Molecular Dynamics & Polymer Physics

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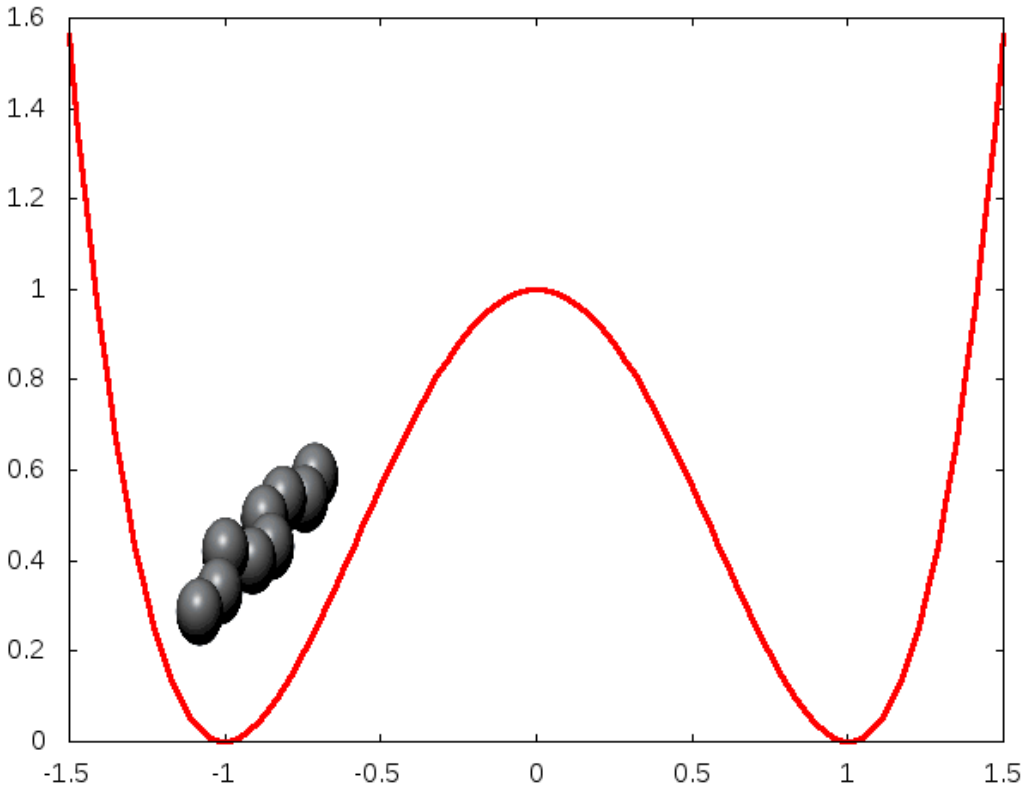
Aim: Statistical properties of polymers in a double-well potential



Overview

- Molecular Dynamics
- Multi-Core Implementation
- Polymer Dynamics

Molecular Dynamics

Langevin equation:

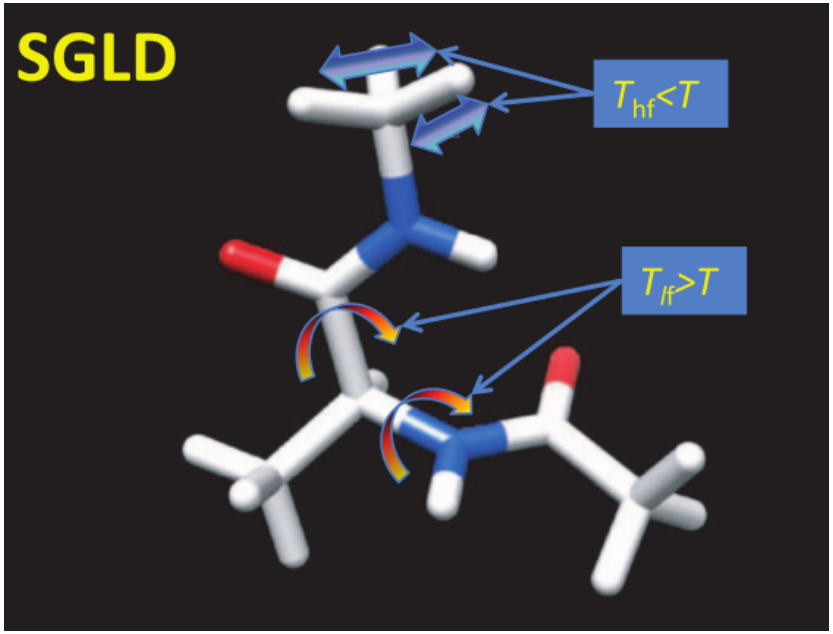
$$m_i \ddot{\vec{x}}_i = \vec{F}(\vec{x}_i(t)) - \underbrace{\gamma_i m_i \dot{\vec{x}}_i}_{\text{friction}} + \underbrace{\vec{R}_i}_{\text{stochastic term}}$$

$$\langle \vec{R}_i(t) \vec{R}_j(t') \rangle = 2 m_l k_B T \gamma_l \delta_{i,j} \delta(t - t') \Rightarrow \text{white noise}$$

Lennard-Jones-Potential:

$$U_{LJ} = \begin{cases} 4\epsilon \left(\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^{6} \right) & r_{ij} < r_c \\ 0 & r_{ij} \geq r_c \end{cases}$$

Self-guided Langevin Dynamics[1]:



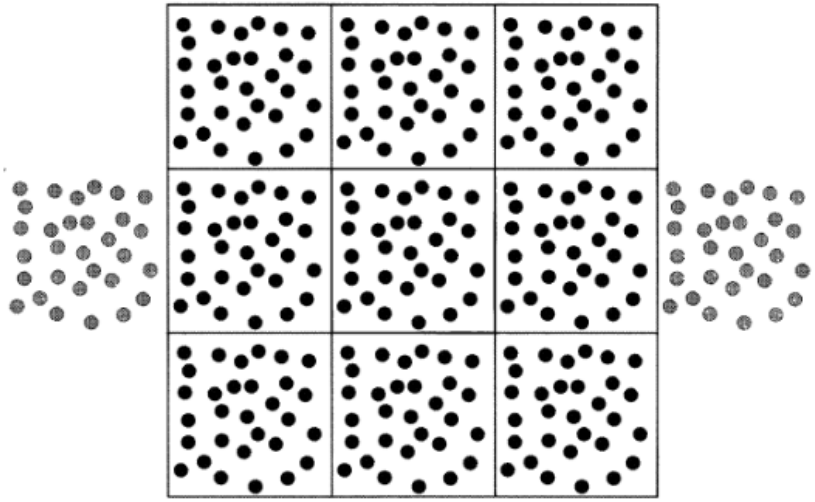
Kinetic energy from high frequency motions to low frequency motions to accelerate conformational searching

[1] Xiongwu Wu, Milan Hodoscek and Bernard R. Brooks: Replica exchanging self-guided Langevin dynamics for efficient and accurate conformational sampling

Implementation details:

- Second order integrator[1]
- Periodic boundary conditions[2]
- Neighborlist[3]
  - $r_b = r_c + \Delta r$
  - $\Delta r \leq n\tilde{v}\Delta t$

[1] Eric Vanden-Eijnden, Giovanni Ciccotti: Second-order integrators for Langevin equations with holonomic constraints



