Simulation of a large polymer with untruncated interaction near the collapse

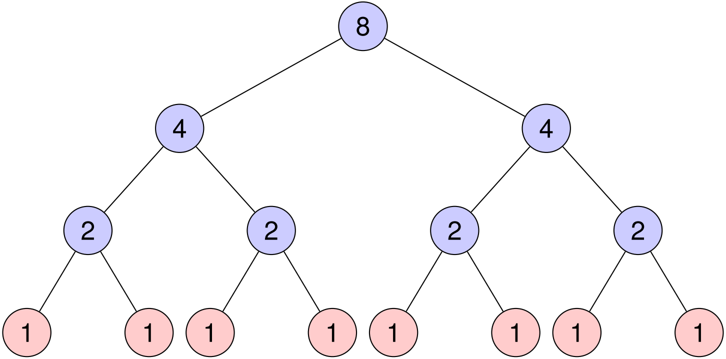
Stefan Schnabel and Wolfhard Janke

CompPhys18

SAW / hard-sphere polymer

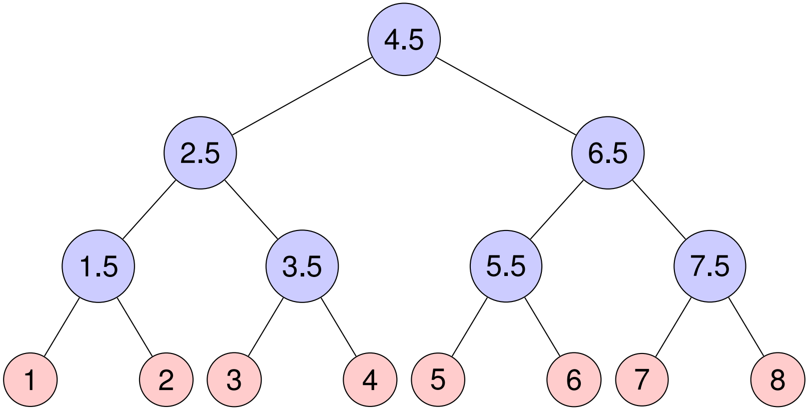
- bead-stick model in continuous space (3d), $\{\mathbf{x}\}$
- bonds (sticks) of length unity: $|\mathbf{x}_{i+1} - \mathbf{x}_i| = 1$
- monomer "interaction potential":
  $$U(r_{ij}) = \begin{cases} 0 & \text{if} \quad r_{ij} > 1 \\ \infty & \text{otherwise} \end{cases}, \qquad r_{ij} = |\mathbf{x}_i - \mathbf{x}_j|$$
- use binary tree, similar to N. Clisby, J. Stat. Phys. **140**, 349 (2010) (on lattice)

Binary tree

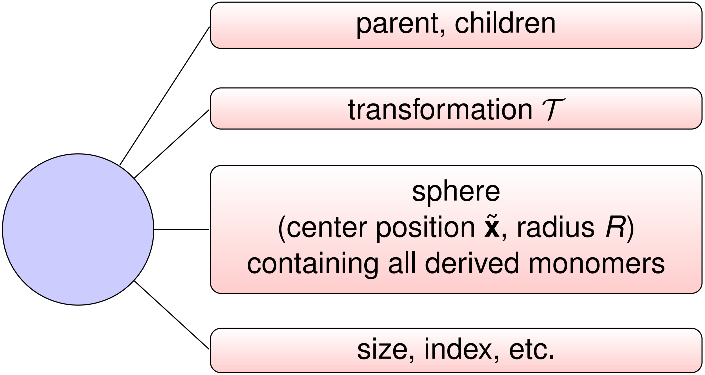


- leaves represent monomers
- inner nodes represent all derived leaves

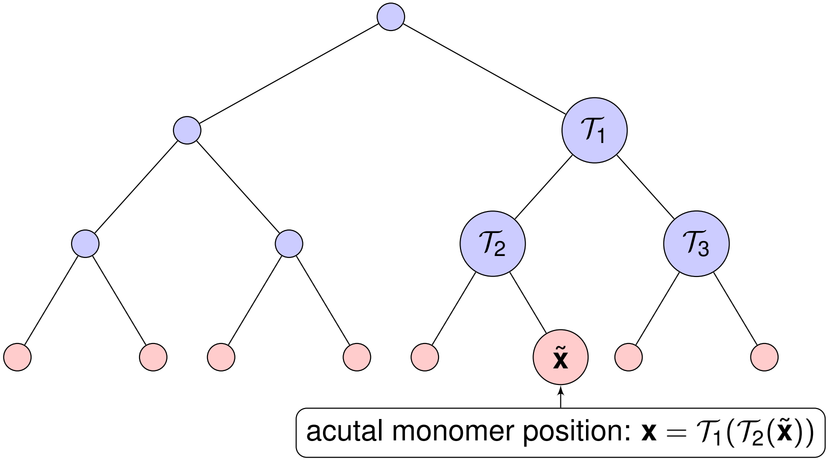
Binary tree



Node content

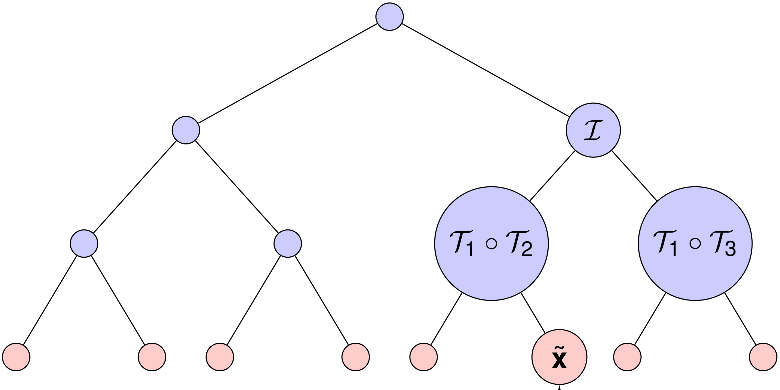


Monomer position



Monomer position

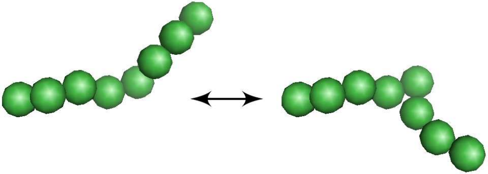
Transformations can be pushed down:



monomer position: $\mathbf{x} = (\mathcal{T}_1 \circ \mathcal{T}_2)(\tilde{\mathbf{x}}) \equiv \mathcal{T}_1(\mathcal{T}_2(\tilde{\mathbf{x}}))$

