

Efficiencies of joint non-local update moves in Monte Carlo simulations of coarse-grained polymers

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ARTICLE INFO

Article history:

Received 5 July 2017

Received in revised form 19 October 2017

Accepted 25 October 2017

Available online 6 December 2017

Keywords:

Polymers

Monte Carlo simulation

Efficiency

Autocorrelation time

Acceptance ratio method

ABSTRACT

In this study four update methods are compared in their performance in a Monte Carlo simulation of polymers in continuum space. The efficiencies of the update methods and combinations thereof are compared with the aid of the autocorrelation time with a fixed (optimal) acceptance ratio. Results are obtained for polymer lengths $N = 14, 28$ and 42 and temperatures below, at and above the collapse transition. In terms of autocorrelation, the optimal acceptance ratio is approximately 0.4 . Furthermore, an overview of the step sizes of the update methods that correspond to this optimal acceptance ratio is given. This shall serve as a guide for future studies that rely on efficient computer simulations.

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1. Introduction

The Monte Carlo method [1], and in particular the Metropolis algorithm [2], is a powerful yet simple tool for a wide range of applications. Therefore, it is of common interest to adjust the simulation parameters such that the highest efficiency possible is achieved. In particular, the size of the update step is of crucial importance, because it determines how a simulation proceeds through the state space of a given (physical) system. This can also be expressed as an acceptance ratio: A small update step yields a high acceptance ratio, whereas a large update step lowers the chance of accepting an update move.

Due to a lack of better knowledge, choosing an optimal acceptance ratio is often done heuristically by simply adjusting it to 0.5 [3]. In the past, a universal optimal acceptance ratio of approximately 0.234 has been proposed for Monte Carlo sampling of models with a large number of degrees of freedom [4,5]. However, the “myth” [6] of this approach rooted in mathematical statistics [7,8] was later debunked, and it was shown that the result is not necessarily applicable in the practical implementation of computer simulations in statistical physics, where the optimal acceptance ratio depends crucially on the dimensionality of the problem, the observable examined, as well as on the (local or global) update scheme implemented [9]. Additionally, the occasionally discussed “dynamic” optimization of the acceptance ratio during the actual simulation can have some pitfalls due to the violation of detailed

balance and lead to a systematic bias [10], if not done with great care [11].

Often it may be useful to implement a combination of local and global (or at least non-local) update schemes, in order to ensure the proper sampling of narrow energy minima, yet still be able to reach systemic distant states. Hence, the question of what acceptance ratio is *universally* optimal seems to remain largely unanswerable. Here we give an overview of how to optimally adjust some of the frequently used update schemes in the area of statistical polymer simulations.

The rest of the paper is structured as follows: We define the polymer model studied here in Section 2. The used update schemes, the acceptance ratio method and computational details are described in Section 3. In Section 4 we present our findings, which we summarize in Section 5.

2. Model

We used a simple bead–stick model, where the polymer is reduced to its monomers, represented by ‘beads’, and its bonds, represented by ‘sticks’. The bonds connecting the monomers are not permitted to change their length. The position vectors \mathbf{r}_i of the monomers point to the centre of the beads. The bonded neighbours all have a distance of unit length,

$$|\mathbf{r}_{i+1} - \mathbf{r}_i| \equiv 1 \quad \forall i = 1, \dots, N - 1. \quad (1)$$

The potential energy E of the system consists of an excluded-volume effect, a Van der Waals attraction, and an effect in which a

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bending of the polymer is penalized. These are described by a 12–6 Lennard-Jones potential and a cosine potential, respectively, i.e.,

$$E = E_{\text{LJ}} + E_{\text{bend}}. \quad (2)$$

The Lennard-Jones potential

$$E_{\text{LJ}} = 4\epsilon \sum_{i=1}^{N-2} \sum_{j=i+1}^N \left[\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^6 \right] \quad (3)$$

is described in terms of the distances r_{ij} between two non-bonded monomers i and j , where at a distance of $r_{ij}^{\text{min}} = \sqrt[6]{2}\sigma \approx 1.122\sigma$ the potential has its minimum. The potential parameters σ and ϵ describe coarse-grained polymer properties of microscopic length scale, which, however, are not of interest here in detail. Throughout this study we set $\sigma = \epsilon = 1$, which means that energies are measured in units of ϵ and distances in units of σ .

The cosine potential

$$E_{\text{bend}} = \kappa \sum_{i=1}^{N-2} (1 - \cos \vartheta_i), \quad (4)$$

with ϑ_i denoting the angle between adjacent bonds, penalizes the bending of the polymers, i.e., those conformations where the polymer is rather stretched out are favoured. In this study we set $\kappa = 0.25$.

