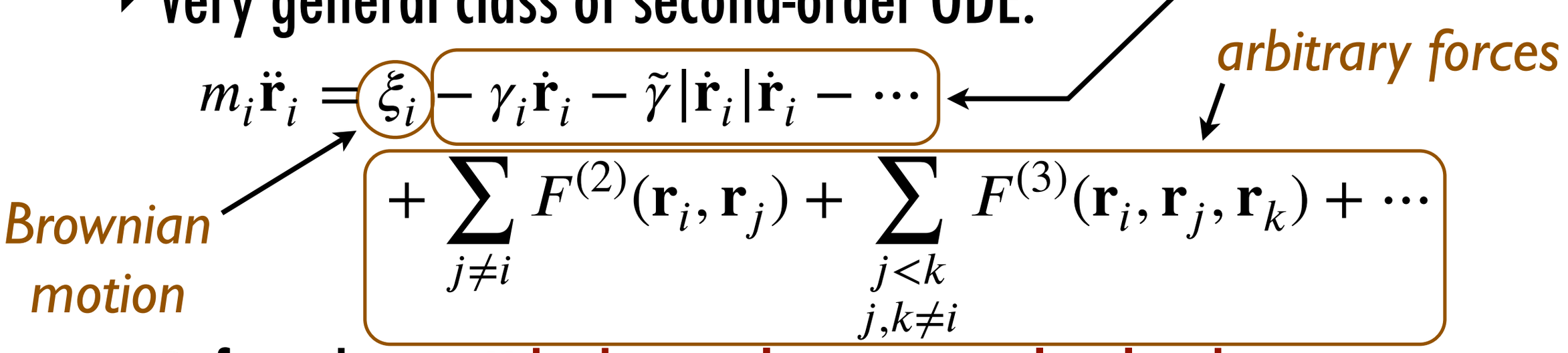
N-body simulations

Phys 750 Lecture 10

N-body simulations

- Forward integration in time of strongly coupled classical particles or (rigid-body composite objects)
- Very general class of second-order ODE:

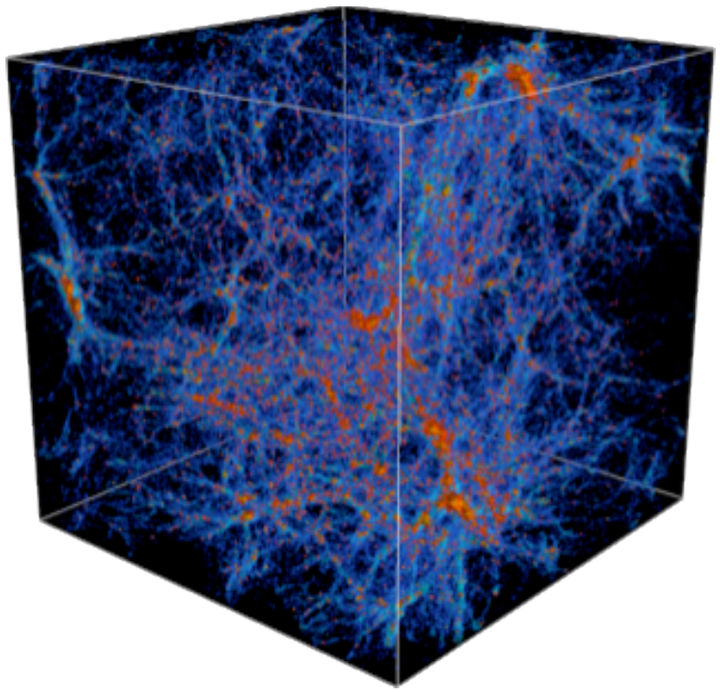


  - Referred to as N-body simulation or molecular dynamics in various scientific communities

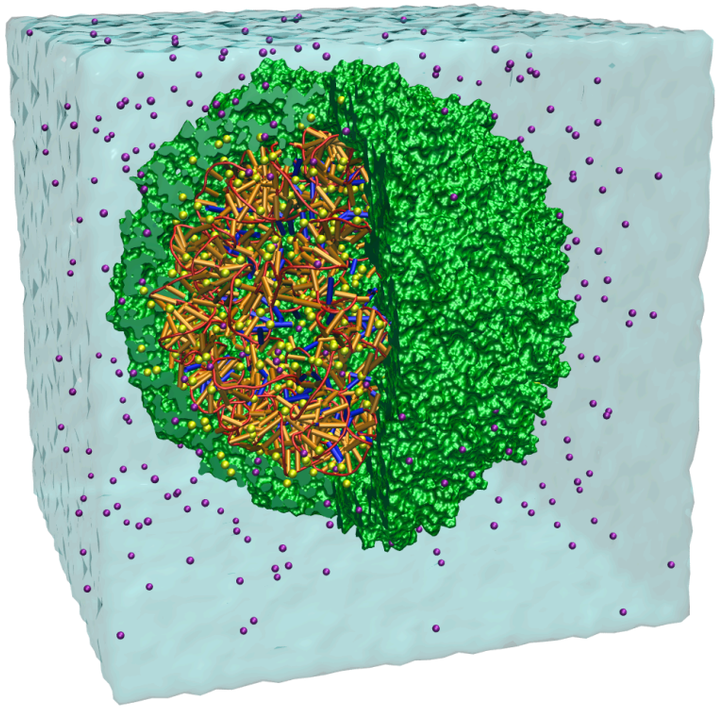
Broad applicability

- Useful in many contexts and over vastly different scales

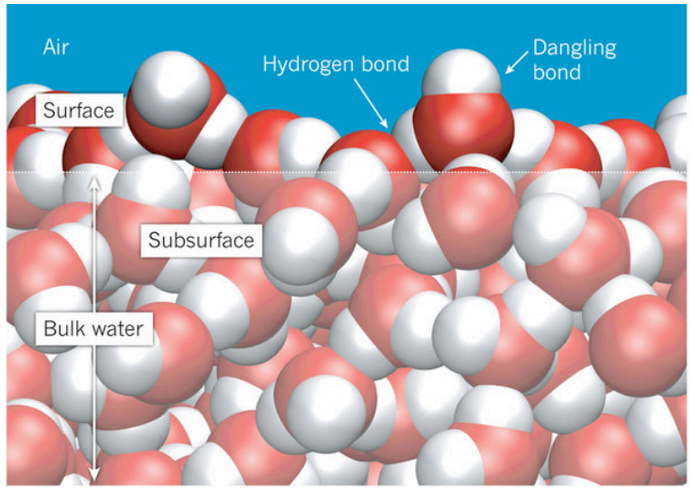
galaxy formation



virus



“classical water”



N-body simulations

- Classical systems of many particles, dissipationless and interacting via central forces, have a Hamiltonian of the form

$$H = \sum_i \frac{p_i^2}{2m_i} + \sum_{i<j} U(r_{ij})$$

- Momentum variables $\mathbf{p}_i = m_i \mathbf{v}_i$ are conjugate to the position variables $\mathbf{r}_i$ ($2DN$-dimensional phase space)
- Interactions determined by the pair potential $U(r)$

N-body simulations

- The set of second-order differential equations maps to a set of coupled first-order equations:

$$\dot{\mathbf{r}}_i = \frac{\partial H}{\partial \mathbf{p}_i} = \frac{\mathbf{p}_i}{m_i} = \mathbf{v}_i$$

$$\dot{\mathbf{p}}_i = -\frac{\partial H}{\partial \mathbf{r}_i} = -\sum_{j \neq i} \frac{\partial U(r_{ij})}{\partial \mathbf{r}_i} = -\sum_{j \neq i} U'(r_{ij}) \hat{\mathbf{r}}_{ij}$$

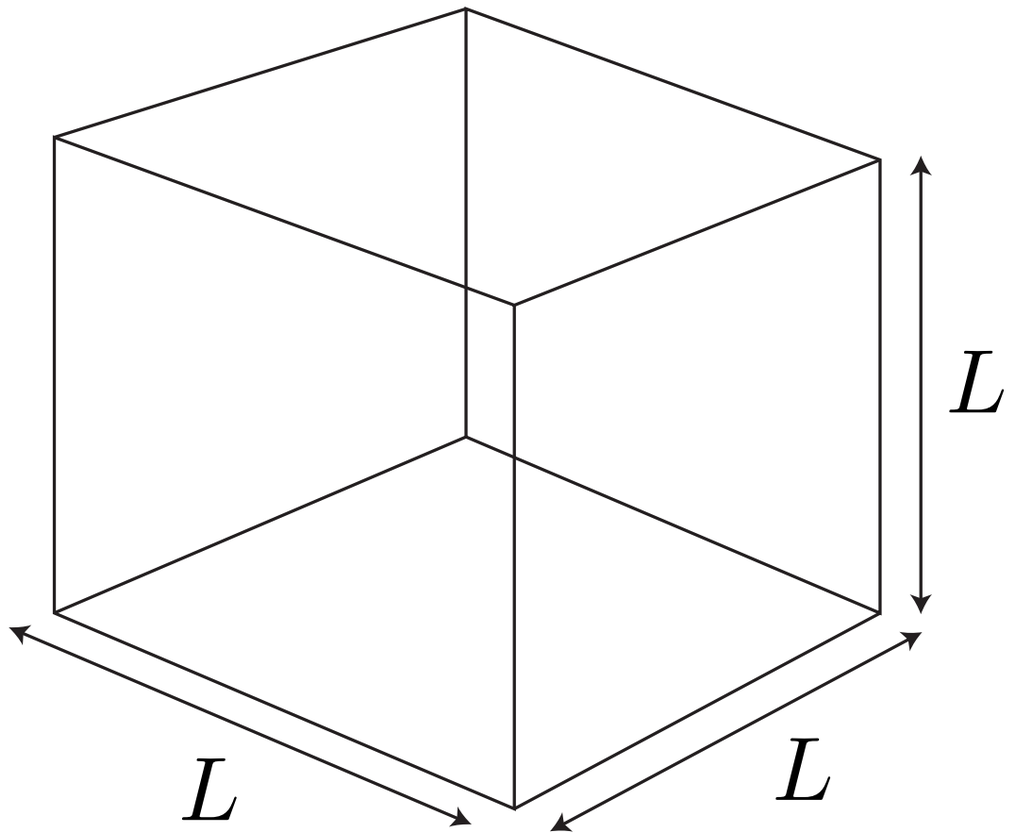
net force exerted by the other $N - 1$ particles

