Parallel Tempering Algorithm for
Conformational Studies of Biological Molecules

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ABSTRACT

The effectiveness of a new algorithm, parallel tempering, is studied for numerical simulations of biological molecules. These molecules suffer from a rough energy landscape. The resulting slowing down in numerical simulations is overcome by the new method. This is demonstrated by performing simulations with high statistics for one of the simplest peptides, Met-enkephalin. The numerical effectiveness of the new technique was found to be much better than traditional methods and is comparable to sophisticated methods like generalized ensemble techniques.

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1. INTRODUCTION

One way of investigating biological molecules is by means of computer experiments. However, such numerical simulations can be notoriously difficult when the molecule is described by “realistic” energy functions where interactions between all atoms are taken into account. For a large class of molecules (for instance, peptides or proteins) the various competing interactions yield to frustration and a rough energy landscape. Hence, at low temperatures simulations based on canonical Monte Carlo [1] or molecular dynamics techniques will get trapped in one of the multitude of local minima separated by high energy barriers. Only small parts of conformational space are sampled and physical quantities cannot be calculated accurately. One way to overcome this difficulty is to perform a simulation in a so-called generalized ensemble, which is based on a non-Boltzmann probability distribution. Multicanonical algorithms [2] and simulated tempering [3] are prominent examples of such an approach which also includes the new ensemble introduced in Refs. [4, 5]. Application of these techniques to the protein folding problem was first addressed in Ref. [6] and over the last few years the generalized ensemble approach has become an often used method for simulation of biological molecules and other complex systems [6]-[10]. A numerical comparison of different generalized ensemble algorithms can be found in Ref. [11].

Another way to alleviate the multiple minima problem is to look for improved updates of configurations in the numerical simulation. The cluster algorithm [12] is an example of global updates that enhances thermalization and has been very successful in spin systems. However, for most other systems with frustration, no such updates are known. Here, a new algorithm, parallel tempering, is described which introduces improved updates by means of constructing a special generalized ensemble. It is shown that the new method can be successfully applied to the simulation of molecules with complex energy landscape. By simulating one of the simplest peptides, Met-enkephalin, with high statistics its effectiveness is compared with canonical simulations and sophisticated generalized ensemble techniques like the multicanonical algorithm [2]. Both Monte Carlo and molecular dynamics versions of parallel tempering are studied and it is shown that the new method can be combined with other generalized ensemble techniques.
2. METHODS:
Let me start by briefly summarizing the parallel tempering algorithm which was originally introduced in the context of spin glass simulations [13]. Similar ideas were also proposed in Refs. [14, 15].

In a regular canonical simulation, a configuration of one copy of the molecule under consideration is updated by Monte Carlo [1] or molecular dynamics. Each configuration $C$ is characterized by a set of (generalized) coordinates and is assigned a Boltzmann weight

$$w_B(\beta, C) = e^{-\beta E(C)},$$

(1)

where we have introduced the inverse temperature $\beta = 1/k_B T$ with $k_B$ the Boltzmann constant. The so realized Markov - chain yields to a canonical distribution at one temperature $T$.

On the other hand, in parallel tempering one considers an artificial system build up of $N$ non–interacting copies of the molecule, each at a different temperature $T_i$. A state of the artificial system is specified by $C = \{C_1, C_2, ..., C_N\}$, where each $C_i$ is a set of (generalized) coordinates which describes the configuration of the $i$–th copy. Since the $N$ copies of the molecule are not interacting with each other, one can assign to a state $C$ of the compound system a weight:

$$w_{PT}(C) = e^{-\sum_i^N \beta_i E(C_i)} = \prod_i^N w_B(\beta_i, E(C_i)).$$

(2)

Without lack of generality one can assume $\beta_1 < \beta_2 < ... < \beta_N$. For a numerical simulation of the artificial system one has to construct a Markov-chain which will ensure that the corresponding equilibrium distribution will be approached. Such a Markov-chain can be realized with the following two sets of moves [13]:

1. Standard MC moves which effect only one, say the $i$-th, copy. These moves are called local updates because they change only one coordinate of the configuration in solely one copy. Since the copies are non-interacting it follows from Eq. 2 that the transition probability depends only on the change in potential energy of the $i$–th
copy. Hence, such local MC moves are accepted or rejected according to the usual Metropolis criterion [1] with probability:

\[ w_{PT}(C^{\text{old}} \rightarrow C^{\text{new}}) = w_B(C^{\text{old}}_i \rightarrow C^{\text{new}}_i) = \min(1, e^{-\beta_i \Delta_i E}) \]  

where \( \Delta_i E \) is defined as \( \Delta_i E = E(C^{\text{new}}_i) - E(C^{\text{old}}_i) \).

