Molecular Dynamics & Polymer Physics

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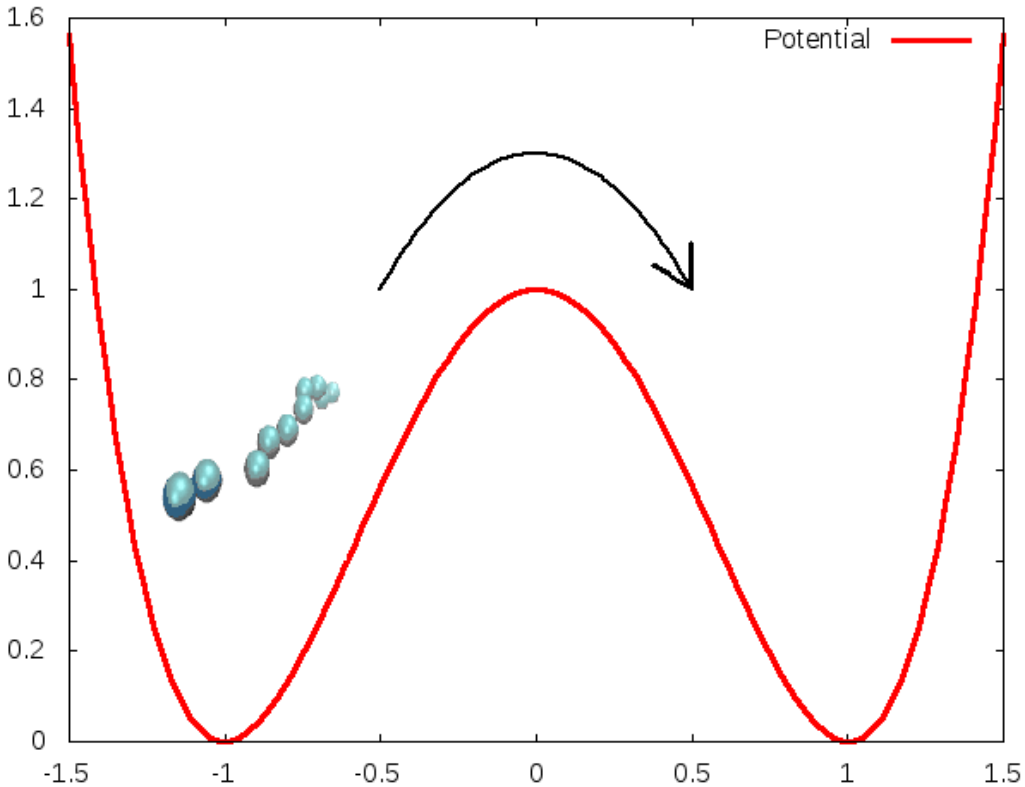
Aim: Transitionrate of polymers in a double-well potential



Overview

- Molecular Dynamics
- Multi-Core Implementation
- Polymer Dynamics

Molecular Dynamics

Langevin equation:

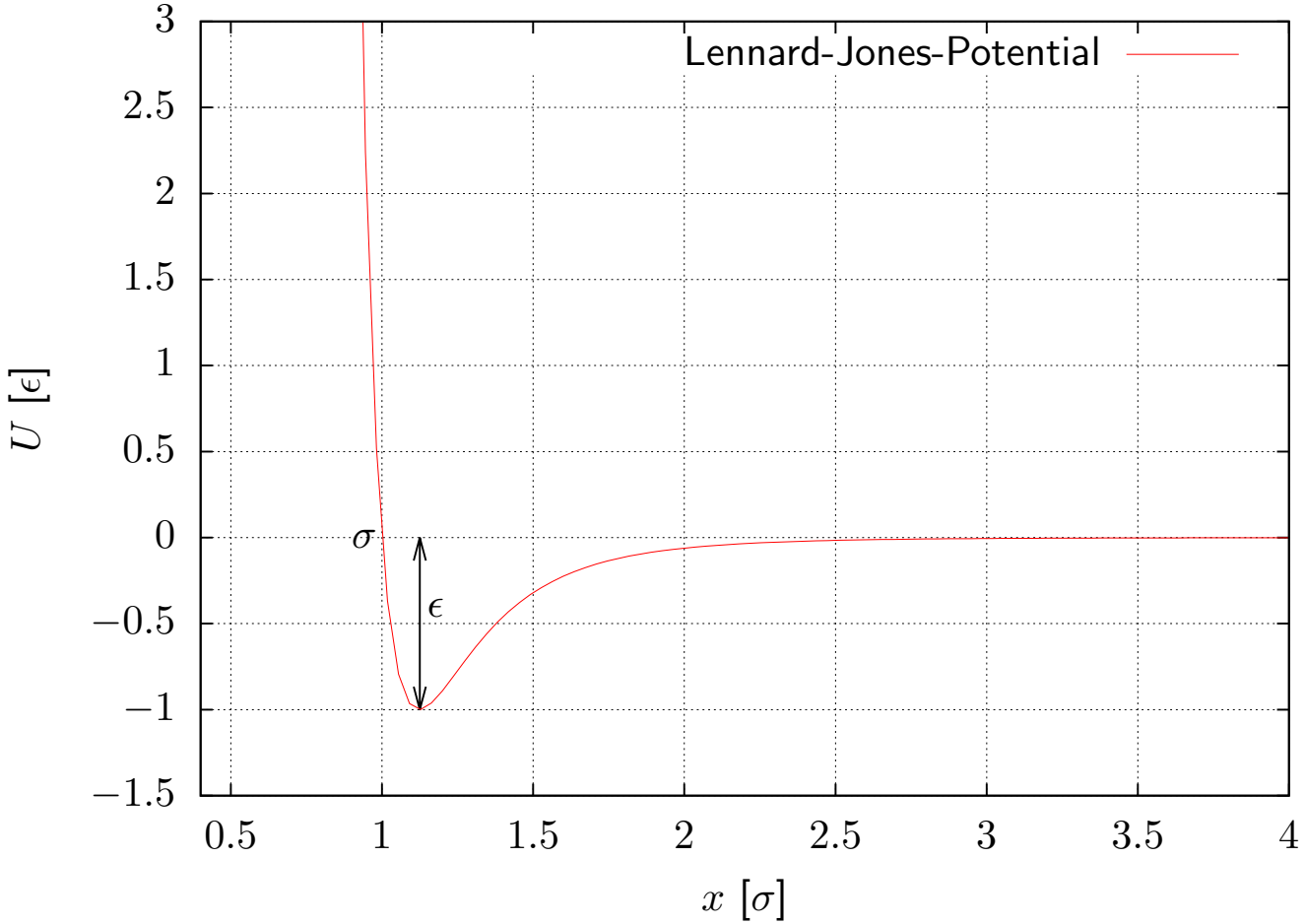
$$m_i \ddot{\vec{x}}_i = \vec{F}(\vec{x}_i(t)) - \underbrace{\gamma_i m_i \dot{\vec{x}}_i}_{\text{friction}} + \underbrace{\vec{R}_i}_{\text{stochastic term}}$$

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

Lennard-Jones-Potential:

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

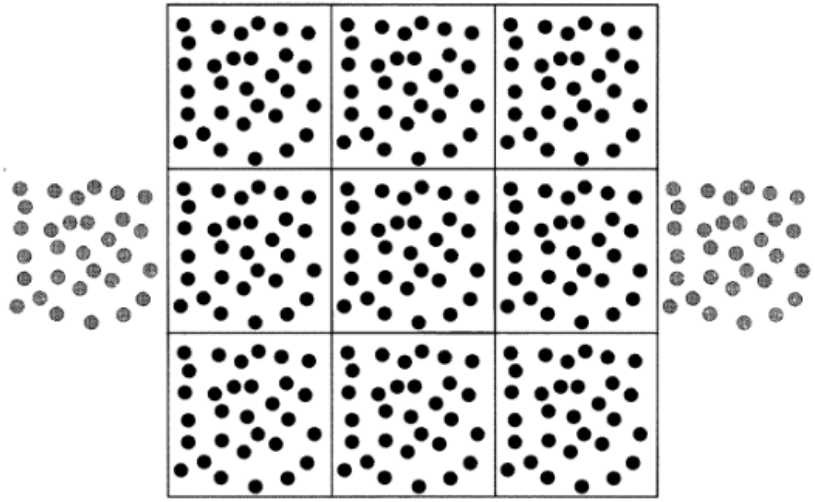
Lennard-Jones-Potential:



Implementation details:

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

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



Implementation details:

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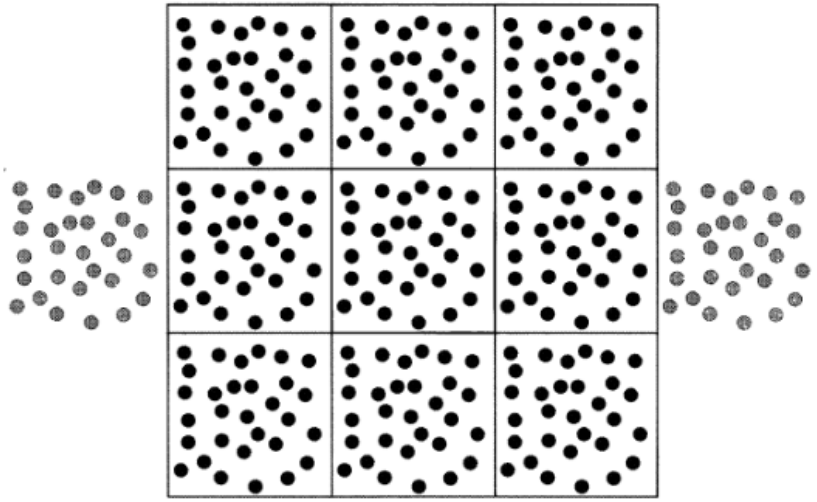
- Neighborlist[3]
  - $r_b = r_c + \Delta r$
  - $\Delta r \leq n\tilde{v}\Delta t$

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



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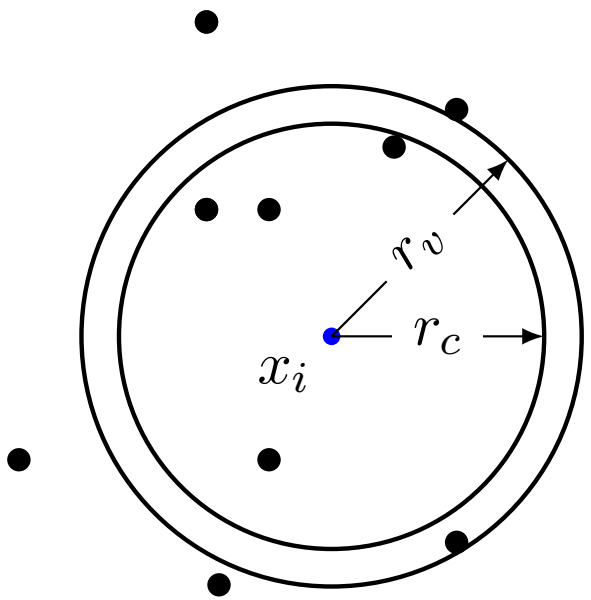
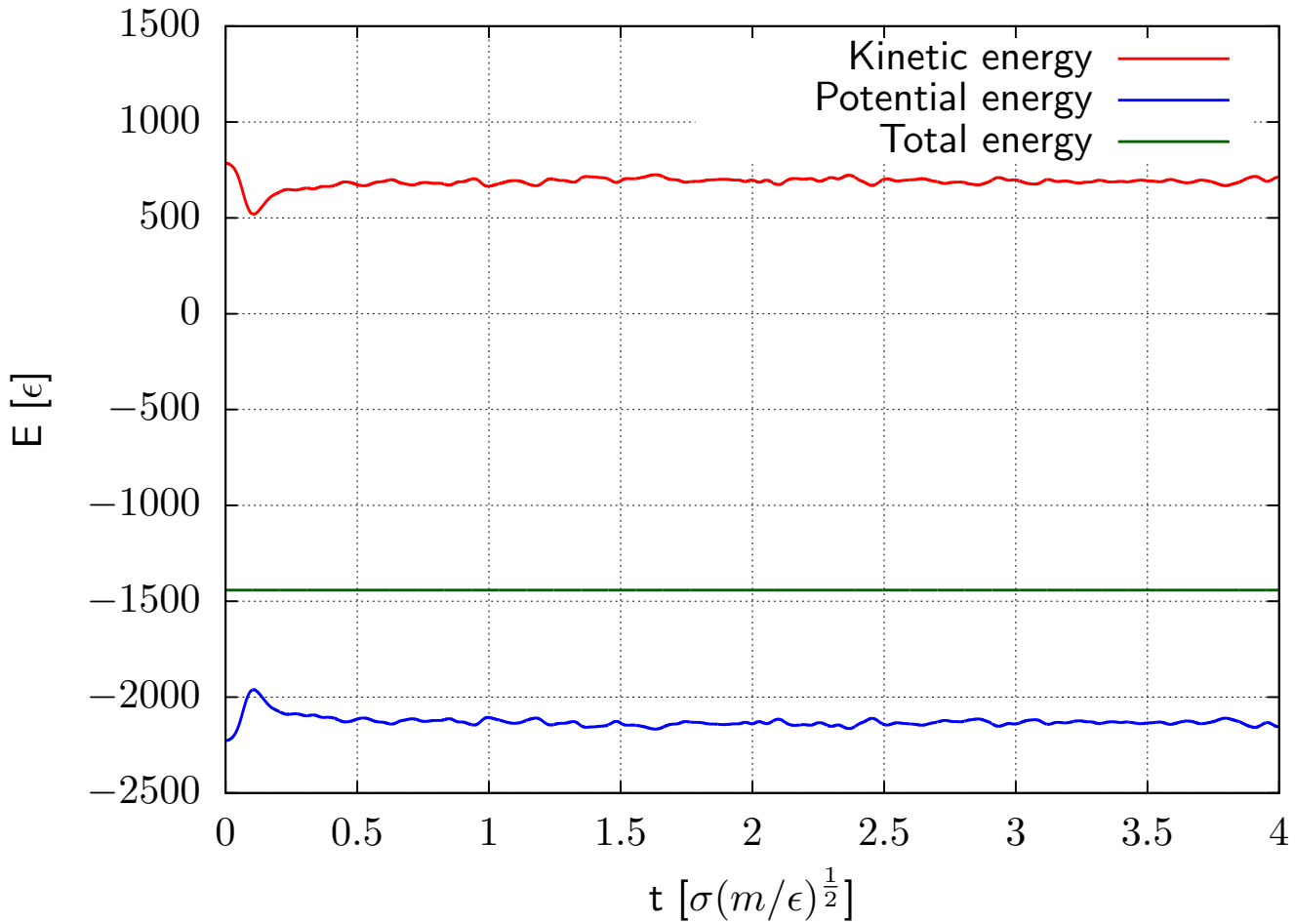