Update

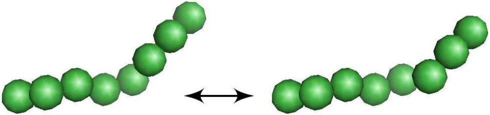
$$(\mathbf{x}_6, \mathbf{x}_7, \mathbf{x}_8) \rightarrow (\mathcal{T}_u(\mathbf{x}_6), \mathcal{T}_u(\mathbf{x}_7), \mathcal{T}_u(\mathbf{x}_8))$$



$$\mathcal{T}_u(\mathbf{x}_i) = \mathcal{R}\mathbf{x}_i + \mathbf{a}$$

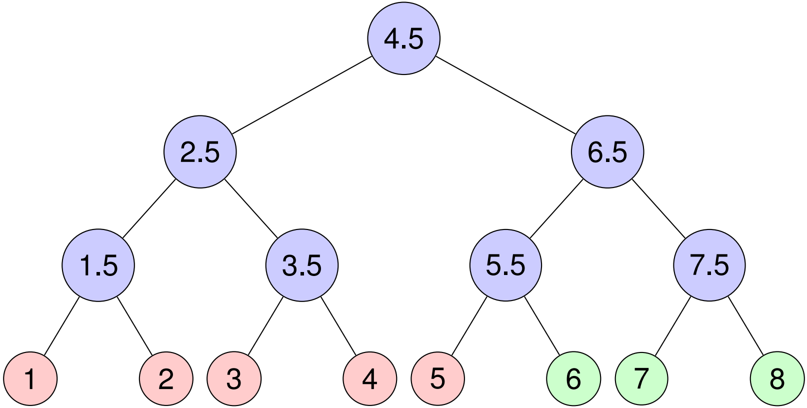
Update

$$(\mathbf{x}_6, \mathbf{x}_7, \mathbf{x}_8) \rightarrow (\mathcal{T}_u(\mathbf{x}_6), \mathcal{T}_u(\mathbf{x}_7), \mathcal{T}_u(\mathbf{x}_8))$$



$$\mathcal{T}_u(\mathbf{x}_i) = \mathbf{x}_i + \mathbf{b}$$

Update $(\mathbf{x}_6, \mathbf{x}_7, \mathbf{x}_8) \to (\mathcal{T}_u(\mathbf{x}_6), \mathcal{T}_u(\mathbf{x}_7), \mathcal{T}_u(\mathbf{x}_8))$



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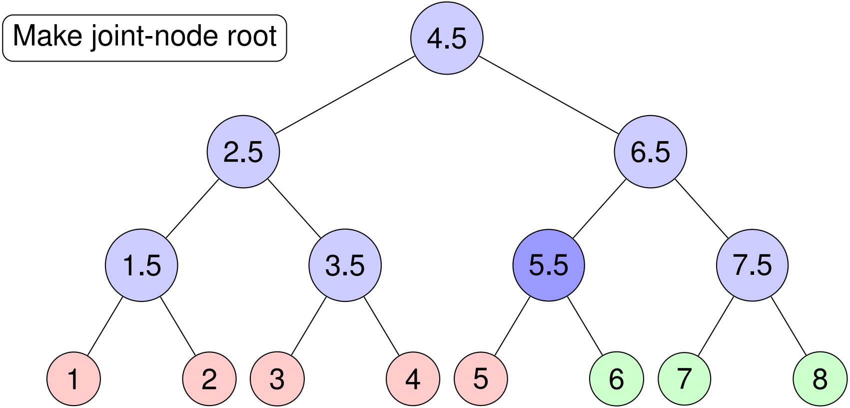

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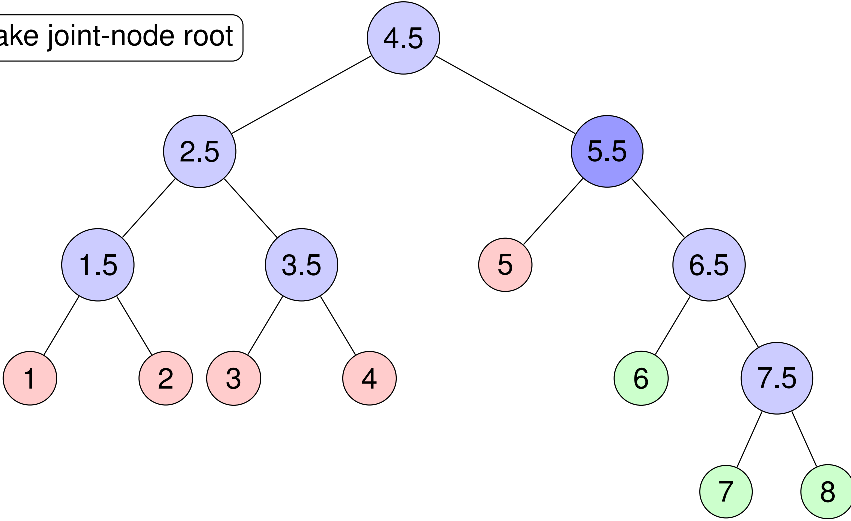
Make joint-node root



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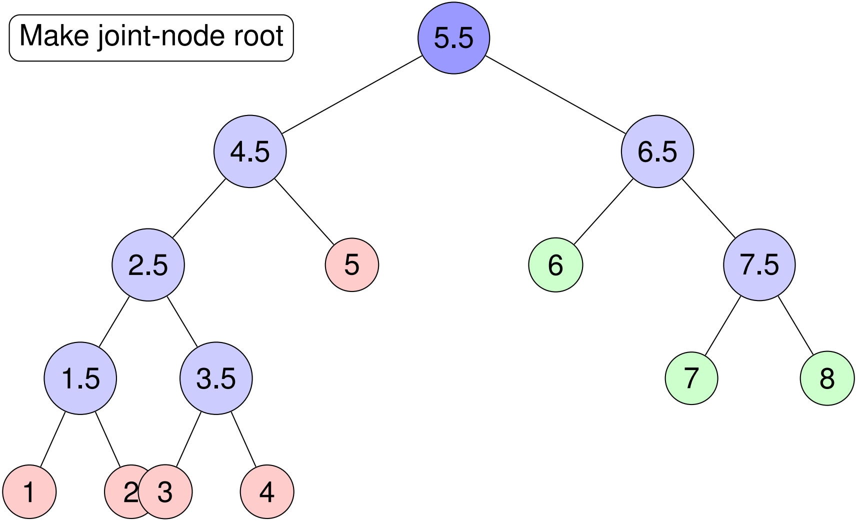