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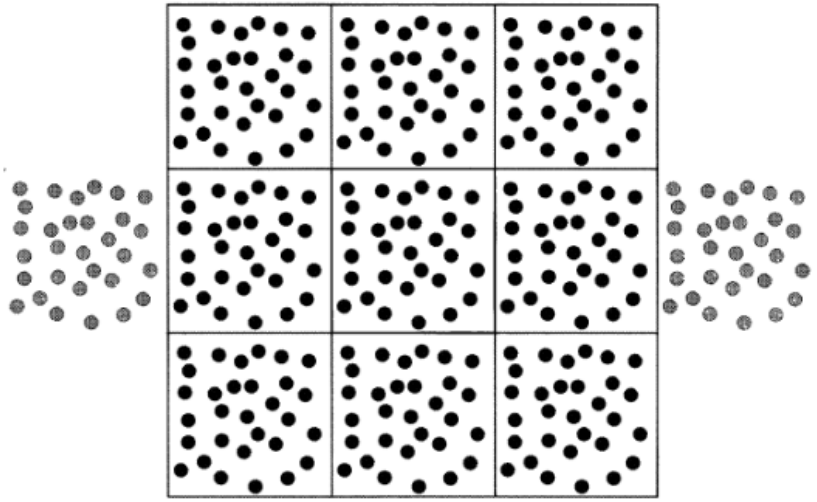
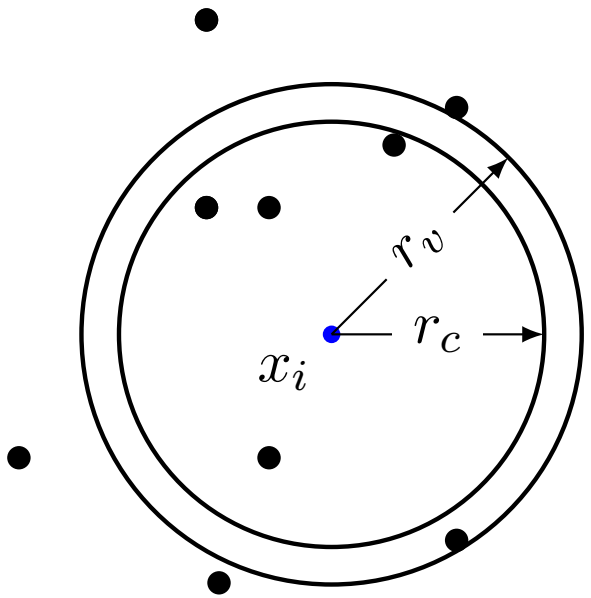
[2]D.C. Rapaport: The Art of Molecular Dynamics Simulation



Implementation details:

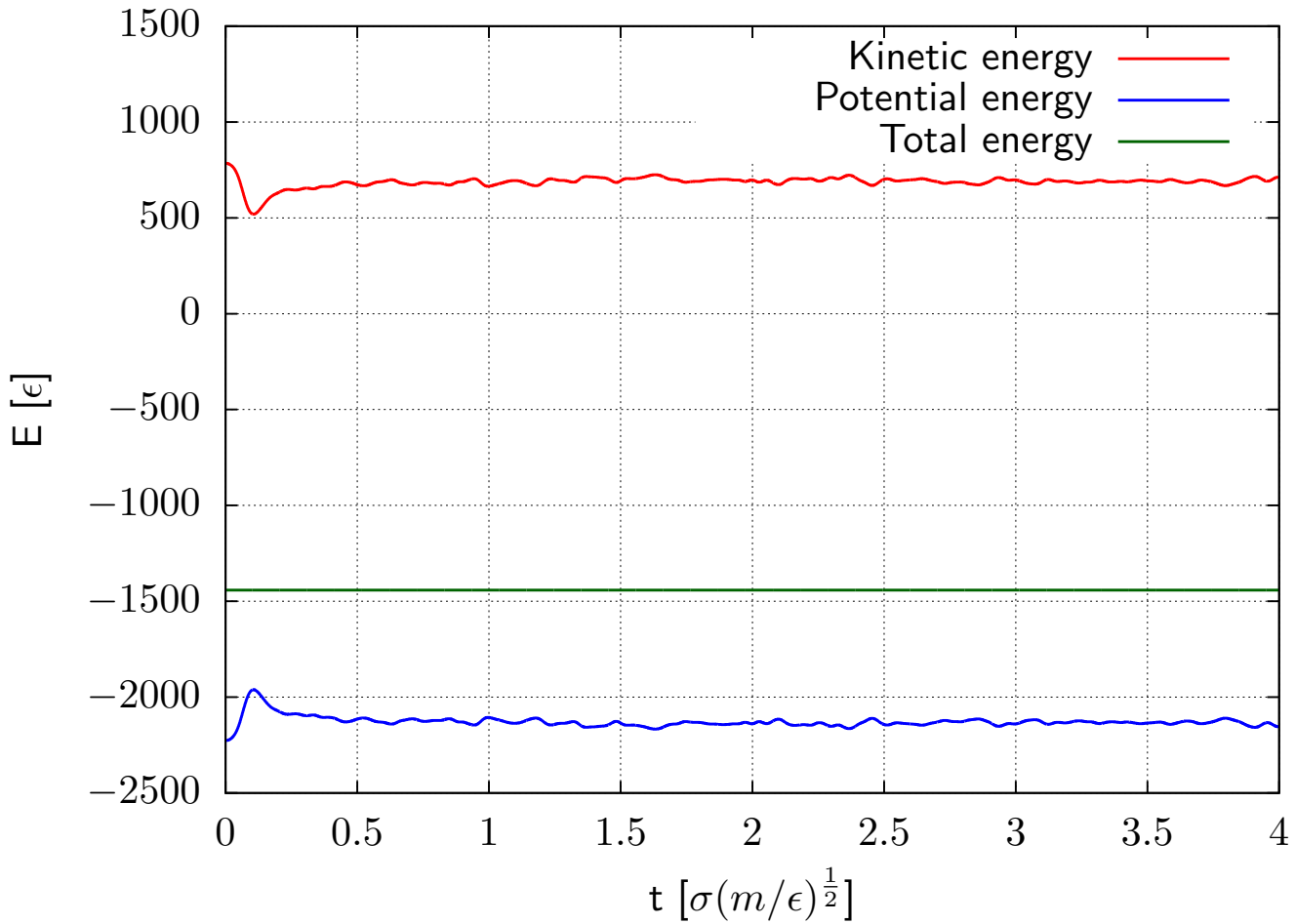
- Second order integrator[1]
- Periodic boundary conditions[2]
- Neighborlist[3]
  - $r_v = r_c + \Delta r$
  - $\Delta r \leq n\tilde{v}\Delta t$