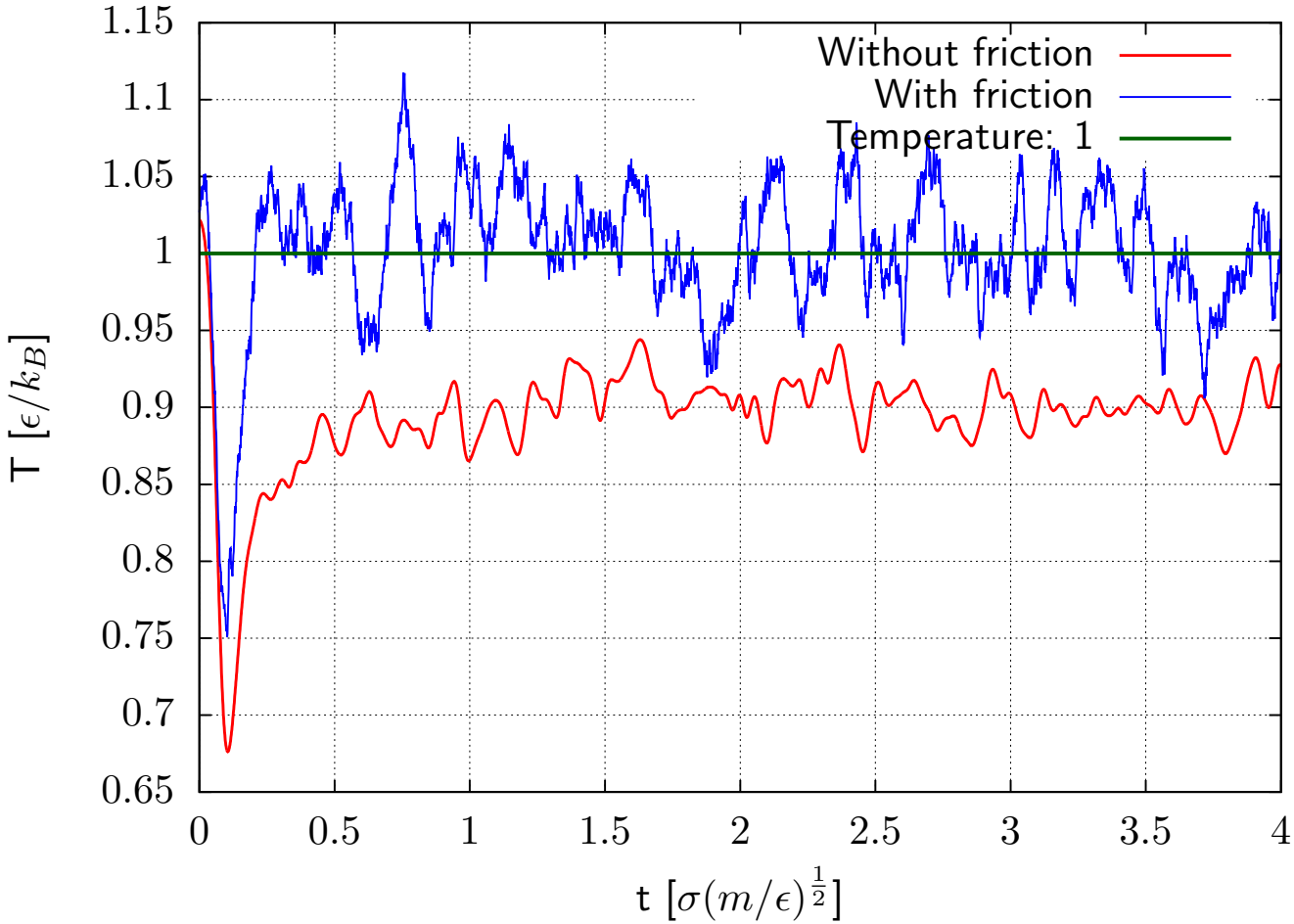
[3]Loup Verlet: Computer "Experiments" on Classical Fluids