2.1. Efficiency measure

To compare the efficiencies of the different update methods, we chose the integrated autocorrelation time $\tau_{\text{int},\mathcal{O}}$ of an observable \mathcal{O} of the system [3]. In particular the potential energy E and the squared radius of gyration R_{gyr}^2 were chosen here, as these two give information about intrinsic as well as structural details of the polymer. The squared radius of gyration is defined as

$$R_{\text{gyr}}^2 = \frac{1}{N} \sum_{i=1}^N (\mathbf{r}_i - \mathbf{r}_{\text{mean}})^2, \quad (5)$$

with \mathbf{r}_i being the positional vector of the i th monomer and $\mathbf{r}_{\text{mean}} = \frac{1}{N} \sum_{i=1}^N \mathbf{r}_i$ the centre of mass. The computation of the integrated autocorrelation time follows [12,13], where

$$\tau_{\text{int},\mathcal{O}} = \frac{1}{2} + \sum_{t=1}^{t_{\text{max}}} \Gamma_{\mathcal{O}}(t) / \Gamma_{\mathcal{O}}(0). \quad (6)$$

The autocorrelation function $\Gamma(t)$ describes the correlations of some observable \mathcal{O} over the recorded time series,

$$\Gamma_{\mathcal{O}}(t) = \langle (\mathcal{O}_i - \langle \mathcal{O} \rangle)(\mathcal{O}_{i+t} - \langle \mathcal{O} \rangle) \rangle. \quad (7)$$

To save computation time in the determination of $\tau_{\text{int},\mathcal{O}}$ it is useful to define an optimal termination point $t_{\text{max}} \rightarrow t_{\text{opt}}$ for the summation in Eq. (6). The point t_{opt} was chosen such that after this point only terms much smaller than $\tau_{\text{int},\mathcal{O}}$ would be summed, contributing virtually nothing to $\tau_{\text{int},\mathcal{O}}$.

To distinguish different phases of polymers, a common practice is to study physical observables \mathcal{O} and their fluctuations $\frac{d}{dT} \langle \mathcal{O} \rangle = \beta^2 (\langle \mathcal{O} E \rangle - \langle \mathcal{O} \rangle \langle E \rangle)$. Typical examples are the derivatives of the energy E or the squared radius of gyration R_{gyr}^2 , depicted in Fig. 1. Recently it was demonstrated that the autocorrelation time can function as an indicator for pseudo-phase transitions of polymers [14]. The autocorrelation time diverges near the freezing transition and peaks near the collapse transition temperature. However, in the latter study a bead-spring polymer model with only local update moves was used, namely a single shift of the monomers which differs from our local crankshaft move in a bead-stick model. Also the dependence of $\tau_{\text{int},\mathcal{O}}$ on the acceptance ratio was not considered.

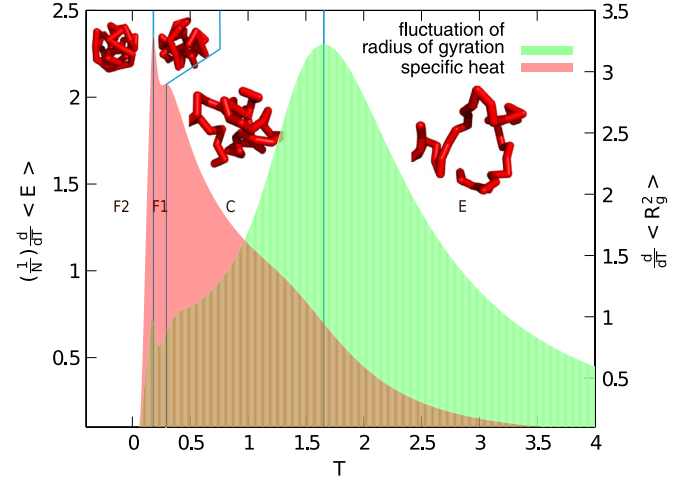


Fig. 1. Phase diagram of a polymer in the bead-stick model of length $N = 28$. The peaks of the derivatives of the energy (the specific heat) and squared radius of gyration indicate transitional changes. The polymer conformations change along temperature from frozen (F), via globule-like compact (C) to elongated (E) states.

3. Simulation setup

3.1. Update methods

We implemented several different simulation programs, where each one uses one or a combination of two update methods. These are the *pivot* and the *spherical* update methods, either combined with the *crankshaft* or the *double-bridge* method. Also, the combination crankshaft/double-bridge move was implemented. In one Monte Carlo sweep the respective computationally costlier method is used only once after updating N times with the less costly method. The most costly of the methods is the double-bridge update, whereas the crankshaft is the least costly. In the following these update methods will be described briefly. For a more comprehensive overview with references to the original literature, see [15].

3.1.1. Crankshaft

The crankshaft update method is the only one that only changes the coordinates of a single monomer. Even though the energy change is also far-reaching, this update method has thus a local nature to it. The crankshaft move picks a random monomer. The two neighbouring and bonded monomers build an axis about which it is then rotated by an angle in the range $[-\omega_{\text{max}}, \omega_{\text{max}})$, with $\omega_{\text{max}} \leq \pi$ (cf. Fig. 2). Note that the two termini can never be picked, because they do not have two bonding neighbours. Thus, not all possible conformations can be reached using solely this update move, i.e., it is nonergodic on itself. This can be fixed, however, by combining it with any of the following non-local update methods.