N-body simulations

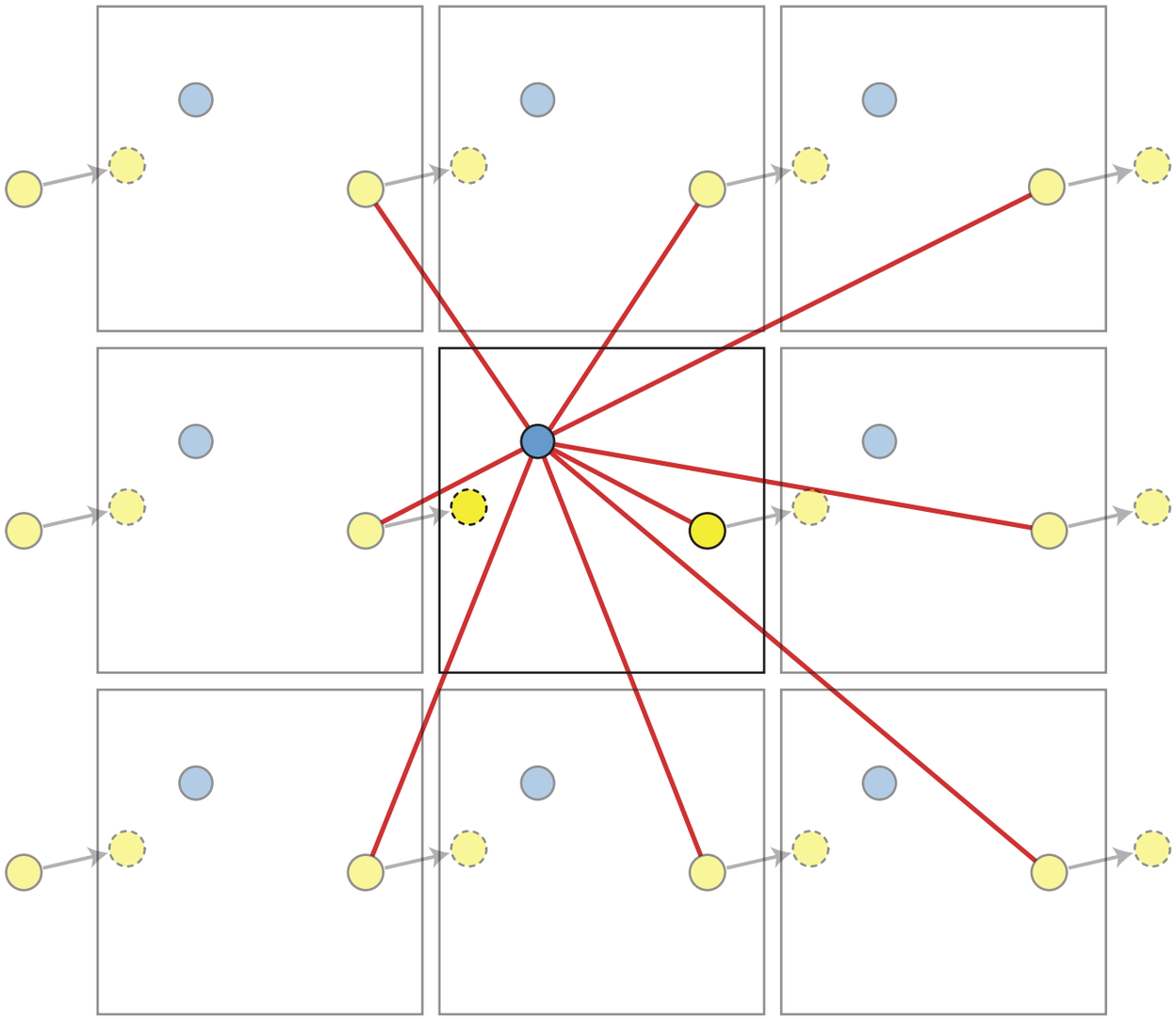
- Special considerations:
  - For long-range forces all particle pairs interact strongly with one another – at best, $N(N-1)/2$ scaling
  - Repulsive interactions require a "container" (via walls or periodic boundary conditions)
  - Time step must be adjusted such that the length scale $v\Delta t$ can resolve the spatial structure of $U(r)$

Finite simulation cell

- Typical setup: finite $L \times L \times L$ periodic cell serves as a representative sample of space
- How to judge distance for the purpose of computing long range forces?



Finite simulation cell



- Periodicity is equivalent to tiling all space with copies of the same cell
- Forces arise from interactions with each of an infinite number of image particles

Finite simulation cell

- Approximating the infinite summation in 1D:

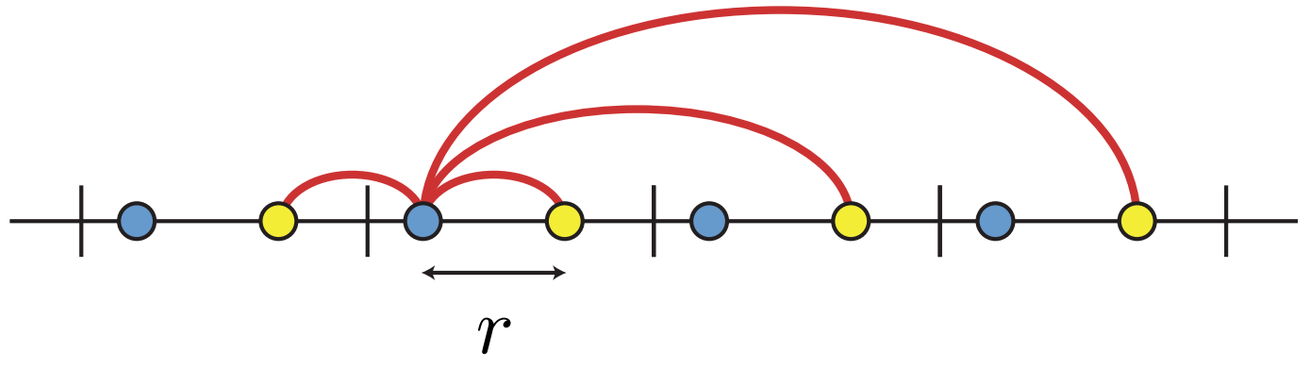
$$F^{\text{eff}}(r) = \sum_{n=-\infty}^{\infty} F(r + nL) = \cdots + F(r - L) + F(r) + F(r + L) + \cdots$$