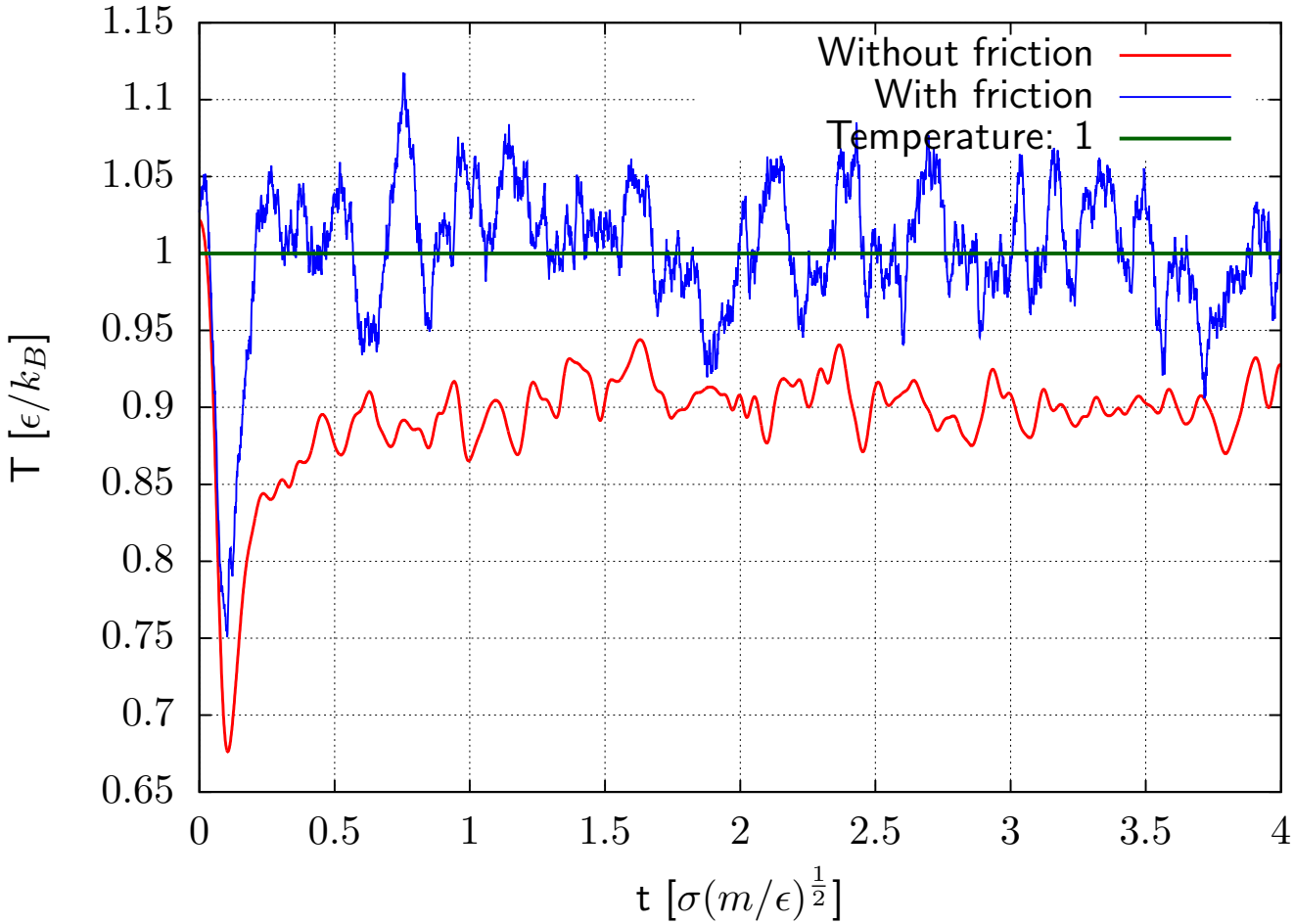
[3] Loup Verlet: Computer "Experiments" on Classical Fluids

Molecular Dynamics: Results

Energy conservation (no stochastic term and friction):



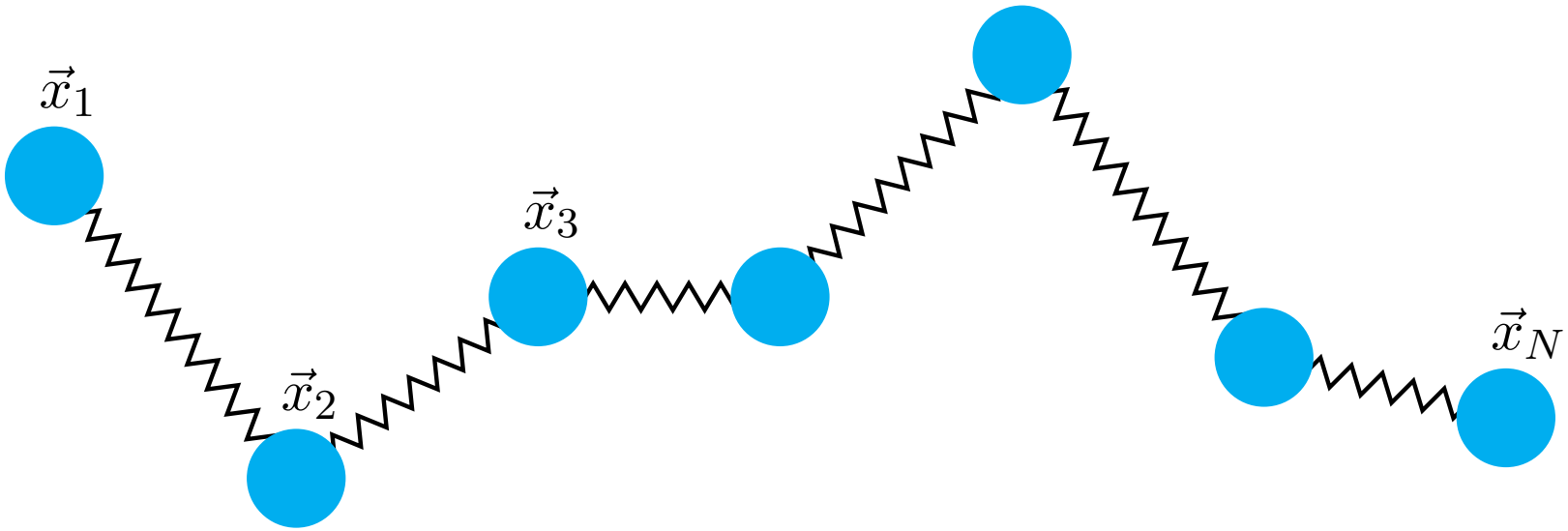
Temperature:



Red: $\gamma = 0$, Blue: $\gamma = 5$, Green: Initial Temperature

Polymer Physics

Rouse-Model:



Potential:

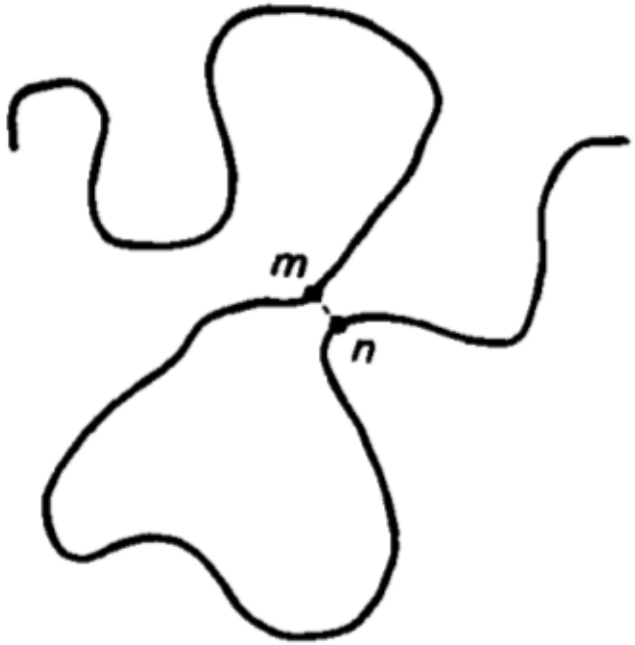
$$U_{ij} = \frac{1}{2} k (\vec{x}_i - \vec{x}_j)^2$$

$k = \frac{3 k_B T}{b^2}$, b ... mean segment length

$\Rightarrow$ Gaussian chain where $\psi(\vec{x}) = \left(\frac{3}{2\pi b^2}\right)^{\frac{3}{2}} \exp\left(-\frac{3\vec{x}^2}{2b^2}\right)$

$\Rightarrow$ End-to-end-distance: $\langle \vec{R}^2 \rangle = \langle (\vec{x}_N - \vec{x}_1)^2 \rangle \propto N - 1$

Excluded volume effect[1]:



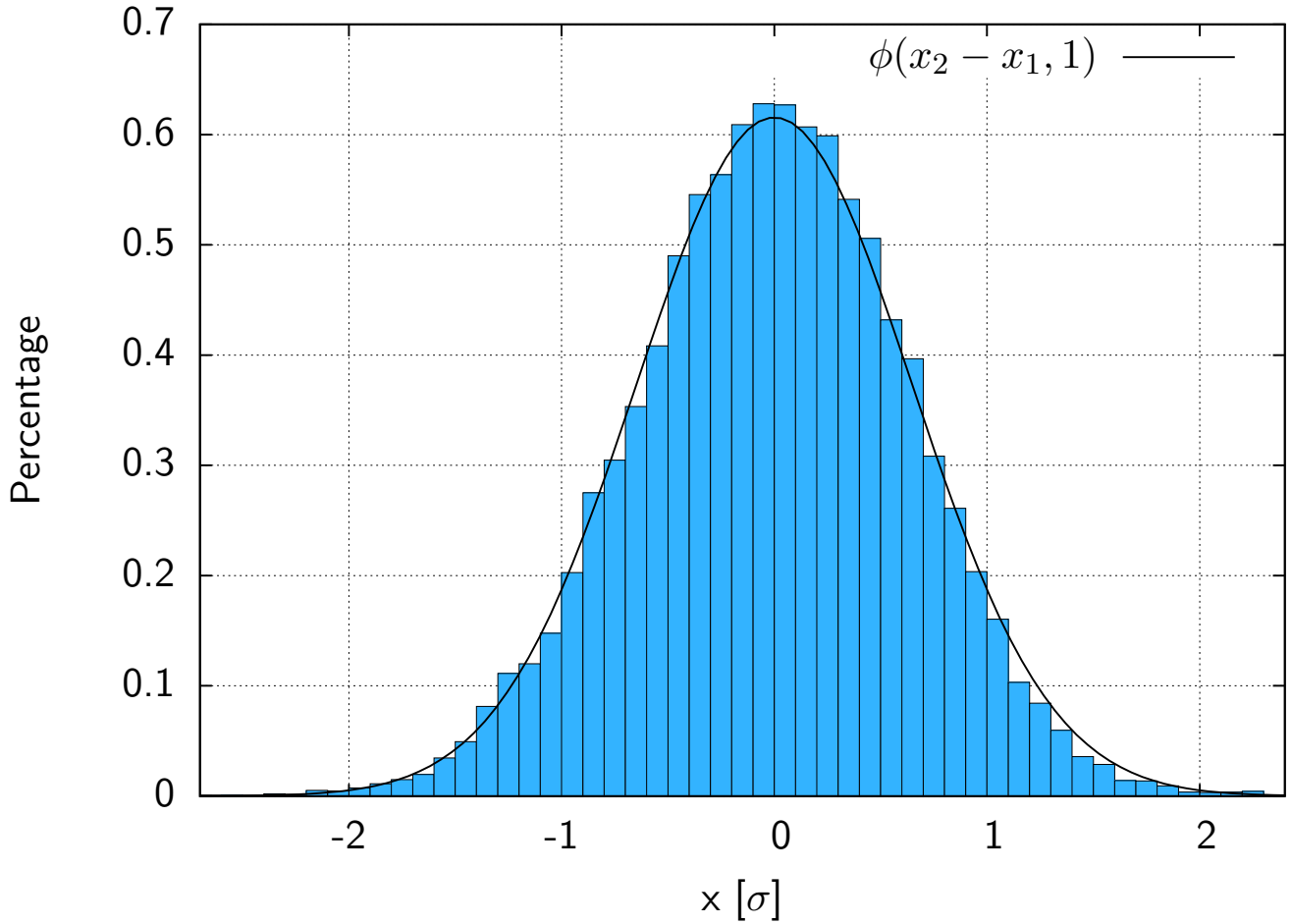
Include Lennard-Jones-Potential $\Rightarrow$ Excluded volume effect

$\Rightarrow$ End-to-end-distance: $\langle \vec{R}^2 \rangle \propto (N-1)^{\frac{6}{5}}$