3.1.2. Pivot

A widely used update method is the pivot move [16,17]. It randomly chooses one of the monomers and lays an axis with random direction through its centre. The whole end tail of the polymer is then rotated about this axis by a randomly chosen angle in $[-\varphi_{\text{max}}, \varphi_{\text{max}})$ with $\varphi_{\text{max}} \leq \pi$ (see Fig. 2). This means that normally all but one pair of bonds keep the same angle relations. It is possible that the orientation of the axis is the same as one of the two bonds at the chosen monomer. In that case the end tail is rather only twisted in a torsion-like movement and it is possible that none of the bond angles change. The pivot update method satisfies detailed balance.

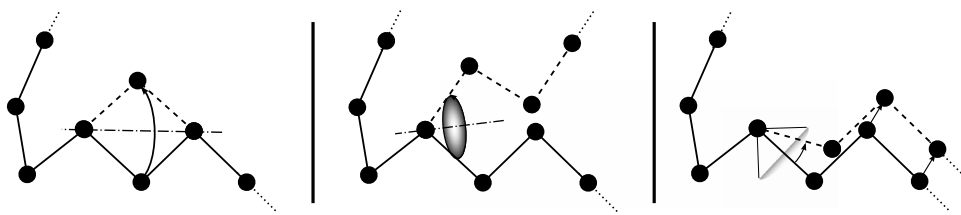


Fig. 2. Illustrations of the crankshaft (left), pivot (centre) and spherical (right) update method. The proposed new conformations are drawn with thick dotted lines while the dashed–dotted lines indicate the rotation axis. See text in Sections 3.1.1–3.1.3 for more information.

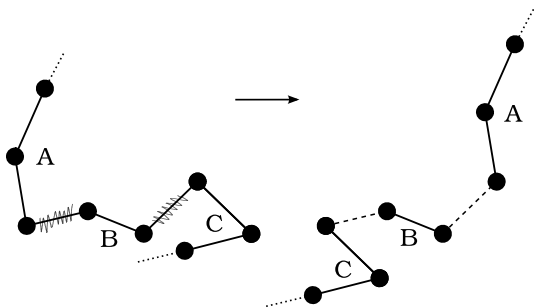


Fig. 3. The double-bridge move with fixed monomer distances. Two bonds are selected randomly and erased (criss–cross lines). The inner part B is shifted and reconnected to the dangling end C. The dangling end A is then shifted and reconnected to the inner part B. The dangling ends A and C have then swapped their bonds to the inner part B.

3.1.3. Spherical

An update proposal similar to the pivot move is the spherical update method [18]. One of the $N - 1$ bonds is picked randomly with all bonds having equal probability. This k th bond is rotated and all following bonds $> k$ (and monomers) are translated. The orientation of these following bonds is not changed. This is illustrated in Fig. 2.

Due to the self-avoidance of the polymer, the acceptance probabilities should not be too small. This can be achieved by restricting the opening angle to a value $2\vartheta_{\max}$. Graphically represented this means that the bond can only move on a spherical cap. For this, two angles have to be evaluated: The bonding angle ϑ and the rotation angle φ , where the correct intervals to choose from are $[0, \vartheta_{\max}]$ with $\vartheta_{\max} \leq \pi$ and $[0, 2\pi)$, respectively. Because every point on this spherical cap can be reached with equal probability, detailed balance is again satisfied.

3.1.4. Double bridge

We introduce here a modified version of the (intramolecular) end-bridging move [19], which we call the double-bridge move. The basic idea of this update method is to exchange two bonds of the polymer. This is done by picking two bonds randomly and removing them. This gives three parts: two dangling ends and one inner part. The latter is shifted such that the monomer of the one dangling end is now connected to the monomer of the inner part, where the other dangling end was connected. The remaining dangling end is now also shifted such that it is connected to the inner monomer, where the first dangling end was connected. This is depicted in Fig. 3. In contrast to the original formulation [19] and to fit our polymer model the new conformations are chosen such that all bonds are kept at a fixed unity length.

3.2. Acceptance ratio method

The acceptance ratio method (ARM) [20] provides a tool to set the probability of accepting an update move in an initial, relatively

short auxiliary run. This probability is defined as the ratio of the number of accepted updates to the total number of updates. The average acceptance probability p_a has an approximately exponential behaviour

$$p_a = \exp(-\delta/\delta_0), \quad (8)$$

where δ generally denotes a step size of an update move (e.g., the rotation angle) and δ_0 is some constant. If an optimal or desired acceptance probability p_a^{opt} is introduced a new step size can be calculated at every update according to

$$\delta_{\text{new}} = \delta_{\text{old}} \frac{\ln(p_a^{\text{opt}})}{\ln(p_a)}. \quad (9)$$

This is tuned in the initial auxiliary run (which due to the fluctuating step size does not satisfy detailed balance). Depending on the update method the respective update range is adjusted such that the desired (optimal) acceptance probability is approximately reached on average. The thus determined optimal step size δ^{opt} is then kept fixed in the actual simulation consisting of a thermalization phase and the data production run.