2. Exchange of conformations between two copies \( i \) and \( j = i + 1 \):

\[ C^{\text{new}}_i = C^{\text{old}}_j \]  
\[ C^{\text{new}}_j = C^{\text{old}}_i \]  

Such exchange is a global update in the sense that for the \( i \)-th copy the whole configuration changes (and the same for the \( j \)-th copy). Since this move introduces configurational changes in two copies of the molecule, it follows from Eq. 2 that the exchange is accepted or rejected according to the Metropolis criterion with probability:

\[ w(C^{\text{old}} \rightarrow C^{\text{new}}) = \min(1, e^{-(\beta_j E(C_j) - \beta_i E(C_i)) + \beta_i E(C_i) + \beta_j E(C_j)}) \]  
\[ = \min(1, e^{(\beta_j - \beta_i)(E(C_j) - E(C_i))}) \]  
\[ = \min(1, e^{\Delta \beta \Delta E}) \]  
\[ = \min(1, e^{\Delta}) \]  

where \( \Delta = \Delta \beta \Delta E \), \( \Delta \beta = \beta_j - \beta_i \) and \( \Delta E = E(C_j) - E(C_i) \). While it is not necessary to restrict the exchange to pairs of copies associated with neighboring inverse temperatures \( \beta_i \) and \( \beta_{i+1} \), this choice will be optimal, since the acceptance ratio will decrease exponentially with the difference \( \Delta \beta = \beta_j - \beta_i \).

It is interesting to observe that from the view point of the artificial compound system the above set of moves realizes a generalized ensemble simulation with (non-canonical) weights given by Eq. 2. However, one can also choose the point of view that parallel tempering realizes for each of the copies a canonical simulation at corresponding temperature \( T_i \). The exchange of conformations is then a new and improved update which decreases the correlation between configurations (for each copy or temperature) and hence increases
thermalization of the *canonical* simulation for each copy (temperature). This guarantees in turn that each of the copies will approach its equilibrium distribution (i.e. the Boltzmann distribution at temperature $T_i$) much faster than without that global update. From this point of view it is also obvious that expectation values of a physical quantity $A$ are calculated as usual according to:

$$<A>_{T_i} = \frac{1}{MES} \sum_k A(C_i(k)),$$

where $MES$ is the number of measurements taken for the $i$-th copy. Using re-weighting techniques \[16\] it is also possible to calculate expectation values for intermediate inverse temperatures $\beta$ with $\beta_i < \beta < \beta_{i+1}$.

While parallel tempering is not restricted to the use on parallel computers, it is obvious that the new technique is well suited for them. A parallel implementation can be easily realized by setting each of the copies on a different node. On each node the molecule is simulated simultaneously and independent from the other nodes with Boltzmann weights $e^{-\beta_i E(C_i)}$ by common Monte Carlo techniques. After a few MC steps pairs of configurations $C_i$ and $C_j$ are exchanged between the nodes $i$ and $j$ with a probability given by Eq. 9.

While the exchange of conformations has to be done by a Monte Carlo procedure, it is not necessary to use Monte Carlo for the *local* updates of the conformations on each node. Instead one can also evaluate on each node for some time $\tau$ a molecular dynamics trajectory, using one of the common canonical molecular dynamics techniques, before an exchange of conformations between two nodes is tried. It is also possible to replace the exchange of configurations between different nodes by an exchange of temperatures between nodes. For a parallel implementation of the algorithm this has the advantage that less messages have to be passed between the different nodes (two temperature values instead of two sets of coordinates).

The main advantage of parallel tempering over generalized ensemble methods is that the weights are *a priori* known, since the weight for a state of the artificial system of non-interacting copies (see Eq. 2) is solely the product of the Boltzmann weights for each of the copies. However, to ensure that an exchange of either conformation or temperatures between two copies will happen with sufficient probability the differences in (inverse) temperatures $\Delta \beta$ in Eq. 9 have to be small. With $\beta_j = \beta_{i+1} = \beta_i + \Delta \beta$ and approximating
the energy $E(C_i) \ (E(C_{i+1}))$ by the thermal expectation value $< E >_{\beta_i} \ (< E >_{\beta_{i+1}})$ one can write the logarithm of probability $e^{-\Delta}$ of an exchange in Eq. 9 as