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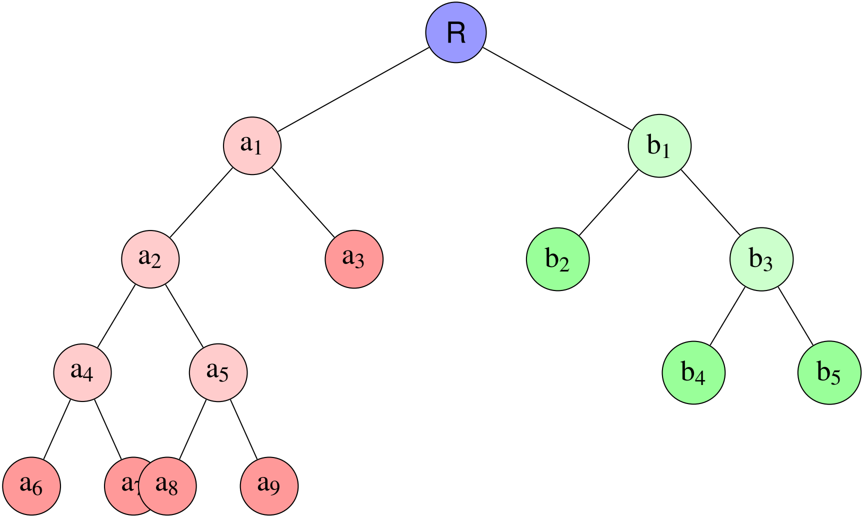

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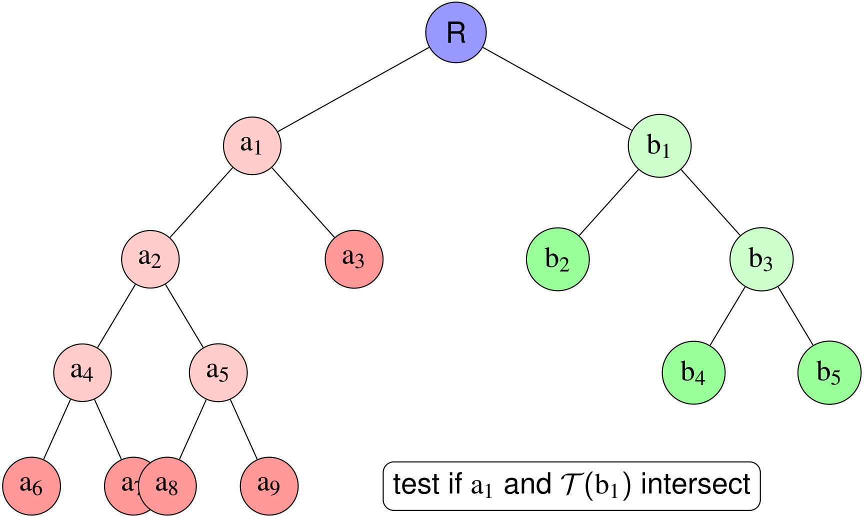
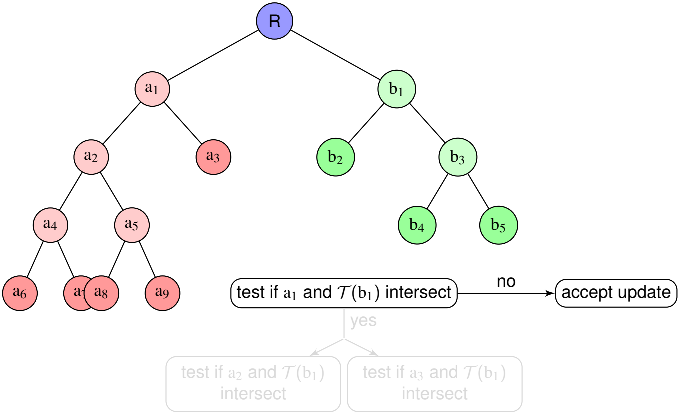


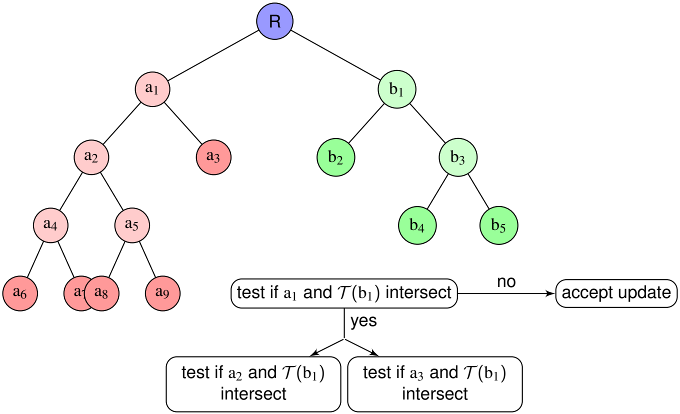
test if a_1 and $\mathcal{T}(\mathrm{b}_1)$ intersect

Update $(\mathbf{x}_6, \mathbf{x}_7, \mathbf{x}_8) \to (\mathcal{T}(\mathbf{x}_6), \mathcal{T}(\mathbf{x}_7), \mathcal{T}(\mathbf{x}_8))$



Split if spheres intersect and reject when intersecting monomers are found.

Update $(\mathbf{x}_6, \mathbf{x}_7, \mathbf{x}_8) \rightarrow (\mathcal{T}(\mathbf{x}_6), \mathcal{T}(\mathbf{x}_7), \mathcal{T}(\mathbf{x}_8))$



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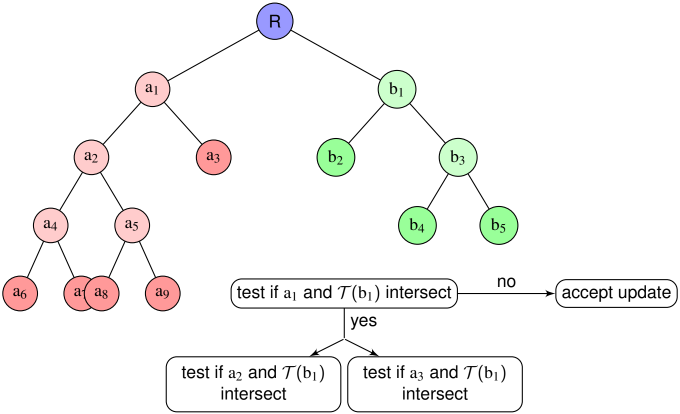

