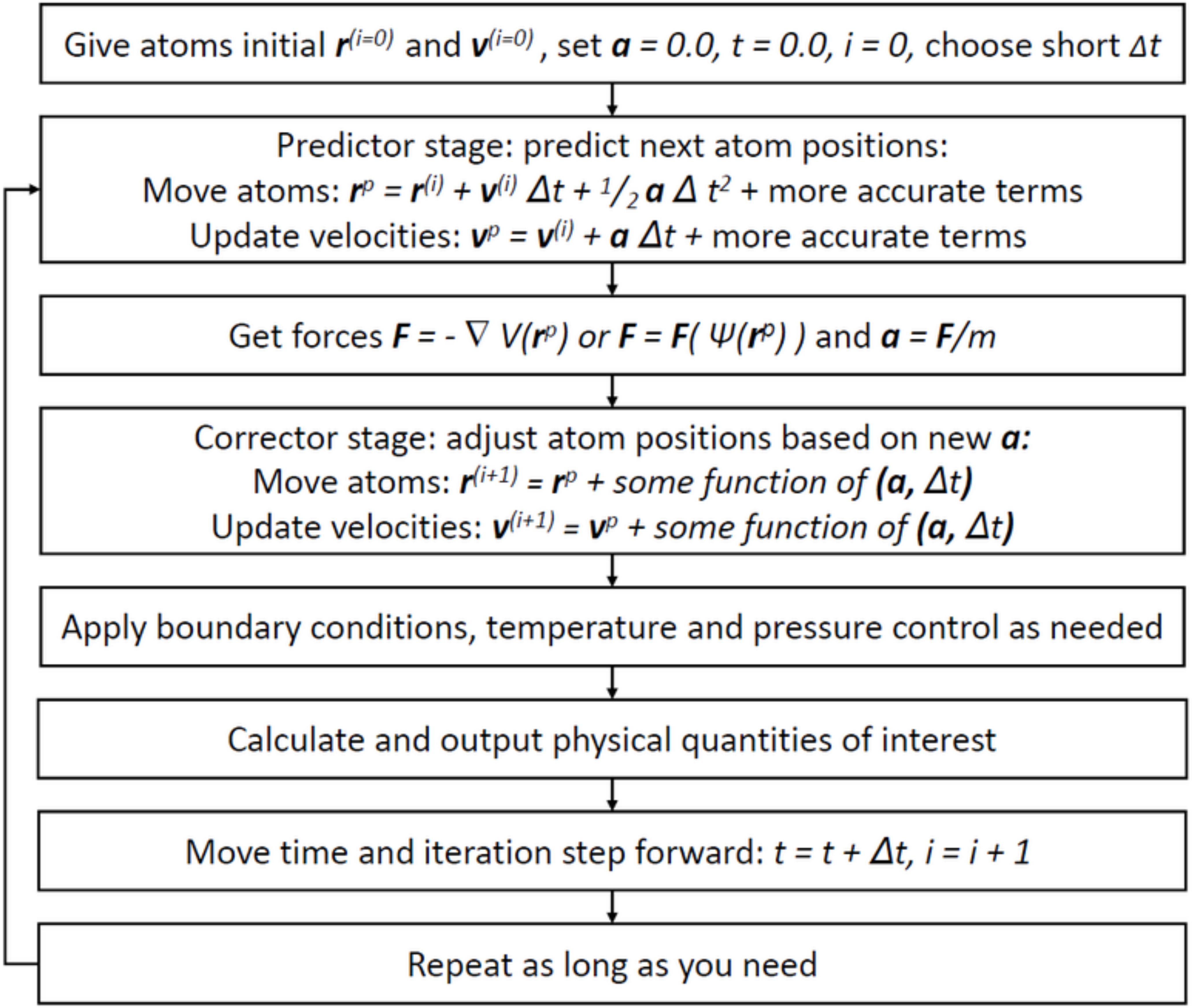
All Forces

$$
\begin{aligned}
U(\vec{R}) \;=\; & \underbrace{\sum_{bonds} k_i^{bond}(r_i - r_0)^2}_{U_{bond}} + \underbrace{\sum_{angles} k_i^{angle}(\theta_i - \theta_0)^2}_{U_{angle}} + \\
& \underbrace{\sum_{dihedrals} k_i^{dihe}[1 + \cos(n_i\phi_i + \delta_i)]}_{U_{dihedral}} + \\
& \underbrace{\sum_i \sum_{j \neq i} 4\epsilon_{ij}\left[\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}}\right)^{6}\right] + \sum_i \sum_{j \neq i} \frac{q_i q_j}{\epsilon r_{ij}}}_{U_{nonbond}}
\end{aligned}
$$