$$\approx F(\min\{|r|, L - |r|\})$$

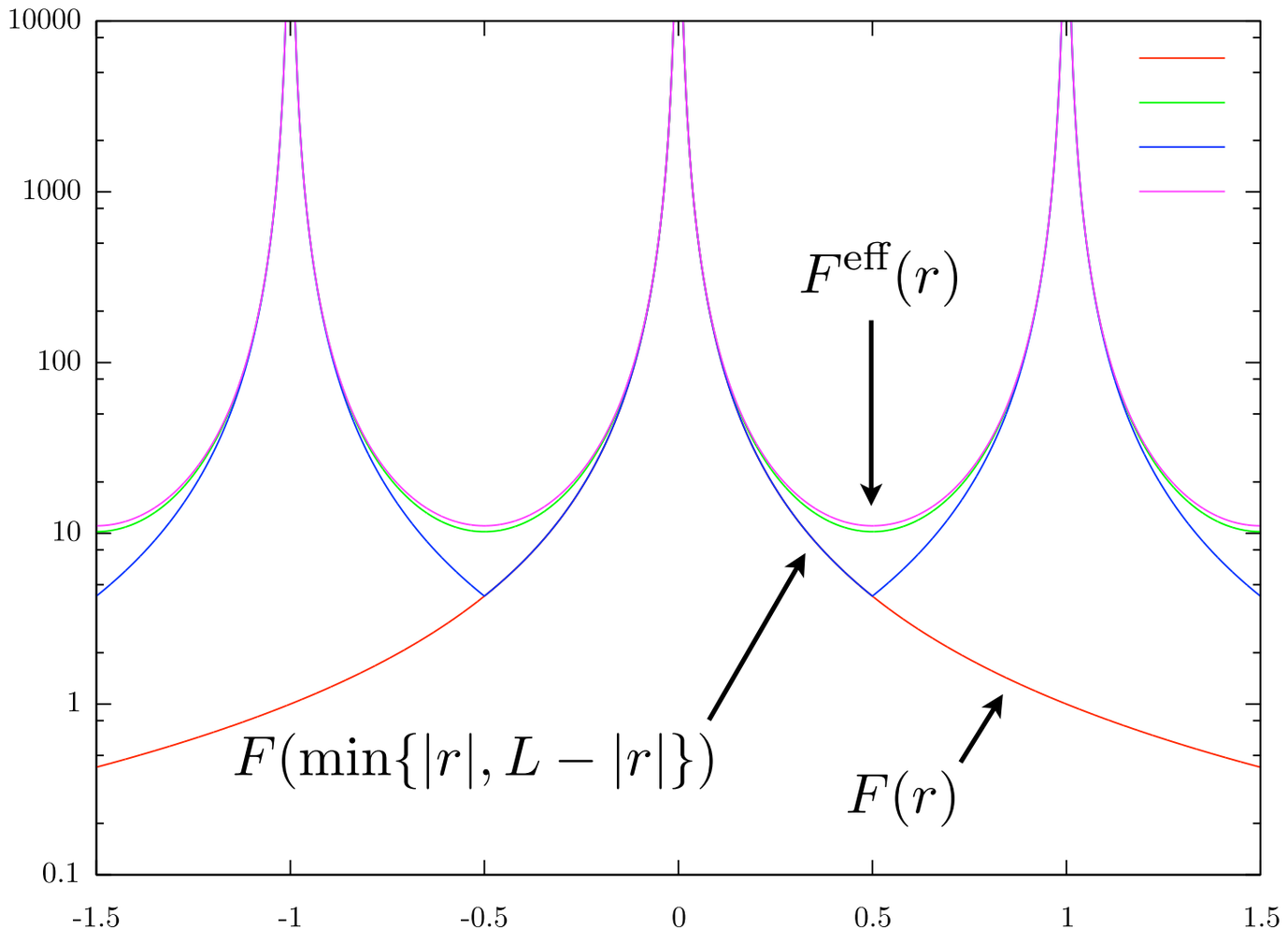
closest-image distance

intra-cell separation

$$-L < r < L$$



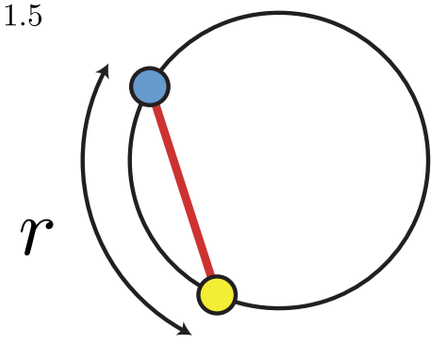
Finite simulation cell



- Summation has an exact form for EM-like and gravity-like interactions

$$F(r) = \frac{1}{r^2}$$

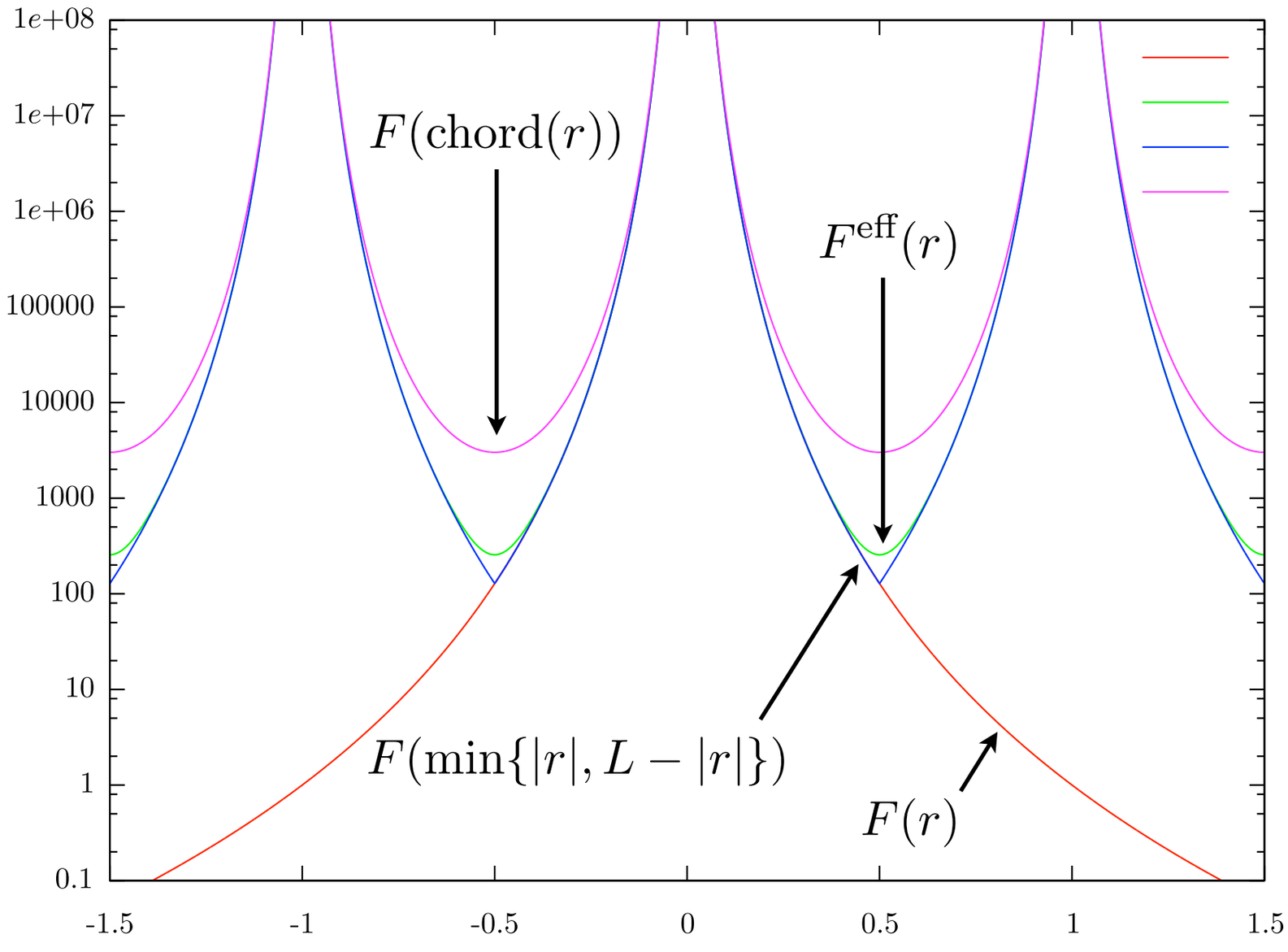
$$F^{\mathrm{eff}}(r) = F(\mathrm{chord}(r))$$



$$\frac{\sin(\pi r/L)}{\pi/L}$$

chord length

Finite simulation cell



- closest-image approximation increasingly good as interactions become short-ranged; e.g.,

$$F(r) = \frac{1}{r^7}$$

Finite simulation cell

- Example distance measure in a 3D orthogonal cell

$$\mathbf{r}_i = (x_i, y_i, z_i)$$

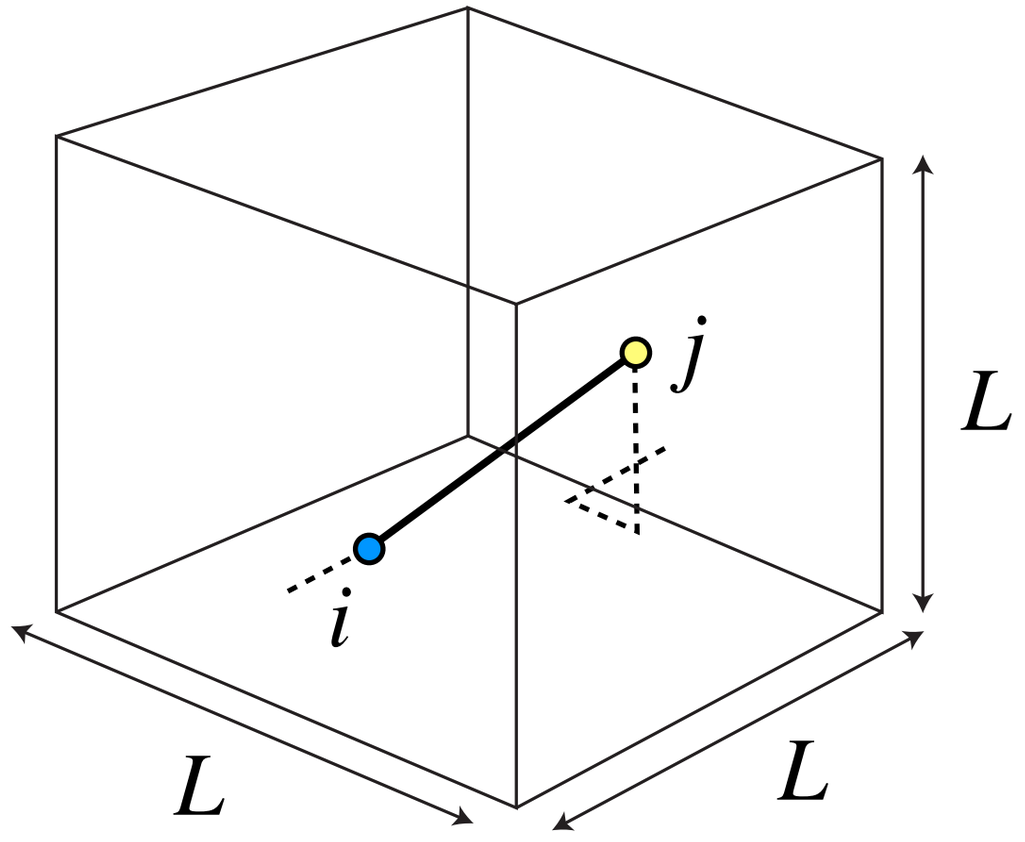
$$\mathbf{r}_j = (x_j, y_j, z_j)$$

$$d_{i,j} = \Big[\min\{|\Delta x|, L - |\Delta x|\}^2 + \min\{|\Delta y|, L - |\Delta y|\}^2 + \min\{|\Delta z|, L - |\Delta z|\}^2\Big]^{1/2}$$