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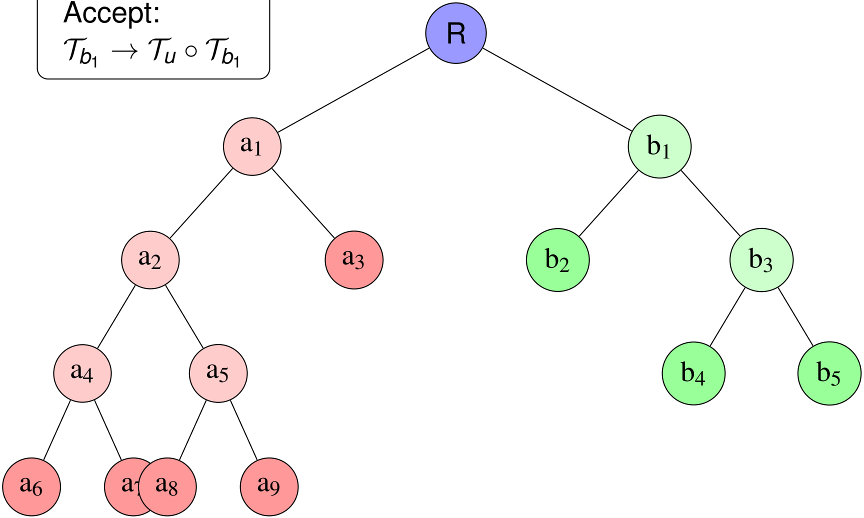
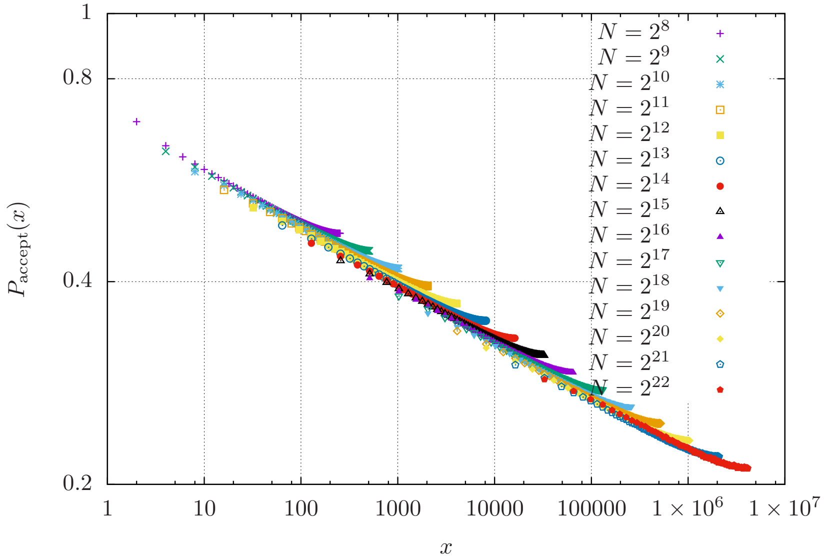
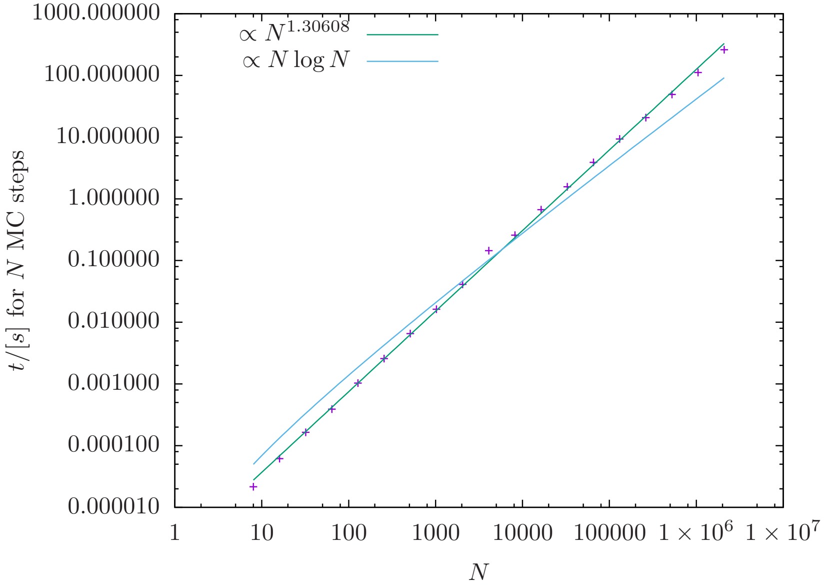
Update $(\mathbf{x}_6, \mathbf{x}_7, \mathbf{x}_8) \rightarrow (\mathcal{T}_u(\mathbf{x}_6), \mathcal{T}_u(\mathbf{x}_7), \mathcal{T}_u(\mathbf{x}_8))$

Accept:
$\mathcal{T}_{b_1} \rightarrow \mathcal{T}_u \circ \mathcal{T}_{b_1}$

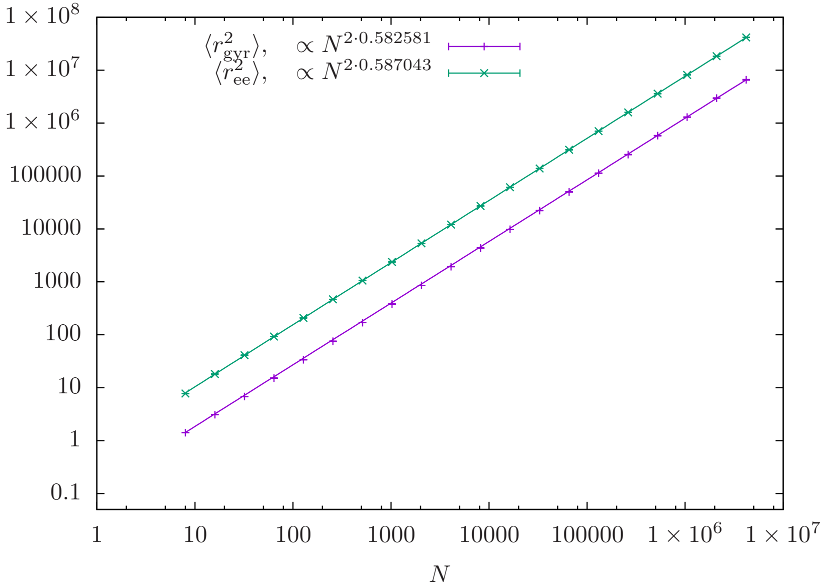



1
0.8
0.4
0.2
$P_{\text{accept}}(x)$
1
10
100
1000
10000
100000
1×10^6
1×10^7
x
$N = 2^8$
$N = 2^9$
$N = 2^{10}$
$N = 2^{11}$
$N = 2^{12}$
$N = 2^{13}$
$N = 2^{14}$
$N = 2^{15}$
$N = 2^{16}$
$N = 2^{17}$
$N = 2^{18}$
$N = 2^{19}$
$N = 2^{20}$
$N = 2^{21}$
$N = 2^{22}$