3.3. Computational details

We performed numerous Monte Carlo simulations of single homopolymers of lengths $N = 14, 28$ and 42 at different temperatures by using the Metropolis update algorithm. For each run the time series of the energy E as well as the squared radius of gyration R_{gyr}^2 were recorded. A measurement was made after every sweep, with a total number of 2 000 000 sweeps for each run. A sweep consists of N update moves or $N + 1$ update moves if two combined moves were used. In the latter, the computationally costlier move was used only once per sweep after updating N times with the less expensive move. All update methods, described in Section 3.1, were compared in their performance.

The simulation temperatures were chosen such that information was gathered below, at and above the critical temperature T_c^θ of the collapse transition, which will be referred to as T_c throughout this study. The estimates for T_c were taken from one of our previous studies [21] and the other temperatures should be well below/above T_c . The critical temperatures for polymer lengths $N = 14, 28$ and 42 were assumed to be $T_c \approx 1.0758, 1.6560$ and 2.0560 , respectively. Below T_c the polymer is in a rather globular state, while above T_c it is in an elongated or expanded state. In a globular state the monomers are closer together, making it difficult for the polymer to ‘untangle’ and thus reaching very different states. These problems can be overcome by using update moves that are non-local, e.g., cutting up some bonds of the polymer and pasting them together again differently. In the low-temperature range the polymer undergoes a first-order like freezing transition at $T_f \approx 0.3$ [22]. Below T_f the polymer is in a very compact state, making it difficult to find accepted new conformations at one update, and thus the autocorrelation time will diverge. In this study the first-order-like freezing transition was not looked at intensively, because this is virtually impossible using the standard Metropolis algorithm.