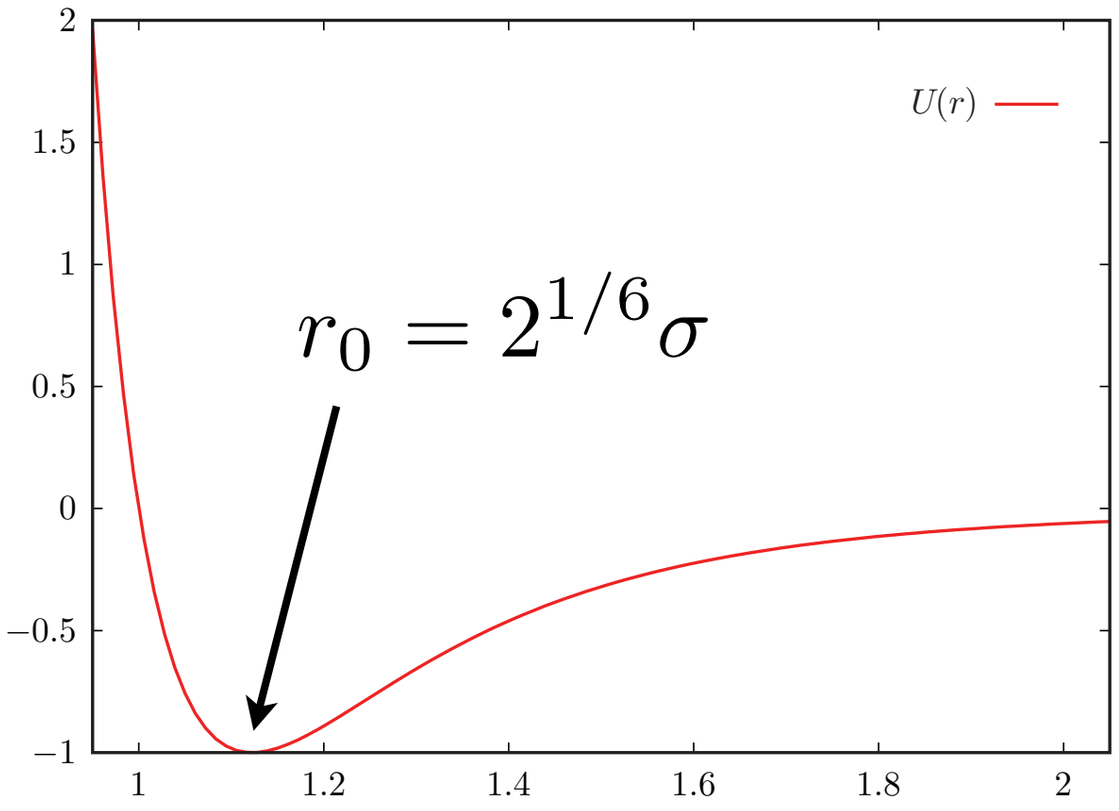
$$\Delta x = x_i - x_j$$

$$\Delta y = y_i - y_j$$

$$\Delta z = z_i - z_j$$



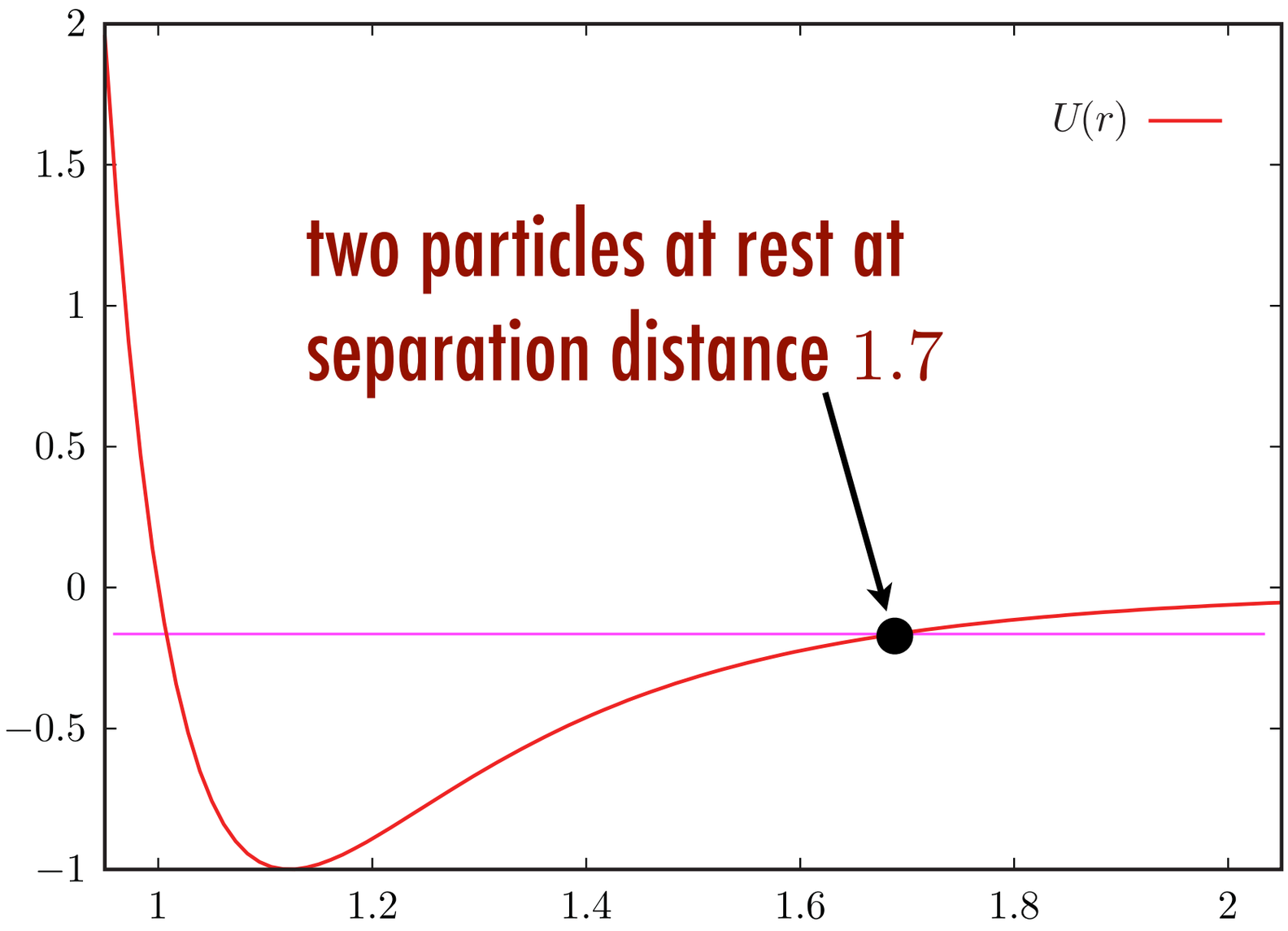
Lennard-Jones Potential



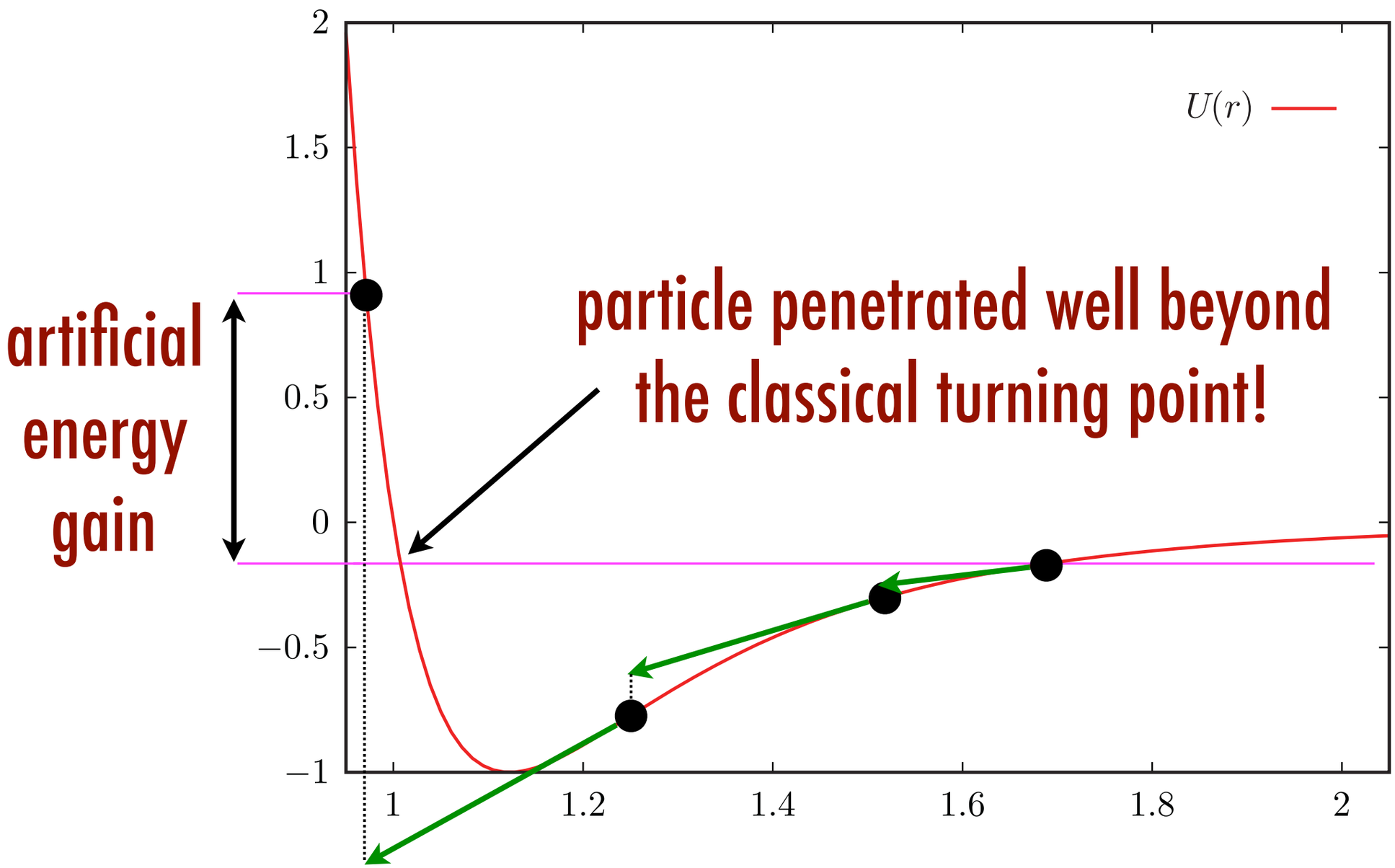
$$U(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