hard-sphere polymer : time per sweep



hard-sphere polymer : results



hard-sphere polymer : results

$$\langle r_{\mathrm{ee}}^2 \rangle_N = D N^{2\nu} \left[1 + \frac{a_1}{N} + \frac{a_2}{N^2} + \dots \right. \\ \left. + \frac{b_1}{N^{\Delta_1}} + \frac{b_2}{N^{2\Delta_1}} + \dots + \frac{c_1}{N^{\Delta_2}} + \dots \right]$$

	I	II	III	[1]
ν	0.58755(1)	0.58763(1)	0.58764(2)	0.587597(7)
Δ_1	0.577(4)	0.493(8)	0.47(4)	0.528(12)

[1] N. Clisby, Phys. Rev. Lett. **104**, 055702 (2010).

Lennard-Jones polymer

- bead-stick model in continuous space (3d), $\{\mathbf{x}\}$
- bonds (sticks) of length unity: $|\mathbf{x}_{i+1} - \mathbf{x}_i| = 1$
- monomer interaction potential: $U(r_{ij}) = \frac{1}{r_{ij}^{12}} - \frac{2}{r_{ij}^{6}}, \quad r_{ij} = |\mathbf{x}_i - \mathbf{x}_j|$
- Hamiltonian: $\mathcal{H} = \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} U(r_{ij})$
- calculating energy or change in energy is of (average) complexity $\mathcal{O}(N^2)$

Metropolis

- $P_{\mathrm{accept}} = \min\left(1, e^{-\beta\Delta E}\right), \quad \Delta E = E_{\mathrm{new}} - E_{\mathrm{old}}$
- chose (uniformly distributed) random number $\xi \in [0, 1)$
- accept if $\xi < P_{\mathrm{accept}}$, i.e., if

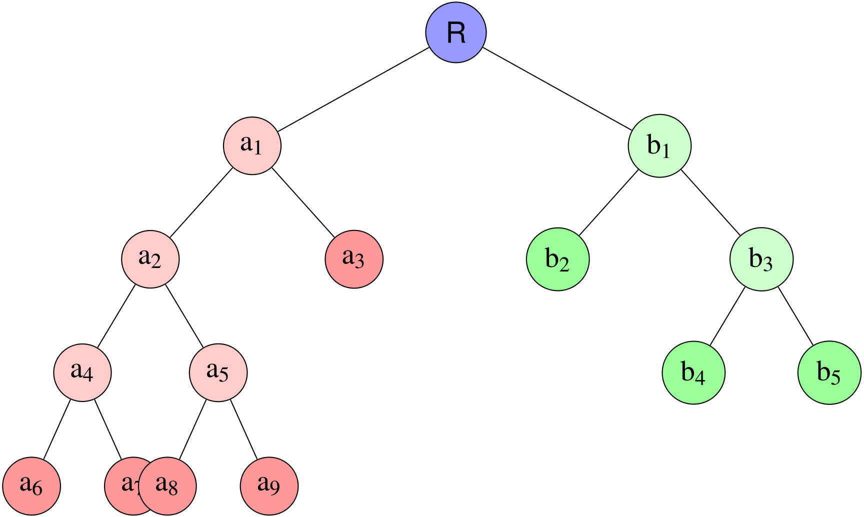
$$\xi < e^{-\beta\Delta E} \tag{1}$$

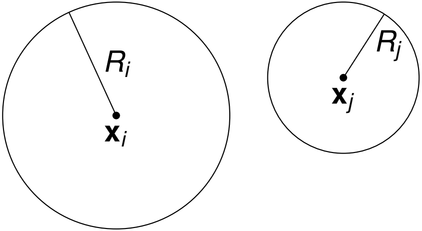
- hence, accept if

$$\Delta E < -\frac{\ln \xi}{\beta} \tag{2}$$

- draw ξ and determine ΔE with increasing precision until (2) can be decided
  $\Delta E \in [E_{\mathrm{new}}^{\mathrm{min}} - E_{\mathrm{old}}^{\mathrm{max}}, E_{\mathrm{new}}^{\mathrm{max}} - E_{\mathrm{old}}^{\mathrm{min}}]$

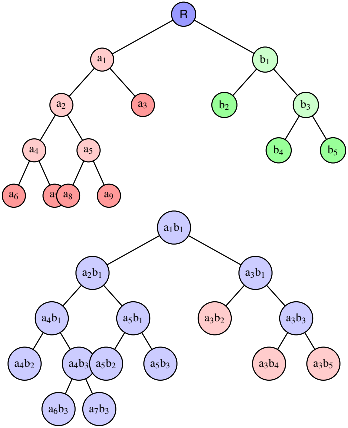
Update $(\mathbf{x}_6, \mathbf{x}_7, \mathbf{x}_8) \rightarrow (\mathcal{T}_u(\mathbf{x}_6), \mathcal{T}_u(\mathbf{x}_7), \mathcal{T}_u(\mathbf{x}_8))$





- node i contains n_i monomers
- minimal distance between node i and j:
  $d_{ij}^{\min} = |\mathbf{x}_i - \mathbf{x}_j| - R_i - R_j$
- maximal distance between node i and j:
  $d_{ij}^{\max} = |\mathbf{x}_i - \mathbf{x}_j| + R_i + R_j$
- if $d_{ij}^{\min} \geq 1$
  then $E_{ij} \geq E_{ij}^{\min} = n_i n_j U(d_{ij}^{\min})$
  and $E_{ij} \leq E_{ij}^{\max} = n_i n_j U(d_{ij}^{\max})$