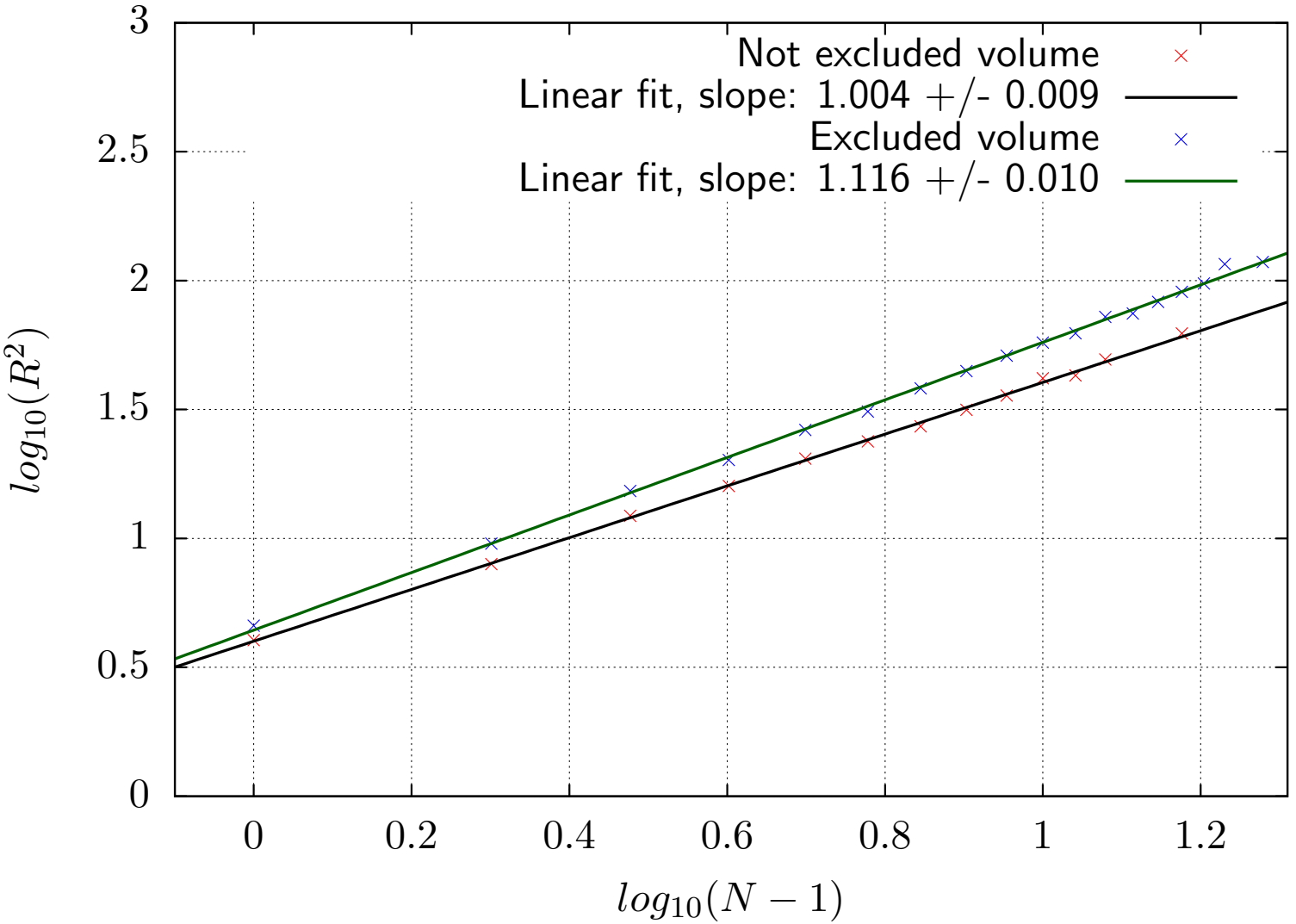
[1] M. Doi, S. F. Edwards: The Theory of Polymer Dynamics

Polymer Physics - Results

Distribution of x-component between two particles:



Not-excluded volume vs. excluded volume:



Todo:

- Implement external double well potential
- Run (long-time) simulations