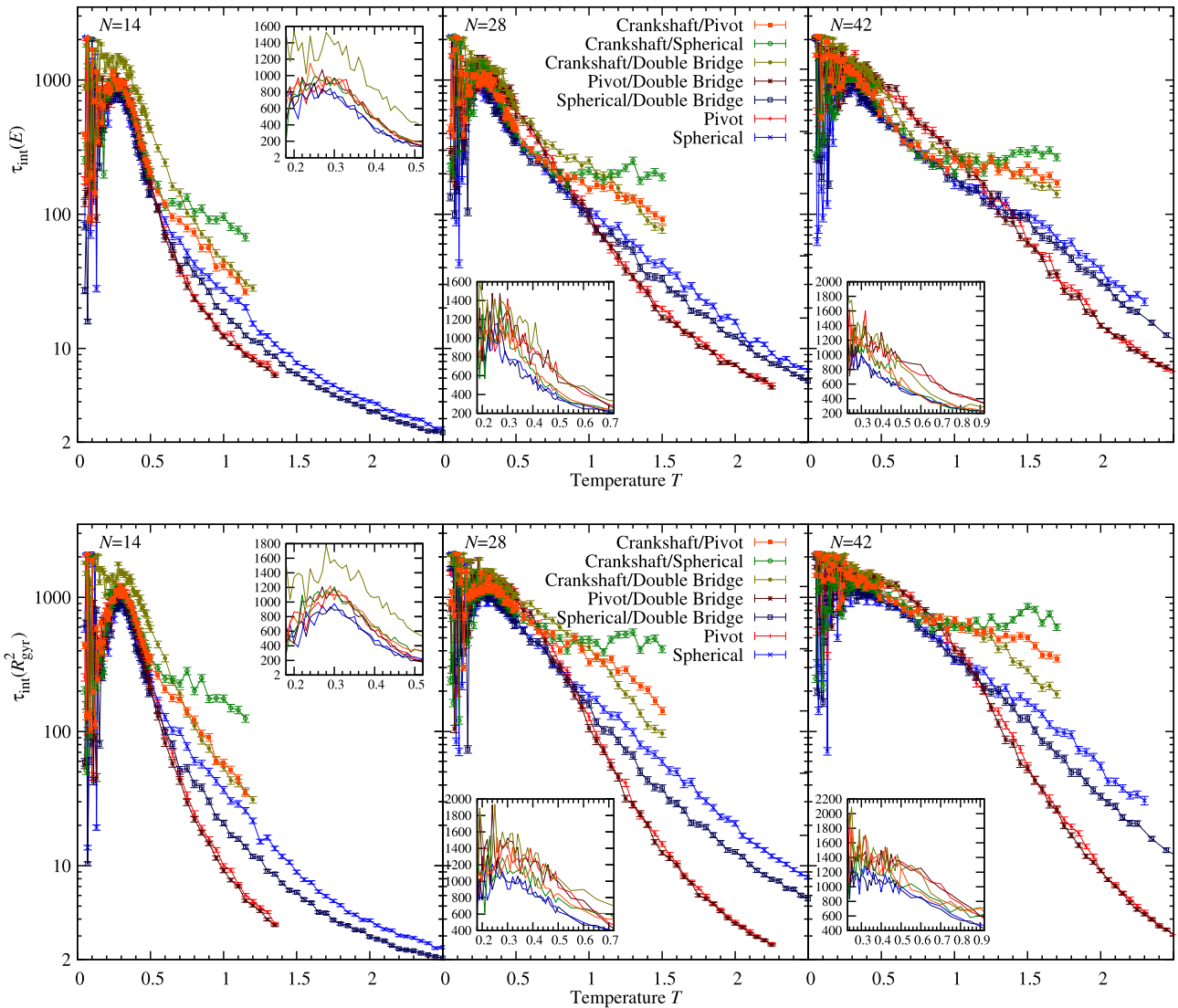


Fig. 4. Autocorrelation times of the energy E (top) and the squared radius of gyration R_{gyr}^2 (bottom) versus temperature on a log-linear scale for the various update methods and polymer lengths. The insets feature the low-temperature range on a linear scale, which gives a better impression of differences between the update-method combinations.

Of course there are also other, more efficient Monte Carlo methods besides the Metropolis algorithm, e.g., the parallel tempering [23,24], multicanonical [25], or the Wang–Landau method [26], of which the latter two can also overcome the problem of (super)critical slowing down at a first-order-like transition [27,28]. The reason why the Metropolis method was chosen here over others is that it was not of interest to carry out highly efficient simulations, but rather to compare the efficiency of update moves. Also, more advanced methods are generally harder to implement and handle. The Metropolis algorithm gives the opportunity to see how the update moves perform in a ‘standard’ Monte Carlo simulation which is widely applicable.

4. Results

4.1. Indications of phase transitions

To better understand how the update-method combinations perform, we show in Fig. 4 the autocorrelation times with respect to the energetic quantity (energy E , top) and the structural quantity (squared radius of gyration R_{gyr}^2 , bottom) over the temperature

range from 0 to 2.5. We observe a strong variation of the autocorrelation times with temperature and also among the different update schemes especially close to the continuous collapse transition around $T = 1.0 - 2.0$. Note that in order to show this behaviour over a broad range we have chosen in Fig. 4 and the following figures a logarithmic scale on the y-axis which, however, veils this strong variation somewhat. In the following we will discuss these figures and compare the various combinations of update methods. We set the acceptance ratio to $p_a = 0.4$. Later on we will show, that this is an (approximately) optimal value in terms of data correlation.

All three chain lengths show a similar behaviour. The most prominent feature are the peaks in the autocorrelation time near the freezing temperature of $T_f \approx 0.3$. Due to the first-order-like behaviour of this transition point the chance of the polymer going from more globule-like to frozen conformations is highly suppressed. This is the case for both, the local and non-local update moves. The non-local moves would change large parts of the conformation but the update proposals are less often accepted the more the monomers are closely packed. The (local) crankshaft move only changes very little in the conformations and the update