Interaction tree



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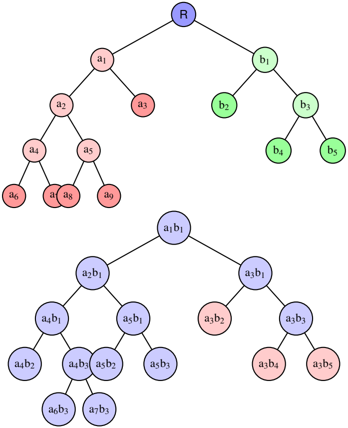
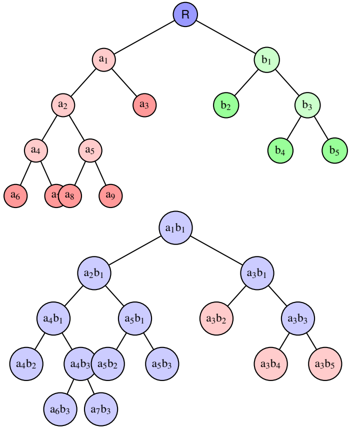


- current estimate for $E_{a_1 b_1}$ is derived by summation over leaves
- nodes with $d^{\min} < 1$ have to be split up
- if $d^{\min} \geq 1$ for all leaves split node with highest uncertainty
- proceed for $E_{a_1 b_1}$ and $E_{a_1 \mathcal{T}(b_1)}$ in parallel until ΔE is precise enough

Interaction tree



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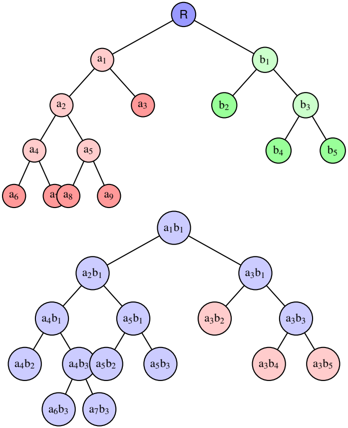

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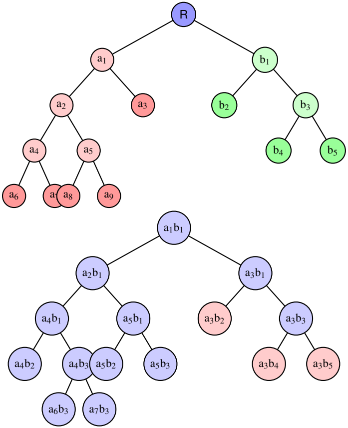

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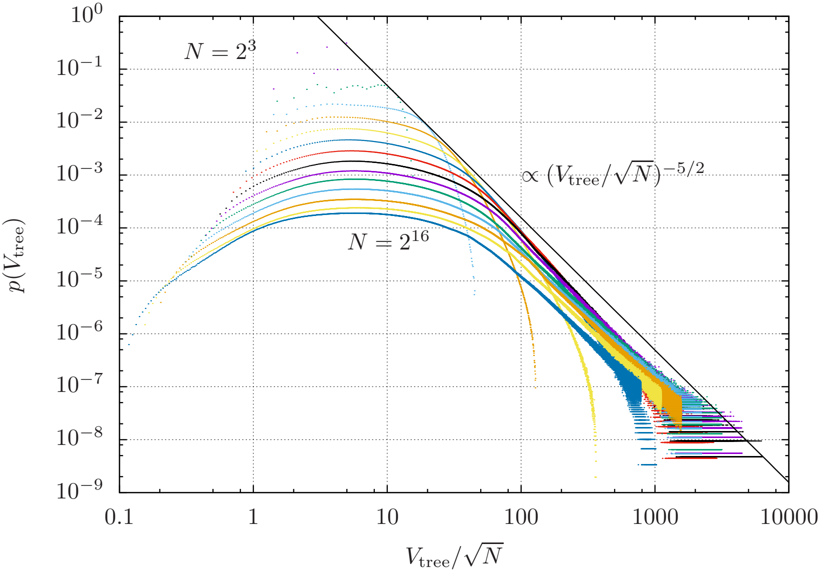
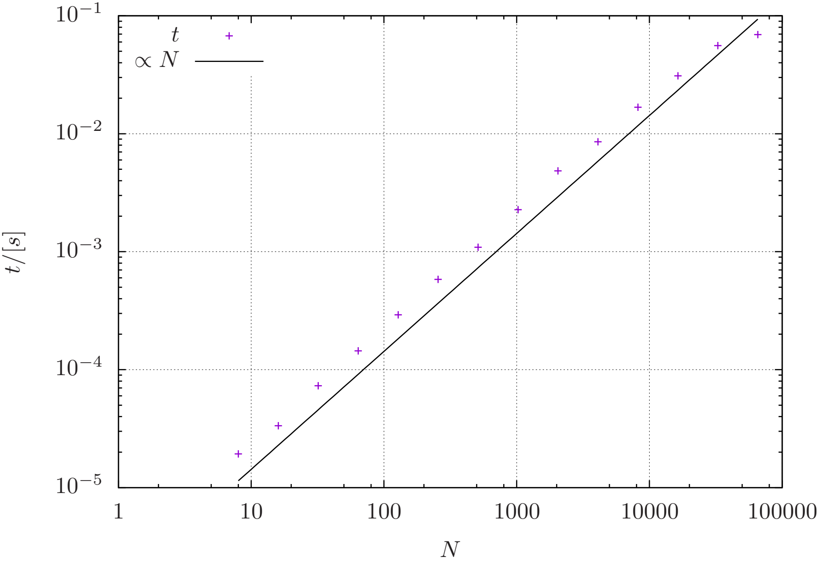
tree size