Time scales

Motion	Time Scale (sec)
Bond stretching	10^{-14} to 10^{-13}
Elastic vibrations	10^{-12} to 10^{-11}
Rotations of surface sidechains	10^{-11} to 10^{-10}
Hinge bending	10^{-11} to 10^{-7}
Rotation of buried side chains	10^{-4} to 1 sec
Allosteric transistions	10^{-5} to 1 sec
Local denaturations	10^{-5} to 10 sec

Simplified schematic of the molecular dynamics algorithm



Equation of state

$$pV = nRT$$

Microcanonical ensemble (NVE)

Adiabatic process

Exchange between potential and kinetic energy

Canonical ensemble (NVT)

Constant temperature

Nosé-Hoover thermostat
Hamiltonian with an extra degree of freedom for heat bath

Use thermostats to remove energy from the system

Isothermal–isobaric ensemble (NPT)

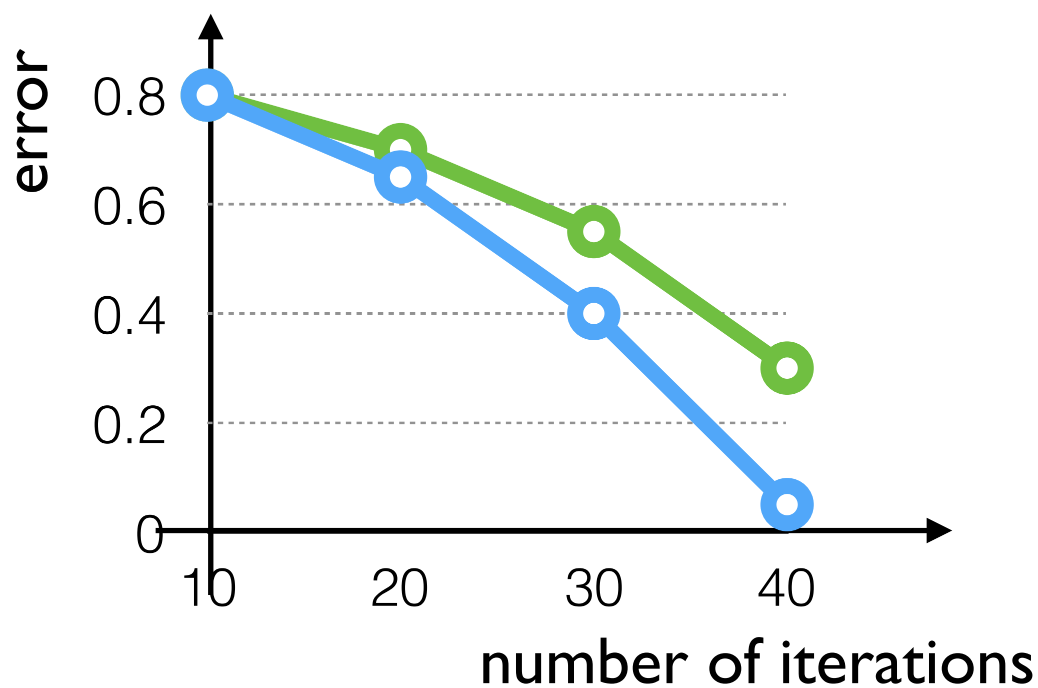
Constant temperature, pressure

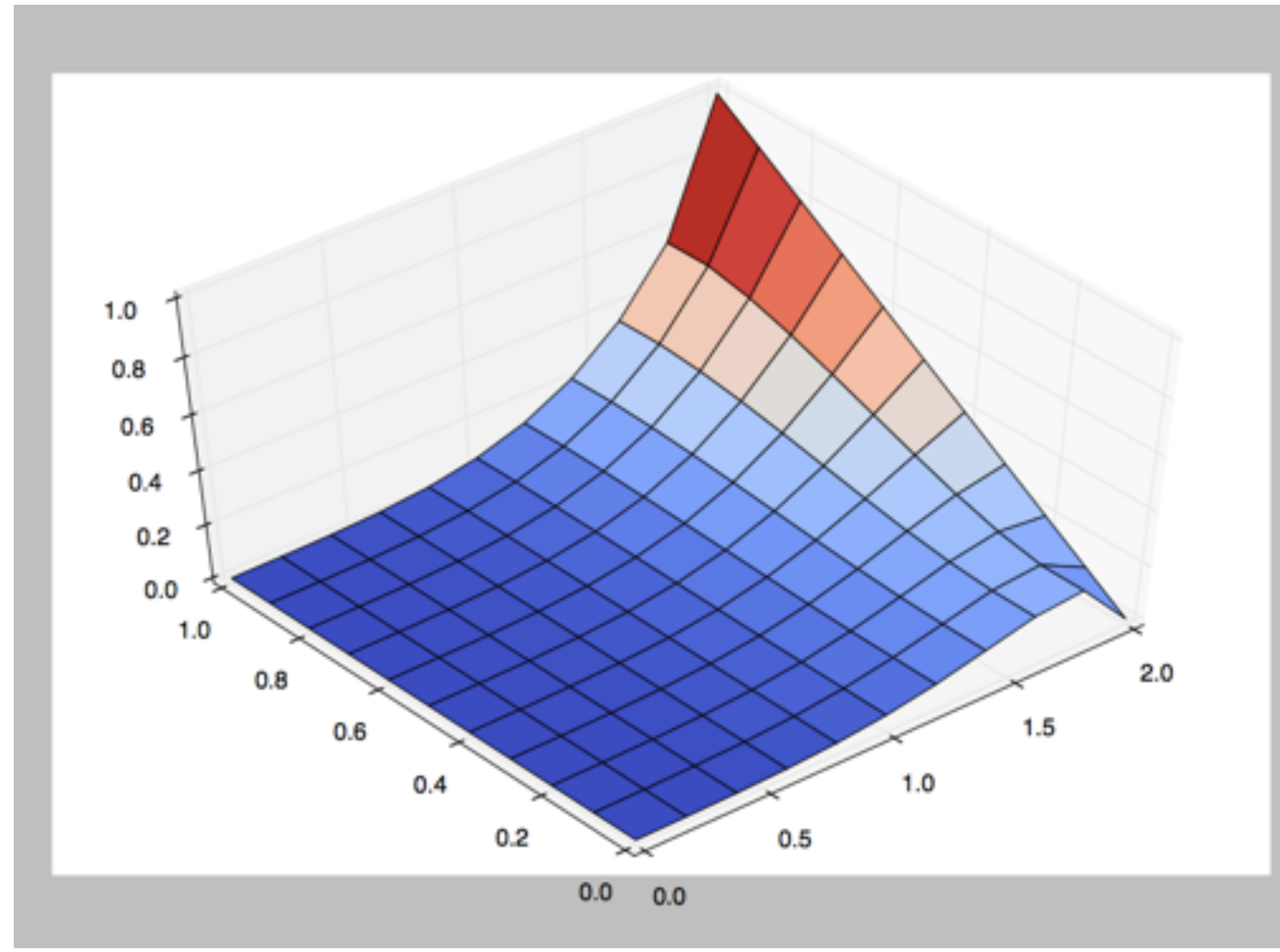
Use barostats to keep pressure constant

Homework

Measure the convergence rate of FDM step09.py

$$error = \sqrt{\sum_{i,j=1}^{nx,ny} \frac{(p_{exact} - p_{approx})^2}{p_{exact}^2}}$$





The exact solution is available from BEM step02.py

$$p_{exact} = \frac{x}{4} - 4 \sum_{n=odd}^{\infty} \frac{1}{(n\pi)^2 \sinh 2n\pi} \sinh n\pi x \cos n\pi y$$

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