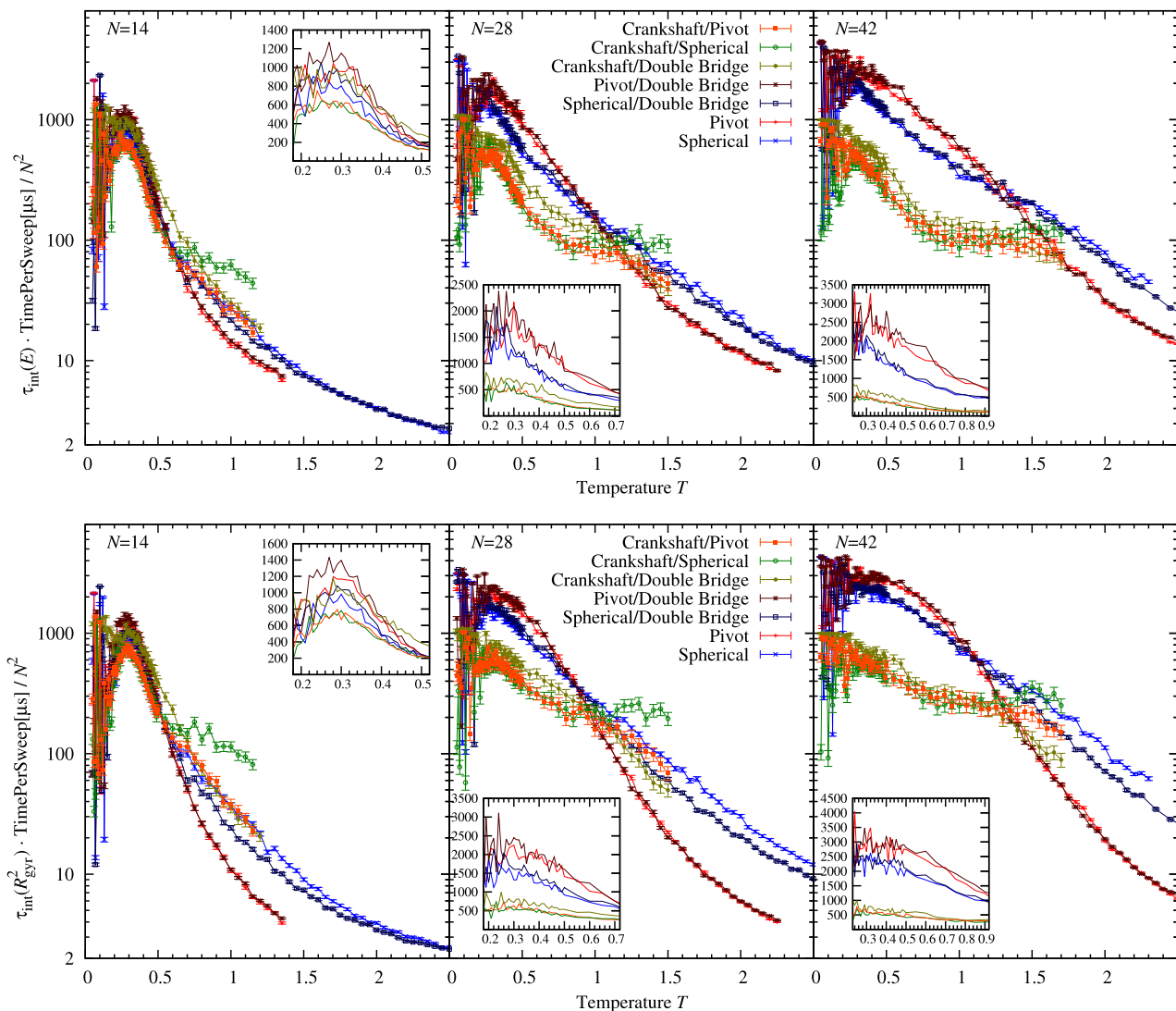


Fig. 5. Real-time autocorrelations per sweep (in μs on a standard PC core) of the energy E (top) and the squared radius of gyration R_{gyr}^2 (bottom) versus temperature on a log-linear scale for the various update methods and polymer lengths. The values are normalized by N^2 for a better fitting of the curves onto the y-axis. The insets focus on the low-temperature data on a linear scale, which gives a better impression of differences between the update-method combinations.

proposals should thus be accepted somewhat more often. However, overcoming the energetic barrier at this point with small structural changes is still highly unlikely.

For temperatures below T_f the values of the autocorrelation time vary across a large range. In this region the Metropolis algorithm cannot produce any reliable data without inefficiently raising the number of sweeps. Above the freezing temperature T_f the autocorrelation times of all non-local update combinations decrease continuously along the temperature range. This is expected, because higher temperatures allow for greater update ranges and thus for greater energetic and structural changes between two consecutive data points. The non-local update combinations show no peak near the collapse transition T_c . The transition here is second-order-like and the polymer continuously expands from globule-like to elongated conformations. Only the combinations with the crankshaft move show a slowing down when approaching the collapse transition point T_c . This effect becomes even clearer for longer chains, as in [14]. The autocorrelation times increase with increasing length N , but also the peak indicating T_c becomes more pronounced. This indicates once more that non-local update methods can cope with the problems arising from pseudo-phase transitions much better than local update methods.

Comparing the autocorrelation times of the pivot and spherical update methods, no fixed relation between the two is evident. The spherical update move is temporally less correlated at low temperatures, while the correlations are greater for high temperatures. This indicates that there must be a point T_\times in the temperature where the efficiencies of the two update methods cross each other. The data also suggest that this crossing point T_\times is a function of the length N of the polymer and seems to decrease for smaller chain lengths. In both cases the combination with the double-bridge move yields generally similar autocorrelation times. For the pivot update, the two curves almost fall on top of each other, whereas the combination of the spherical update with the double-bridge move reduces the autocorrelation times.

To better understand the real-time efficiency of the various updates, we show the autocorrelation times multiplied by the time per sweep of the various update combinations in Fig. 5. In one sweep the positions of all N monomers should be changed at least once on average. The representation in Fig. 5 gives therefore a better impression of how long it takes with a certain combination of update methods to reach an independent conformation. The non-local updates vary very little qualitatively from the pure autocorrelation times, while the local move (i.e., the crankshaft move)