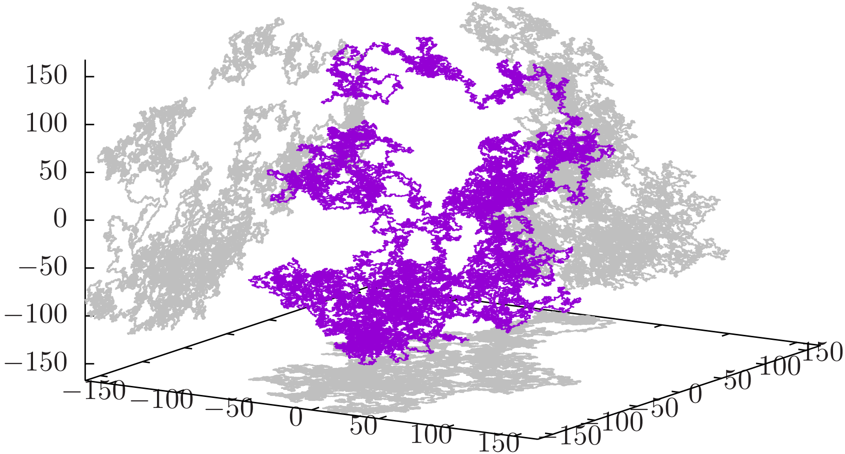


$N = 2^3$
$\propto (V_{\mathrm{tree}}/\sqrt{N})^{-5/2}$
$N = 2^{16}$
$p(V_{\mathrm{tree}})$
10^0
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
10^{-8}
10^{-9}
0.1
1
10
100
1000
10000
$V_{\mathrm{tree}}/\sqrt{N}$

speed



LJ-polymer : configuration



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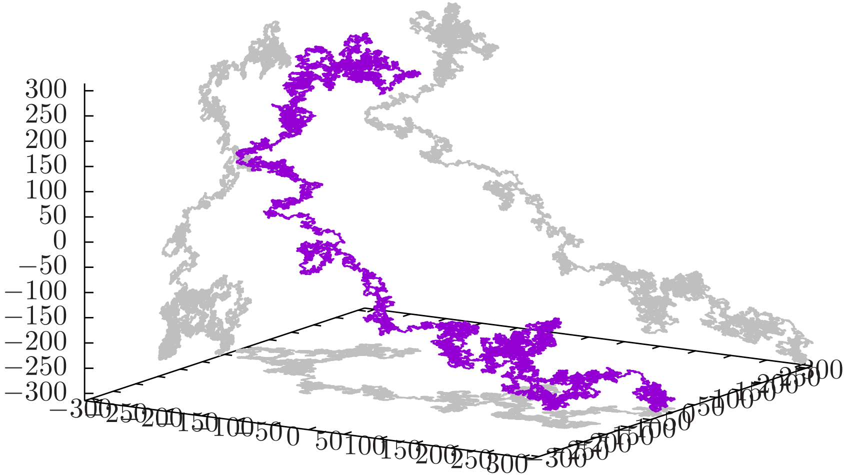
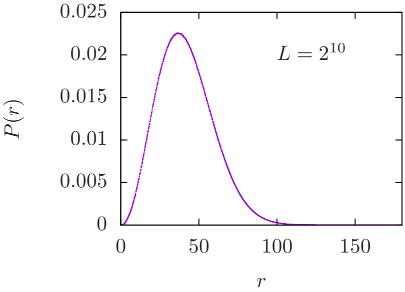


distribution of end-to-end distance

- Gaussian distributed:
  $P(\mathbf{r}) \propto e^{-\mathbf{r}^2/2\sigma^2}$
- radial distribution:
  $P(r) \propto r^2 e^{-r^2/2\sigma^2}$
- radial distribution:
  $P(r)/r^2 \propto e^{-r^2/2\sigma^2}$
- logarithmic:
  $\ln\left(P(r)/r^2\right) = -r^2/2\sigma^2 + c$



- At T_c the quadratic component of the fit of $\ln\left(P(r)/r^2\right)$ against r^2 is zero.

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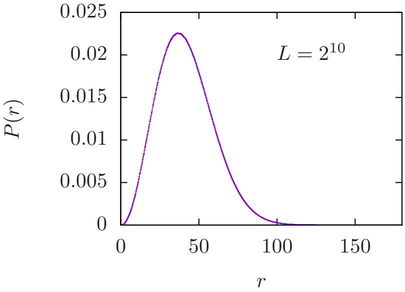

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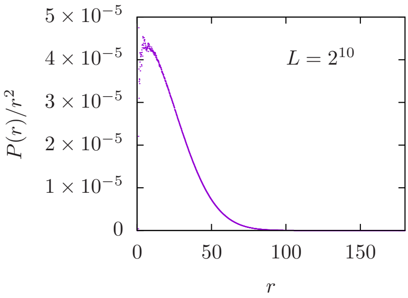

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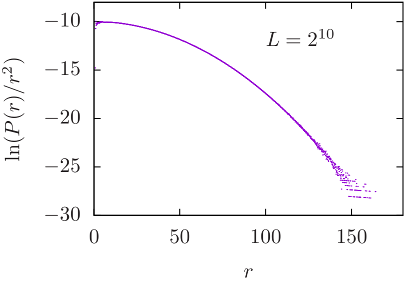

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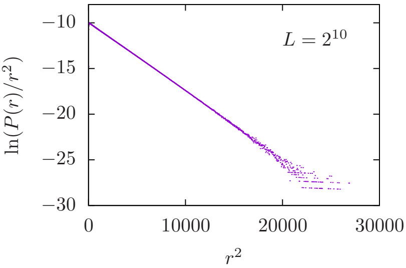

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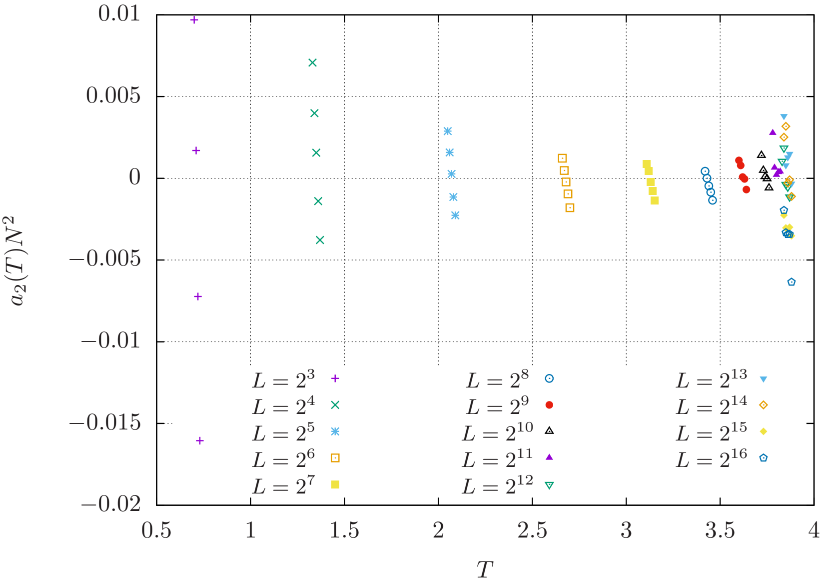
second order components