- Model of Van der Waal's attraction between neutral atoms plus an inner core repulsion
- Equilibrium point $U'(r_0) = 0$ separates the attractive and repulsive regions

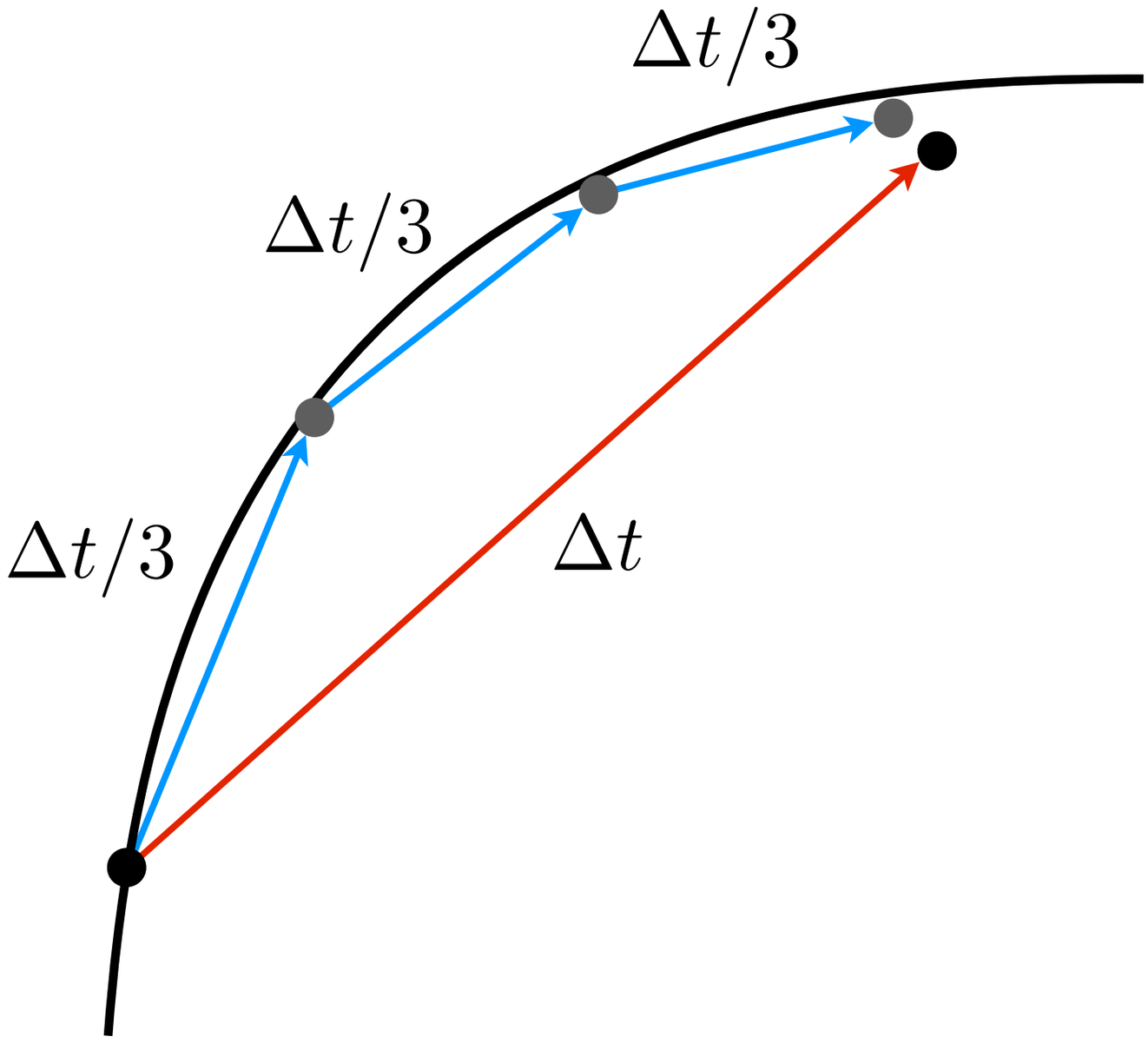
Choice of Time Step



Choice of Time Step



Adaptive Time Step



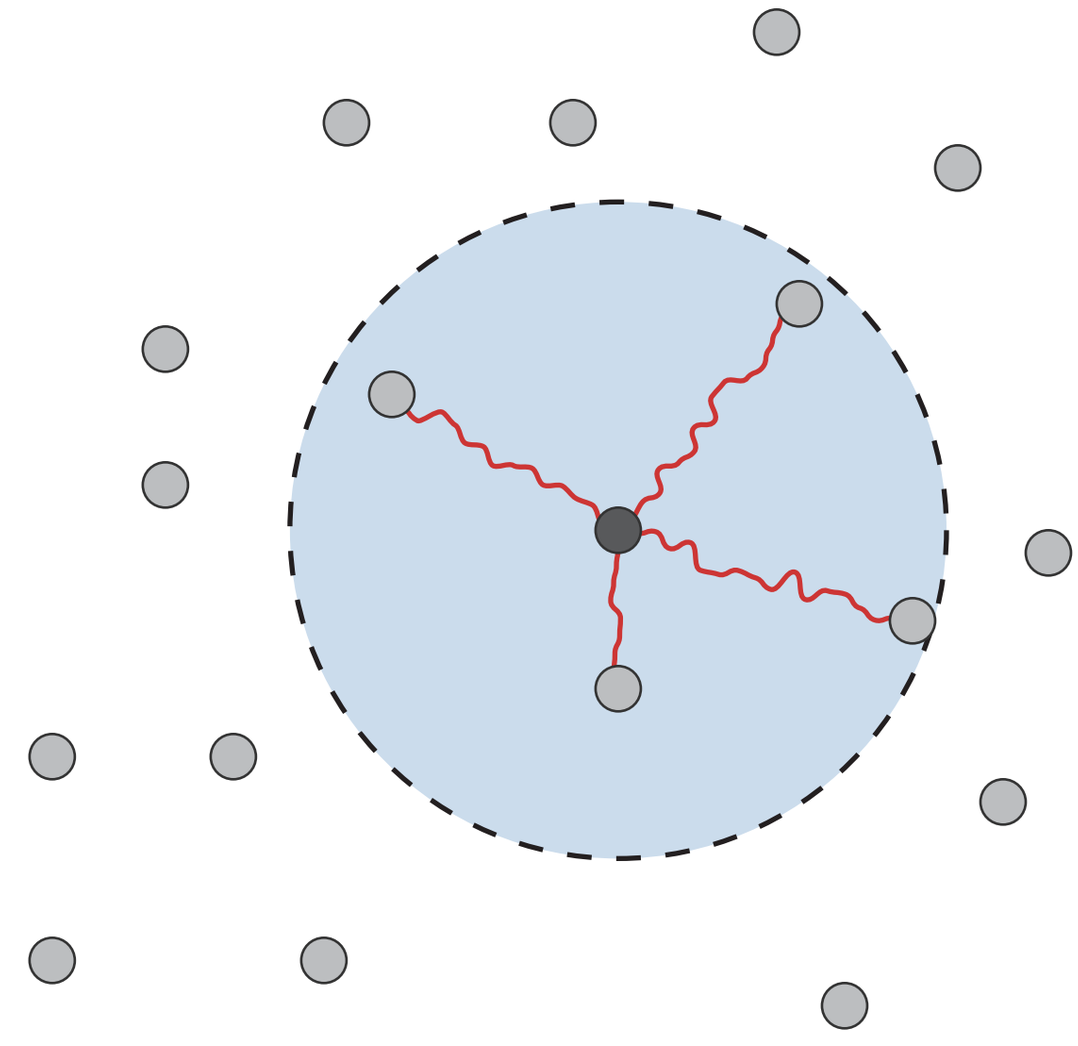
- Allow time step to vary dynamically within the simulation
- Check convergence by comparing evolution of two otherwise identical copies of the system

Range Truncation

- If interactions are finite-range, there are only a small number of forces acting on each particle (unless the particles have coalesced)
  - Algorithm now scales as