Molecular Dynamics: Results

Energy conservation (no stochastic term and friction):



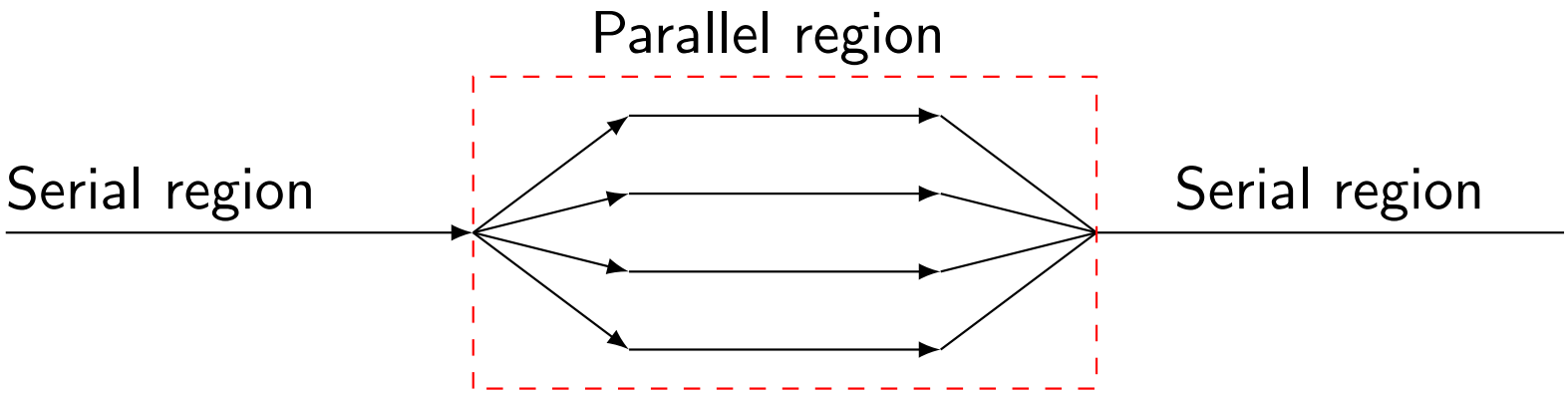
Temperature:



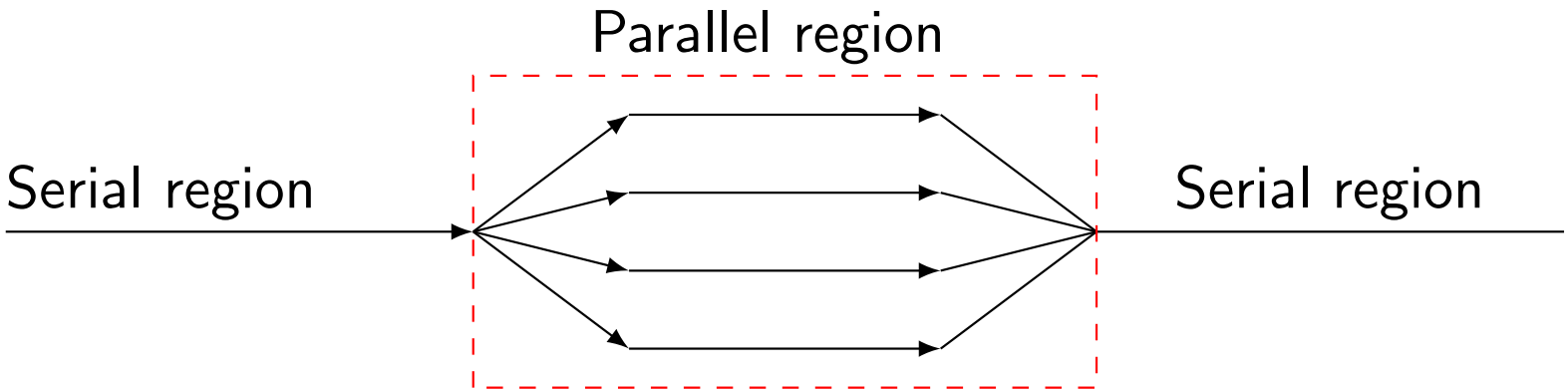
Red: $\gamma = 0$, Blue: $\gamma = 5$, Green: Initial Temperature

Multi-Core Implementation with OpenMP

OpenMP:



OpenMP:

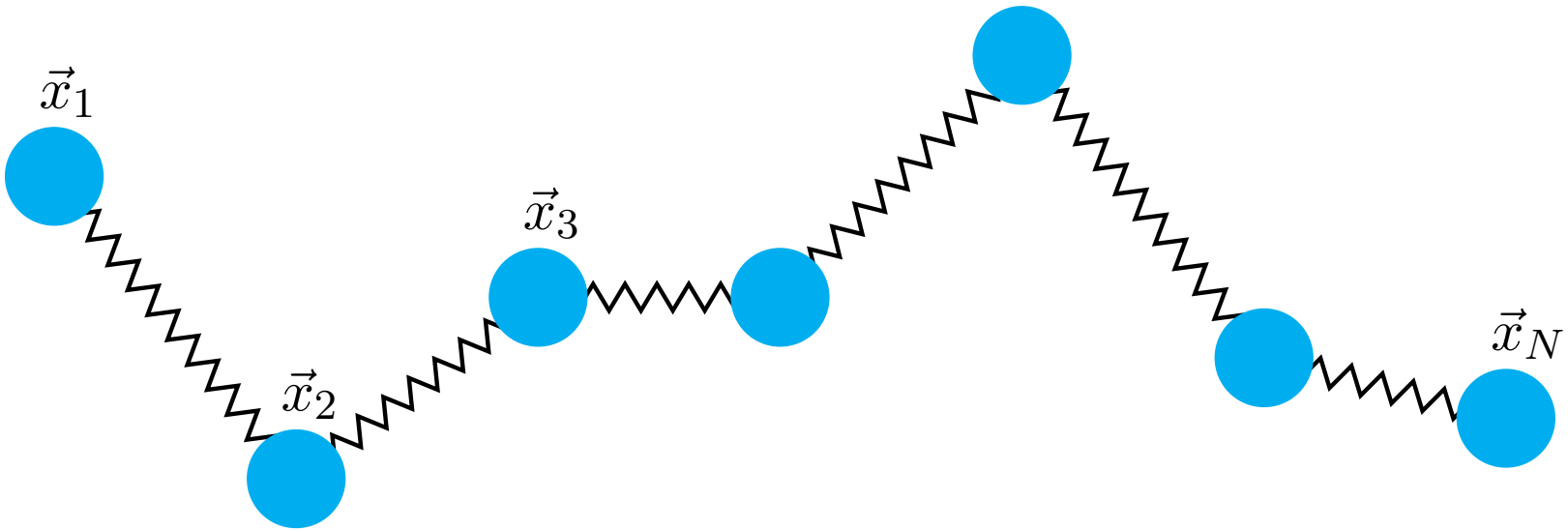


Implementation:

```
omp_set_num_threads(NUM_THREADS);
#pragma omp parallel for
  for (i=0; i<amount; i++){
    // CALCULATIONS
  }
#pragma omp barrier
```