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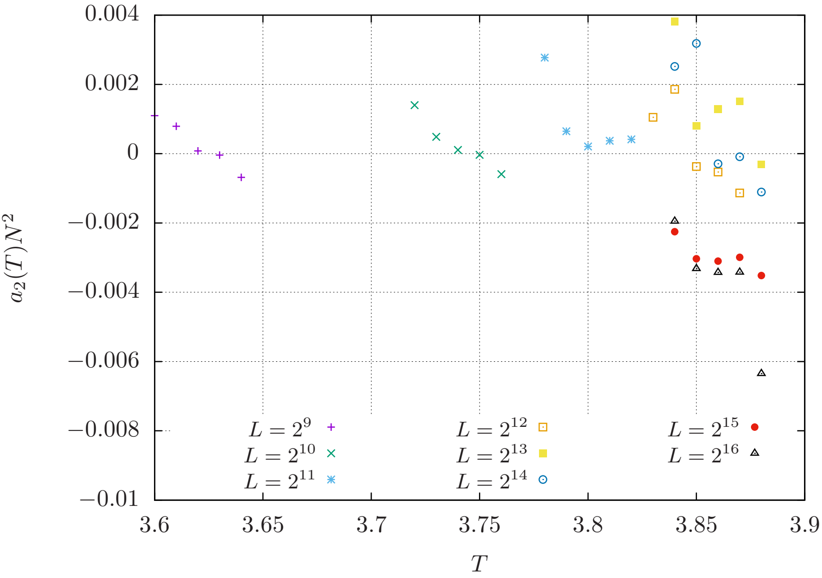
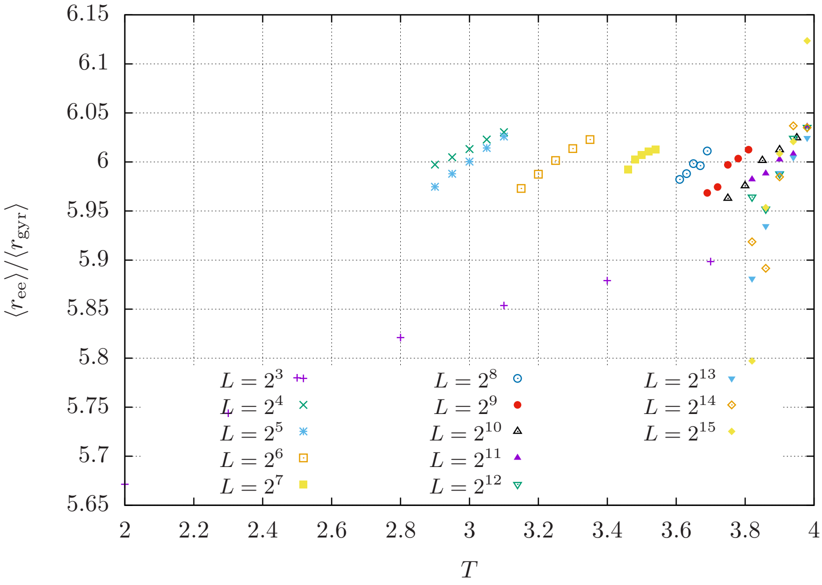
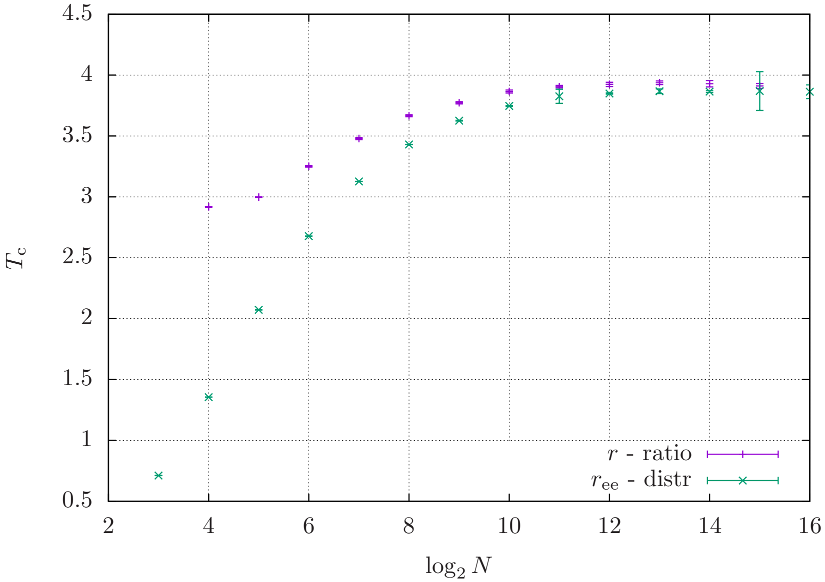


Ratio r_{ee}/r_{gyr}



critical temperature



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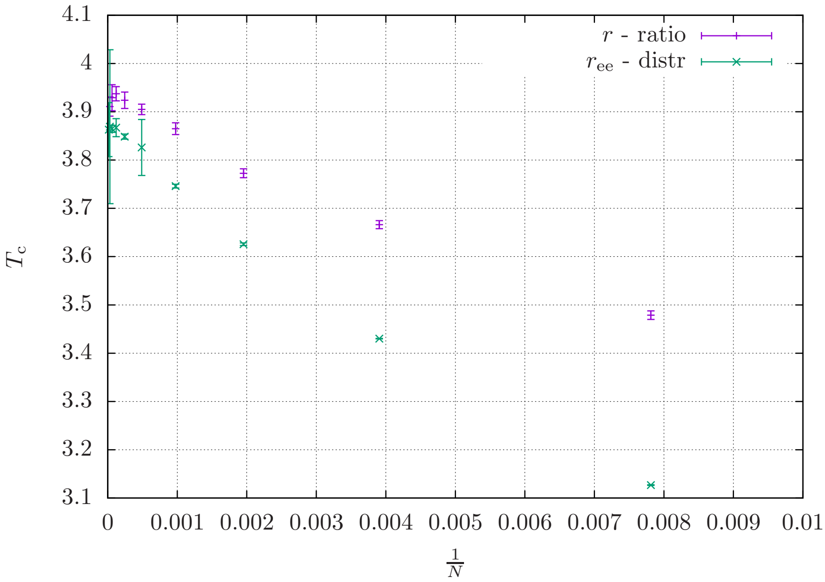

concluding remarks

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concluding remarks

- Binary trees help a lot.
- Metropolis works great with imprecise ΔE.
- Single update now has complexity $\mathcal{O}(N)$.

Thanks for your attention