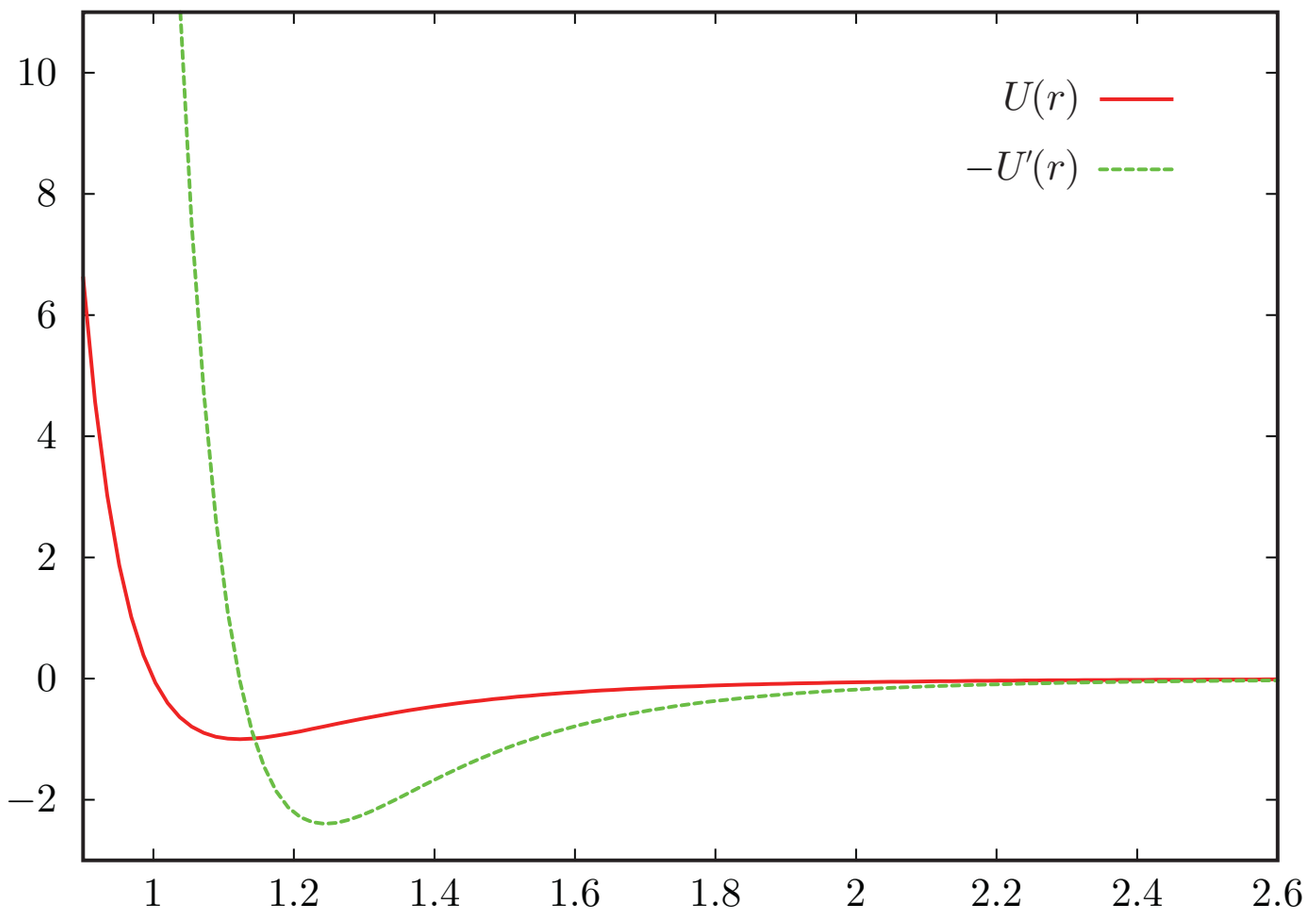
$$\frac{1}{2}\sum_{i=1}^{N} N_{\text{nearby}}^{(i)} \ll \frac{N(N-1)}{2}$$

  - Can we impose a cutoff?



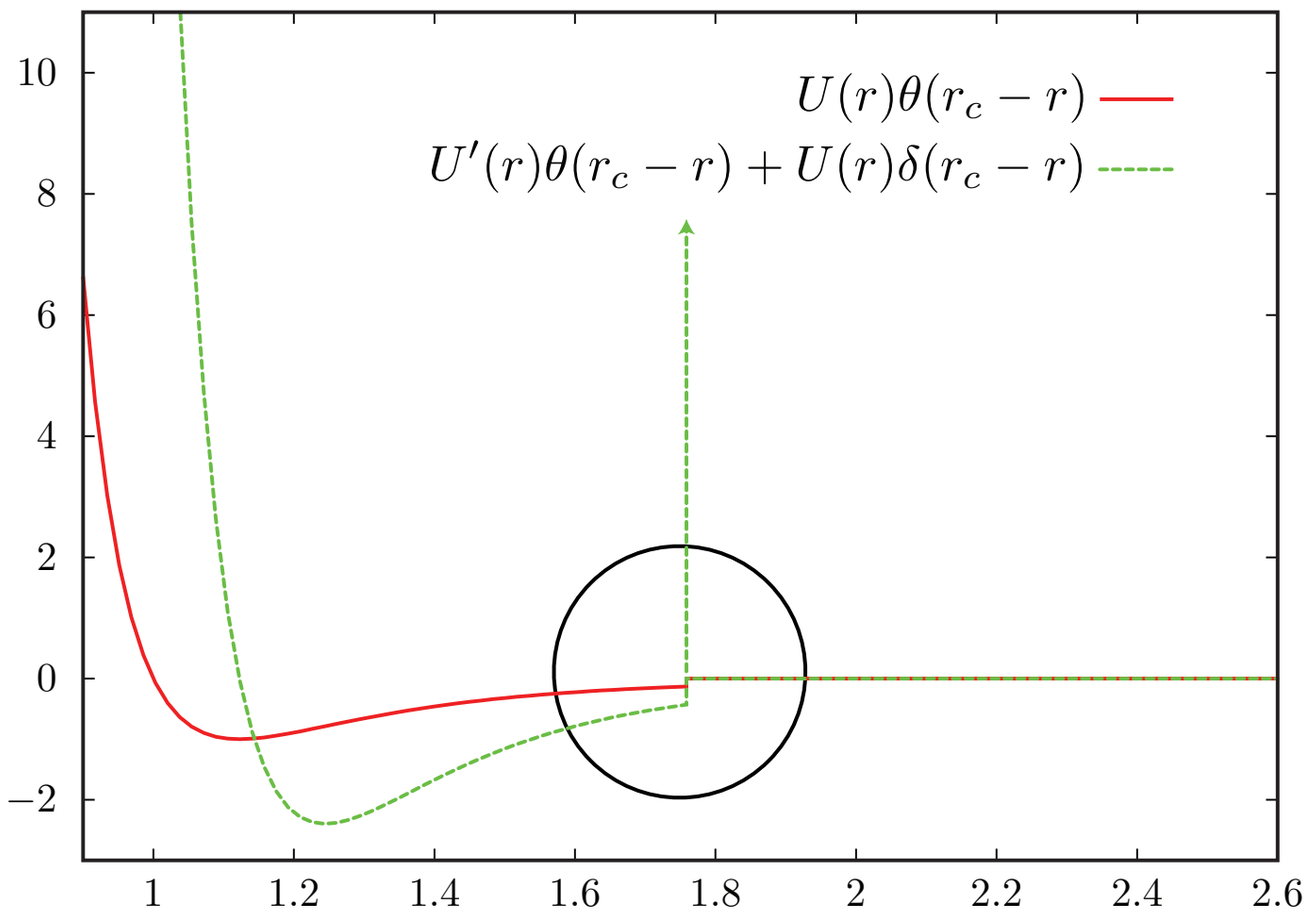
Range Truncation

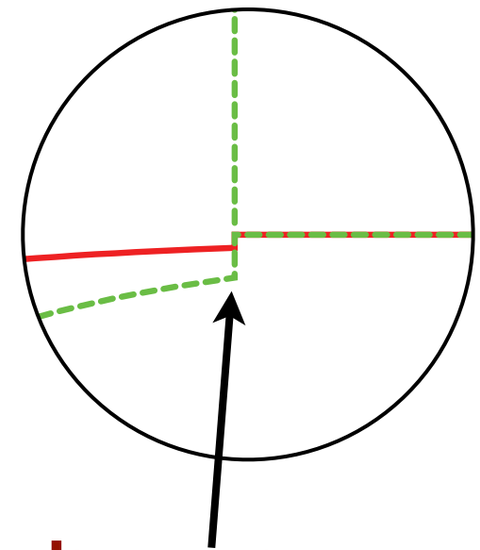
- E.g., Lennard-Jones tail is very weak beyond $r_c \sim 2\sigma - 3\sigma$