Polymer Physics

Rouse-Model:



Potential:

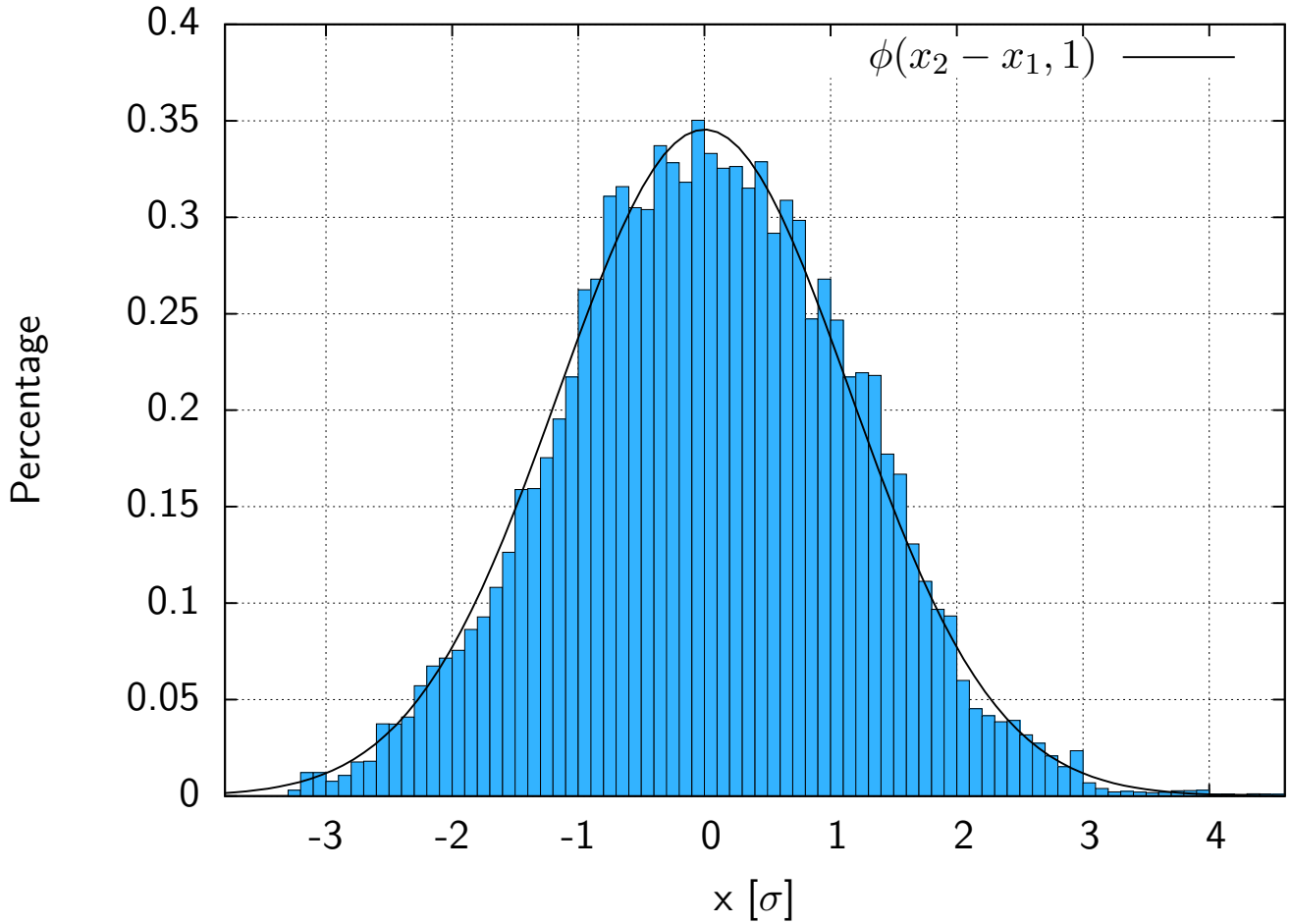
$$U_{ij} = \frac{1}{2} k (\vec{x}_i - \vec{x}_j)^2$$

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

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

Polymer Physics - Results

Distribution of x-component between the first two beads:



Todo:

- Implement external double well potential
- A way to classify transitions
- Run simulations