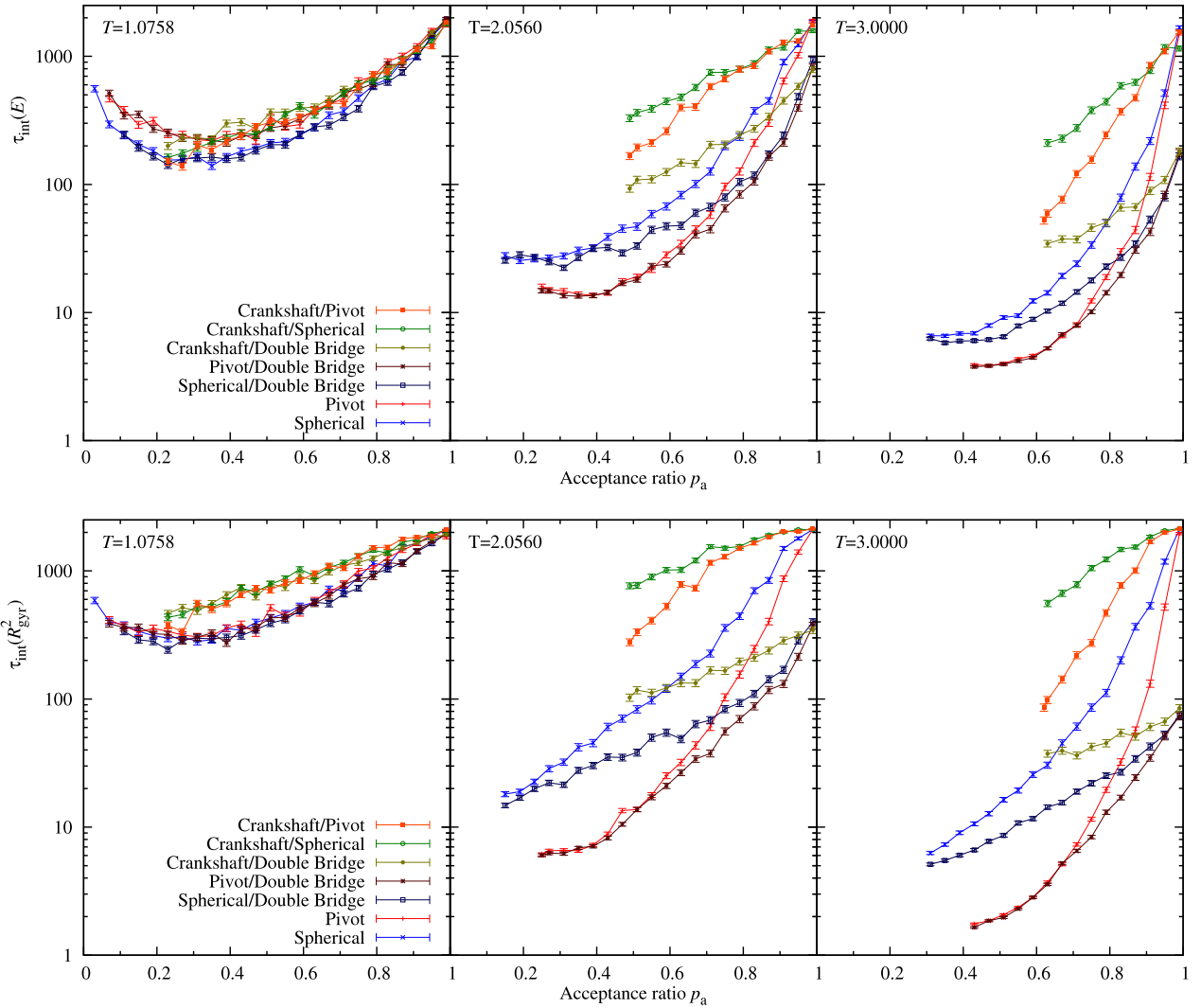


Fig. 6. Dependence of autocorrelation times of energy E (top) and squared radius of gyration R_{gyr}^2 (bottom) on the acceptance ratio p_a for the various update methods for a polymer of length $N = 42$, where $T_c \approx 2$. The optimal acceptance ratio turns out to be quite universally around $p_a^{\text{opt}} \approx 0.4$.

gains in efficiency for longer chains. Because of its local nature, the computational costs of performing this move once are very low. Thus, this sweep can be used relatively more often per sweep than the non-local moves without a large increase in computation time.

4.2. Optimal acceptance ratios

One central purpose of this study was to discover an optimal acceptance ratio. For this we evaluated the autocorrelation times over the acceptance ratios for a polymer of length $N = 42$, depicted in Fig. 6. No sharp minimum can be found in any of the curves. Rather, the curves are nearly ‘flat’ over a broad range of the acceptance ratio around the empirically found value $p_a^{\text{opt}} \approx 0.4$. Low temperatures are particularly insensitive to a change in the acceptance ratio. At higher temperatures though, it is clear that adjustments in the acceptance ratio can be important. In this respect the update moves do not differ qualitatively, but certainly quantitatively, given that the same set of parameters was chosen in the simulation runs. Adding the double-bridge method to any other update method leads to a gain of uncorrelated data for very high acceptance ratios. At the optimal level of acceptance ratio it has very little effect though, because there it is accepted very seldom relative to the other update method used.

The curves are truncated below a certain value of the acceptance ratio. This effect increases at higher temperatures. This may be caused by the interplay between the algorithm to determine the acceptance ratio, the underlying Monte Carlo algorithm, and the definition of the physical system. For instance, for small acceptance ratios the opening angle of the spherical update method increases until $\vartheta_{\text{max}} \approx \pi$ is reached and no angle can be found to push the acceptance ratio below some threshold. This, of course, applies analogously also to the other update schemes. Above some temperature, but certainly above T_c , the polymer tends to be in the elongated phase [22]. Most monomer–monomer distances r_{ij} in this phase are quite large and most values of the pairwise Lennard-Jones potentials are $\lesssim 0$. For the pivot and spherical update methods a rotation about a large angle would drop the monomer–monomer distances into the valley of the Lennard-Jones potential, meaning a great reduction of the energy. Virtually all those moves would be accepted by the Monte Carlo algorithm, because the Boltzmann probabilities $\exp(-\beta \Delta E)$ would tend to values > 1 . Large temperatures strengthen the likelihood of an elongated polymer and thus the likelihood of this happening. The spherical update move can still reach lower thresholds because only very few monomers are moved closer together. The crankshaft update method reaches the highest acceptance ratios. It is limited in this way, because the

Table 1

The update angles of the different update moves at the approximately optimal acceptance ratio $p_a \approx 0.4$ for the three polymer lengths at different temperatures. Where the algorithm could not reach an acceptance probability close to 0.4 the entry is left blank. This corresponds to a maximal update angle. It is important to note that the acceptance probability for these cases is higher than 0.4.