Range Truncation

- Care must be taken not to introduce unphysical forces



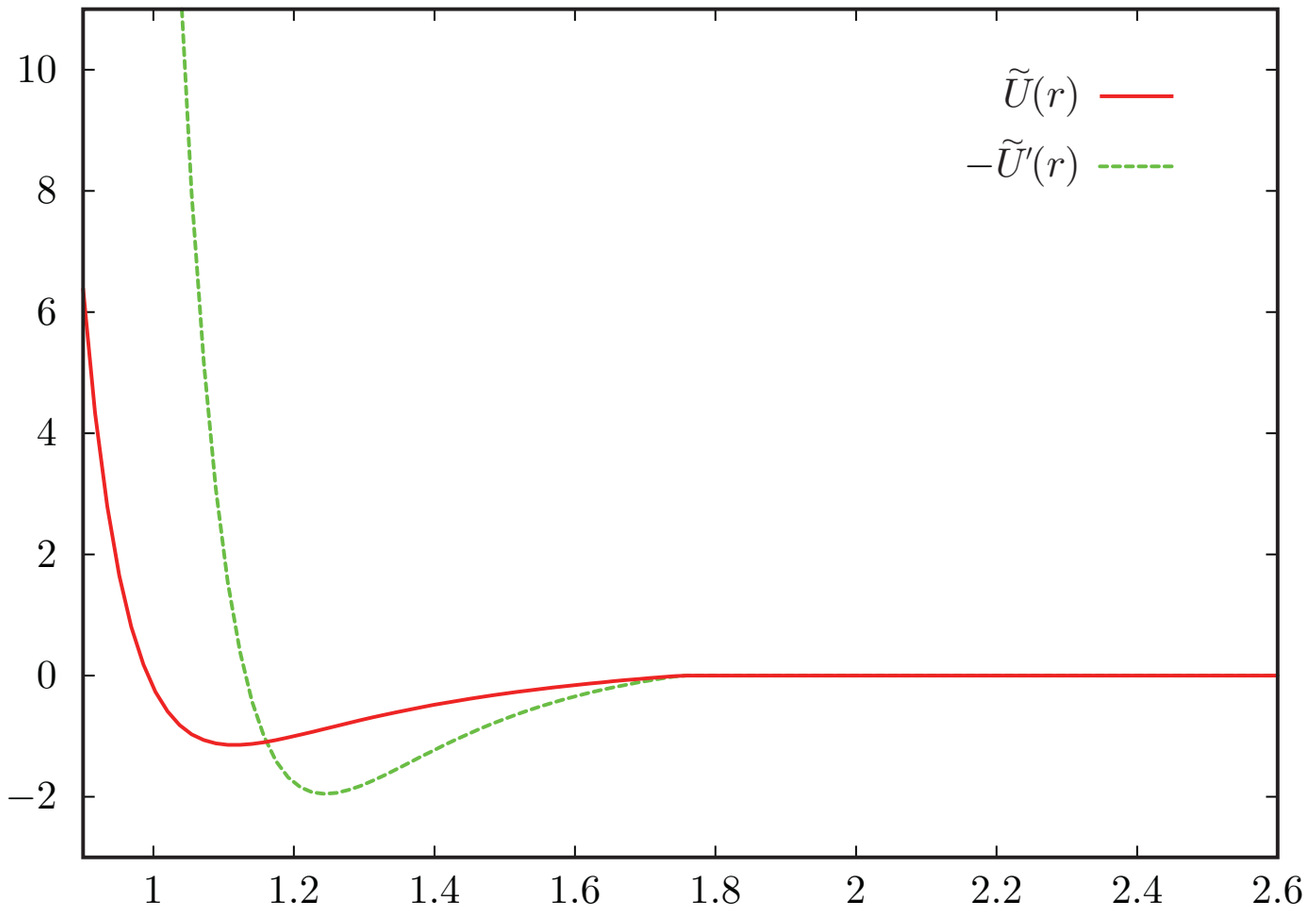


discontinuous, impulsive force

Range Truncation

$$\tilde{U}(r) \equiv \big[U(r) - U(r_{\rm c}) + (r - r_{\rm c})U'(r_{\rm c})\big]\theta(r_{\rm c} - r)$$

$$\tilde{F}(r) = -\tilde{U}'(r) = \big[-U'(r) + U'(r_{\rm c})\big]\theta(r_{\rm c} - r)$$



Ewald summation

- Naive truncation is not possible in the case of truly long-ranged interactions
- Ewald summation is a useful Fourier space trick
- E.g., consider non-self electrostatic interactions between particles in all image cells:

$$U_{\mathrm{Coulomb}} = \frac{1}{2} \sum_{i,j} \sum_{\mathbf{n} \in \mathbb{Z}^3} \frac{q_i q_j (1 - \delta_{\mathbf{r}_i - \mathbf{r}_j, \mathbf{n}L})}{|\mathbf{r}_i - \mathbf{r}_j + \mathbf{n}L|}$$

$$\equiv \frac{1}{2} {\sum_{i,j,\mathbf{n}}}' \frac{q_i q_j}{r_{i,j,\mathbf{n}}}$$

Ewald summation

- Exact rewriting in terms of a background constant, a direct space sum, and a dual space sum:

$$U_0 = -\frac{1}{\sqrt{\pi}} \sum_i \frac{q_i^2}{\rho_0}$$

$$U_1 = \frac{1}{2} \sum_{i,j,\mathbf{n}}{}' q_i q_j \frac{\operatorname{erfc}(r_{i,j,\mathbf{n}}/\rho_0)}{r_{i,j,\mathbf{n}}}$$

$$U_2 = \frac{1}{2\pi L^3} \sum_{i,j} q_i q_j \sum_{\substack{\mathbf{m}\in\mathbb{Z}^3 \\ \mathbf{m}\neq\mathbf{0}}} \frac{\exp\left[-(\pi\mathbf{m}\rho)^2 + 2\pi \mathrm{i}\mathbf{m}\cdot(\mathbf{r}_i - \mathbf{r}_j)\right]}{\mathbf{m}^2}$$

exponentially decaying envelope

real lattice

reciprocal lattice

Ewald summation

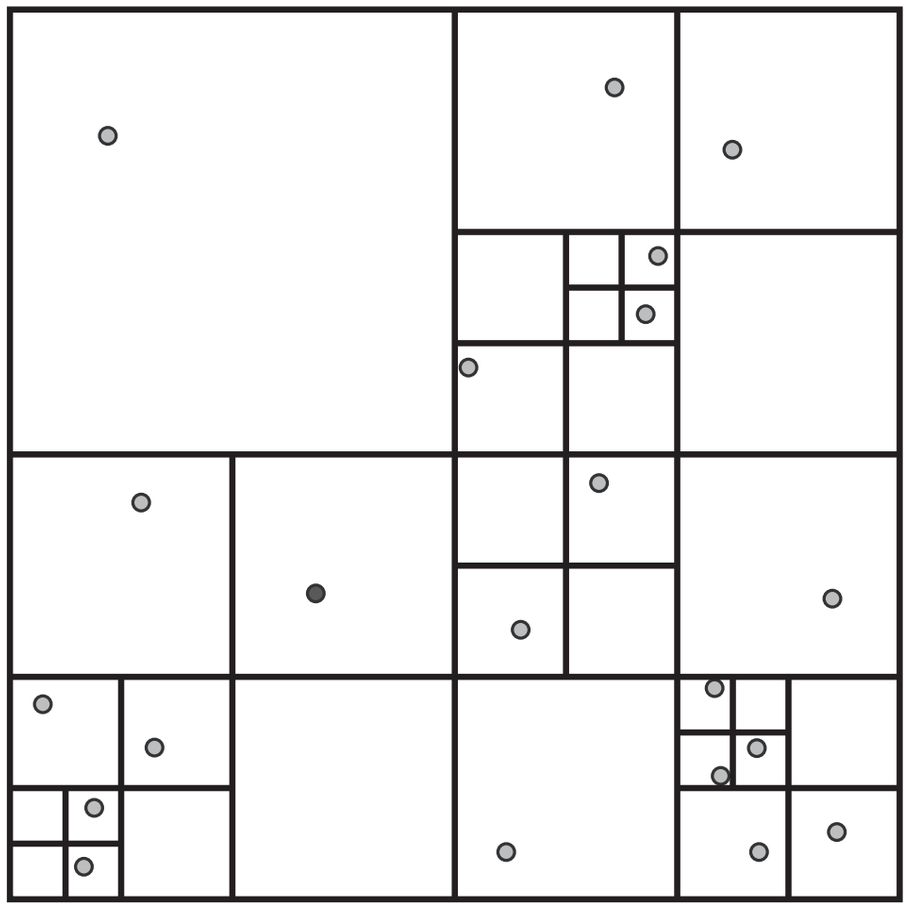
- Safe to truncate the sum in U_1 at separations above ρ_0
- Order N^2 sum over particle indices in U_2 can be evaluated as two order N sums:

$$U_2 = \frac{1}{2\pi L^3} \sum_{\mathbf{m}\neq 0} \frac{\exp\left[-(\pi \mathbf{m}\rho)^2\right]}{\mathbf{m}^2} |S(\mathbf{m})|^2$$

$$S(\mathbf{m}) = \sum_j q_j \exp(2\pi \mathrm{i} \mathbf{m}\cdot\mathbf{r}_j)$$

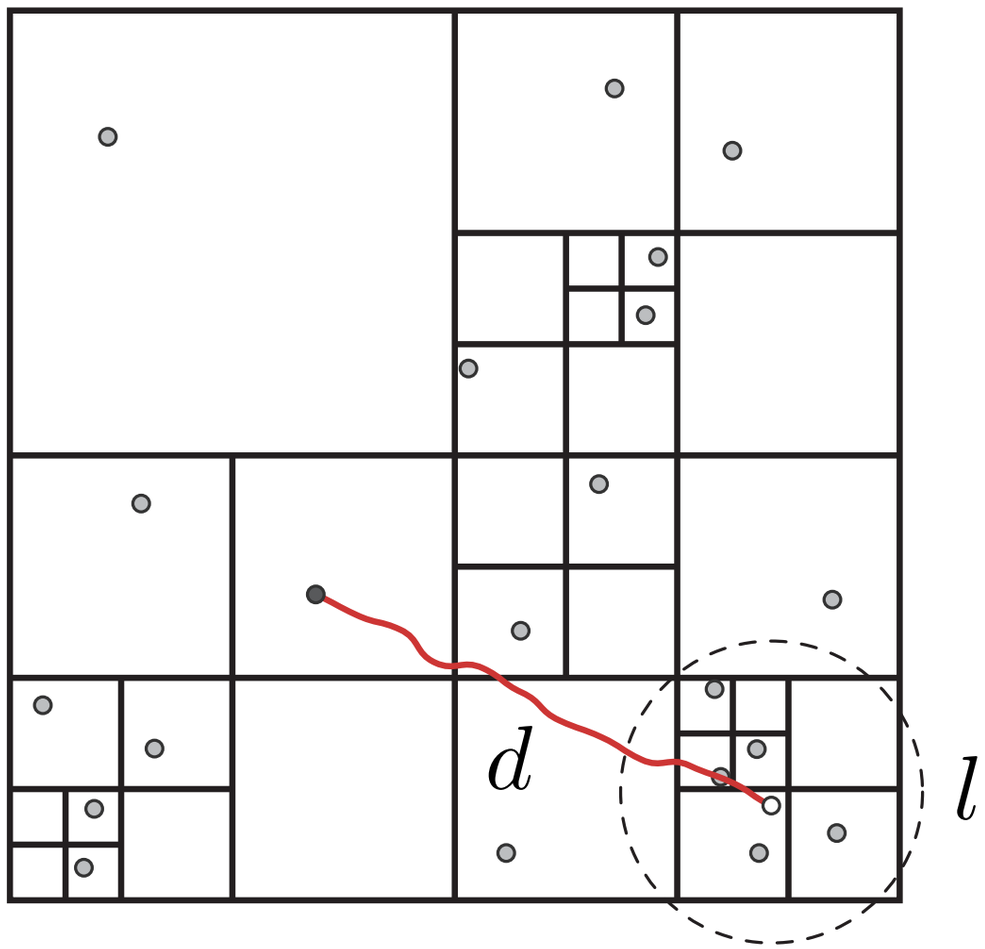
"structure factor"