	N	$T =$	0.5500	1.0758	1.6560	2.0560	2.4000	3.0000
Crankshaft	42	$p_a =$	0.408	0.393	0.398	–	–	–
		$\omega_{\max} =$	0.570	1.381	3.126	–	–	–
	28	$p_a =$	0.433	0.393	–	–	–	–
		$\omega_{\max} =$	0.580	1.646	–	–	–	–
	14	$p_a =$	0.401	0.396	–	–	–	–
		$\omega_{\max} =$	0.827	2.687	–	–	–	–
Pivot	42	$p_a =$	0.392	0.391	0.406	0.388	0.395	0.432
		$\varphi_{\max} =$	0.101	0.201	0.440	1.128	2.005	$\approx \pi$
	28	$p_a =$	0.407	0.388	0.401	0.390	–	–
		$\varphi_{\max} =$	0.148	0.356	1.074	2.514	–	–
	14	$p_a =$	0.395	0.395	–	–	–	–
		$\varphi_{\max} =$	0.376	1.472	–	–	–	–
Spherical	42	$p_a =$	0.431	0.380	0.387	0.383	0.391	0.389
		$\vartheta_{\max} =$	0.081	0.166	0.342	0.616	0.915	1.538
	28	$p_a =$	0.404	0.400	0.384	0.388	0.387	0.392
		$\vartheta_{\max} =$	0.106	0.229	0.567	0.970	1.382	1.977
	14	$p_a =$	0.383	0.391	0.391	0.391	0.392	–
		$\vartheta_{\max} =$	0.196	0.529	1.359	1.992	2.539	–

energy change is even smaller per update and is thus accepted even more often.

In Table 1 we present the update ranges of the crankshaft, pivot and spherical update moves that lead to an approximate acceptance ratio of 0.4. They are shown for the polymer lengths $N = 14, 28$ and 42. Due to the relatively low number of updates in the auxiliary run the desired acceptance ratios of 0.4 are met only roughly, which, however, is not of crucial importance, as discussed above. The overview given in Table 1 will serve as a rough guide for future studies that need an idea of how to set an update range to more efficiently sample the phase space, and thus minimize computational costs.

5. Summary and conclusion

We analysed bead–stick polymers of different chain lengths $N = 14, 28$ and 42 in Monte Carlo simulations employing the Metropolis algorithm. We implemented various update methods and compared their various combinations by means of the statistical autocorrelation time of the energy E and the squared radius of gyration R_{gyr}^2 .

With this we found some indications that allow us to identify phase transitions. The autocorrelation times show clear peaks for all combinations of update methods at the freezing transition at low temperatures which is first-order-like. Further, the combinations including a local update method (i.e., crankshaft) show peaks in the autocorrelation times at the second-order-like collapse transition at higher temperature. This shows that non-local update methods can overcome energetic barriers far more rapidly. However, the real-time autocorrelation times reveal that employing a combination incorporating a local update method can have an advantage in the low-temperature regime, in the sense of efficiency and total run time of a simulation program.

Furthermore, we sought optimal acceptance ratios for the combinations of update methods below, at and above the critical temperature of a polymer of length $N = 14, 28$ and 42. Our results suggest that the most efficient simulation run can be accomplished with the acceptance probability tuned to $p_a^{\text{opt}} \approx 0.4$. An overview is given on how to set the update ranges to accomplish this optimal acceptance probability.

The methodology discussed here could be also applied to other (polymer) models. As described in the Introduction, the existence

of a universal optimal acceptance ratio seems to be implausible. It would thus be interesting to determine optimal acceptance ratios also for other (polymer) models. To this end, several simulations are needed, where each run comprises an auxiliary and data production part. In each auxiliary run the acceptance ratio is systematically adjusted to different values, and subsequently the autocorrelation time is determined. The minimal autocorrelation time of all runs then yields the most efficient setting.

Acknowledgements

This work was in part funded by the European Union and the Free State of Saxony via the “Sächsische AufbauBank” and by the Deutsche Forschungsgemeinschaft (DFG) through SFB/TRR 102 (project B04) and Grant No. JA 483/33-1. Additional support was obtained by the Leipzig Graduate School of Natural Sciences “BuildMoNa” and the Deutsch-Französische Hochschule (DFH-UFA) through the Doctoral College “IL⁴” under Grant No. CDFA-02-07.

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