Barnes-Hut tree



- dynamic data structure: recursive subdivision of space into “quads” containing at most one particle
- The centre-of-mass position is calculated at each tree level and passed up the linked-list hierarchy

Barnes-Hut tree

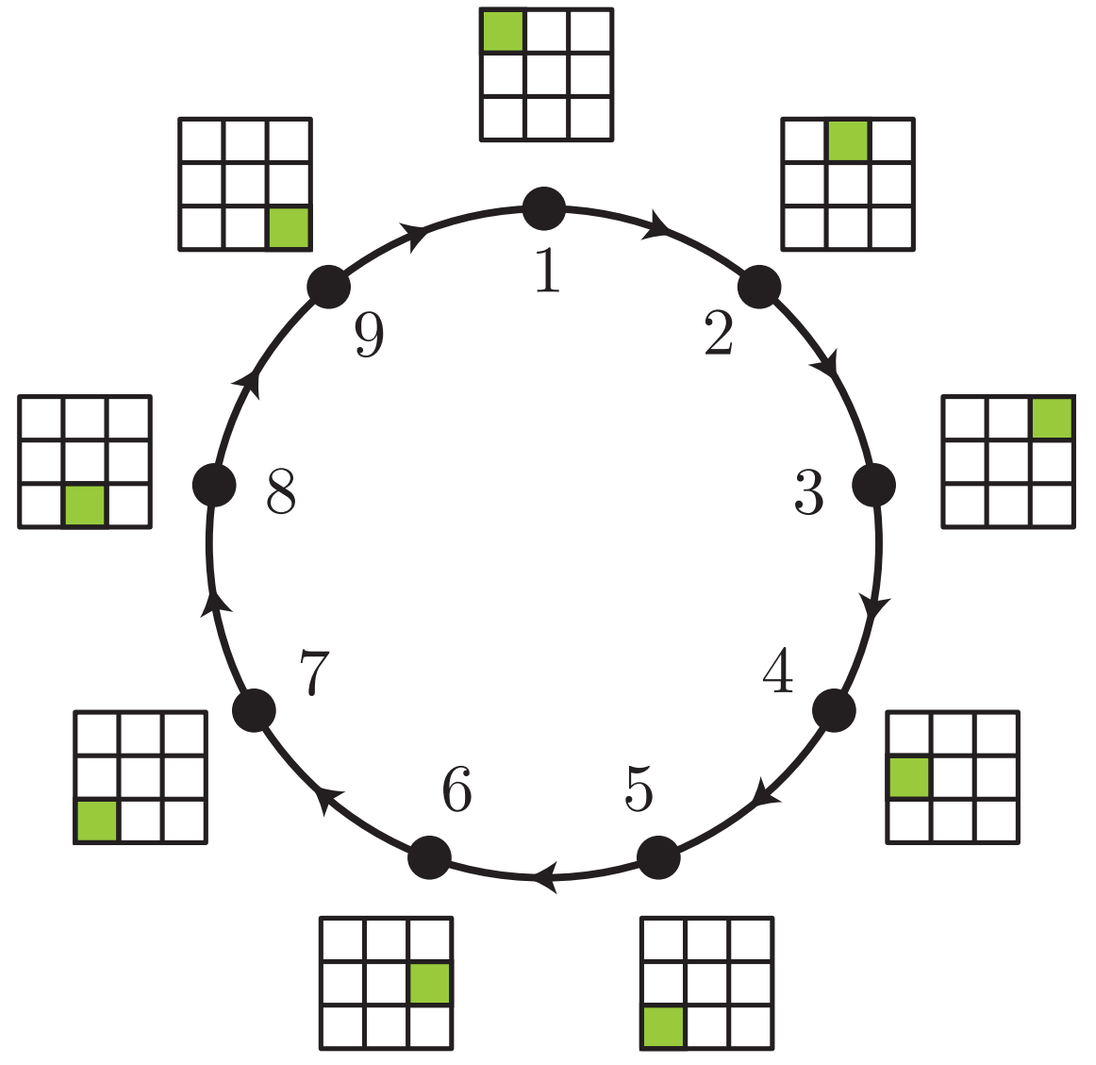


$l/d < \theta_{\mathrm{c}}$

- Assume that a particle cluster sufficiently far away can be represented by a single representative particle at the centre-of-mass (neglects tidal forces)
- Distance judged by the size of the "opening angle"
- Scales as $N \log N$

Parallel Computation

- Simulate on many CPUs simultaneously
- Each machine updates the particles in a sub-region of the full space
- Position information passed as "messages" passed around the ring

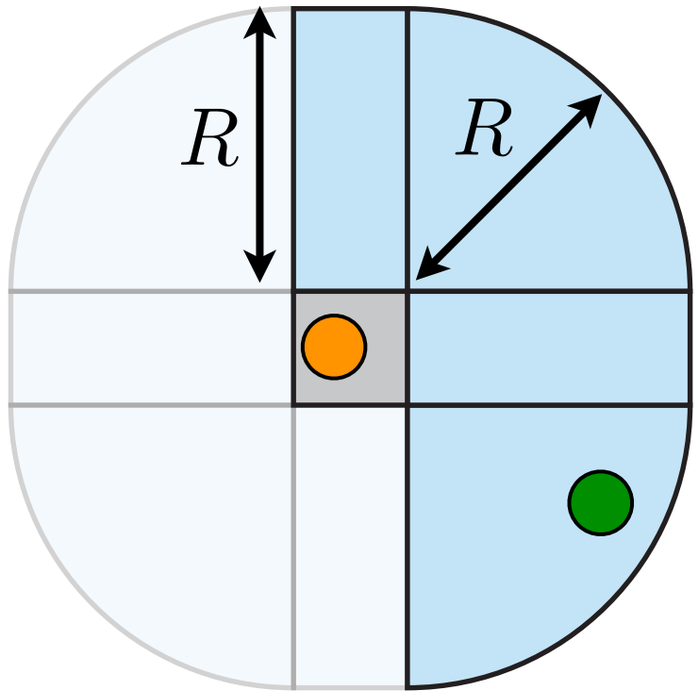


Parallel Computation

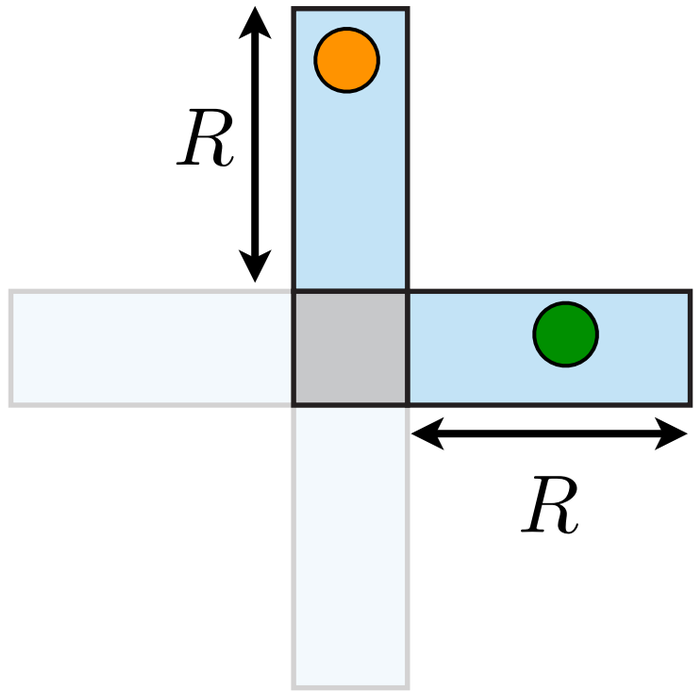
- Because of message-passing overhead, the algorithm scales somewhat worse than $N(N-1)/2N_{\mathrm{CPU}}$:

- Each CPU is numbered cyclically $n = 0, 1, \ldots, N_{\mathrm{CPU}} - 1$
- Loop for each time step:
  - Node n computes forces exerted by its own particles
  - Repeat $n - 1$ times:
    - Node n sends positions to node $n+1$ and receives positions from node $n - 1$
    - Uses received positions to compute forces on its own particles
  - Each node updates its own positions and velocities

Neutral territory methods



traditional half-shell



neutral territory

message passing overhead

$\sim \frac{1}{2}\pi R^2 + 2R$

$\sim 2R$