$$\Delta \approx (\Delta \beta)^2 \frac{d}{d\beta} < E > . \quad (11)$$

It is obvious from this equation that parallel tempering is not suitable for simulations of first order phase transitions, since in that case $< E >$ is not continuous at the critical temperature $T_c$ (and the distribution of energies $P(E)$ bimodal). For all other cases it follows from the above equation that an exchange of configurations between two copies will happen with sufficient probability, as long as $\Delta$ is of order of one. Since the average energy grows roughly proportional with the number of residues $N$, $\Delta \beta$ should be of order of $1/\sqrt{N}$ to satisfy that condition. Hence, the number of temperatures to simulate should also increase roughly proportional to $\sqrt{N}$ with the number of residues. However, the problem remains of finding the number and distribution of temperatures which guarantees optimal performance of the algorithm. The lowest temperature will depend on the molecule under consideration and physical quantities one is interested, but it will in general be a temperature where usual canonical simulations get trapped in local minima. In the present algorithm, escape from these minima is possible through the exchange of conformation between two copies associated with different temperatures. Hence, the highest temperature has to be chosen such that any energy barrier can be crossed at this temperature. In this way it is guaranteed that by the successive exchange of conformations between copies any energy barrier can be overcome and all of the replica will thermalize.

It is easy to combine parallel tempering with other generalized ensemble techniques, since the algorithm only requires that the copies are non interacting and therefore the weight of the compound system factorizable into a product of weights for each copy. Hence, one can generalize Eq. 2 to

$$w_{PT}(C) = \prod_{i=1}^{N} w_{GE}(f(C_i)) , \quad (12)$$

where $w_{GE}(f(C_i))$ is a generalized ensemble weight for the $i$-th copy. The modifications in the transition probabilities Eq. 3 and 8 which follow from this generalization are straightforward. Performing a parallel tempering simulation with generalized ensemble weights
for the copies will yield to corresponding non-canonical distributions. Hence, to calculate thermodynamic quantities at temperatures $T_i$ one has to use re-weighting techniques [16].

In the present article one examples of such a combination of parallel tempering with generalized ensemble techniques is studied. For this the ensemble of Refs. [4, 5] (which is closely related to Tsalis generalized mechanics formalism [17]) was chosen and to some of the copies the following weight

$$w_{GE}(E(\beta_i, C_i)) = \left(1 + \beta_i \frac{E(C_i) - E_0}{m}\right)^{-m}$$

(13)

was assigned. Here, $E_0$ is an estimate for the ground state energy of the molecule and $m$ a free parameter. Obviously, the new weight reduces in the low-energy region to the canonical Boltzmann weight $\exp(-\beta E)$ for $\frac{\beta(E-E_0)}{m} \ll 1$. On the other hand, high-energy regions are no longer exponentially suppressed but only according to a power law, which enhances excursions to high-energy regions. It is expected that the so-defined weights increase the probability of an exchange of configurations between copies.

3. RESULTS AND DISCUSSION

The effectiveness of the new simulation technique was tested for Met-enkephalin, one of the simplest peptides, which has become a often used model to examine new algorithms. Met-enkephalin has the amino-acid sequence Tyr-Gly-Gly-Phe-Met. The potential energy function $E_{tot}$ that was used is given by the sum of the electrostatic term $E_{es}$, 12-6 Lennard-Jones term $E_{vdW}$, and hydrogen-bond term $E_{hb}$ for all pairs of atoms in the peptide together with the torsion term $E_{tors}$ for all torsion angles:

$$E_{tot} = E_{es} + E_{vdW} + E_{hb} + E_{tors},$$

(14)

$$E_{es} = \sum_{(i,j)} \frac{332q_i q_j}{r_{ij}},$$

(15)

$$E_{vdW} = \sum_{(i,j)} \left( \frac{A_{ij}}{r_{ij}^{12}} - \frac{B_{ij}}{r_{ij}^{6}} \right),$$

(16)

$$E_{hb} = \sum_{(i,j)} \left( \frac{C_{ij}}{r_{ij}^{12}} - \frac{D_{ij}}{r_{ij}^{10}} \right),$$

(17)

$$E_{tors} = \sum_l U_l \left(1 \pm \cos(n_t \chi_l)\right),$$

(18)

where $r_{ij}$ is the distance between the atoms $i$ and $j$, and $\chi_l$ is the $l$-th torsion angle. The
parameters \((q_i, A_{ij}, B_{ij}, C_{ij}, D_{ij}, U_i\) and \(n_i)\) for the energy function were adopted from ECEPP/2.\(^{[18]}\) The computer code SMC\(^2\) was used. The peptide-bond dihedral angles \(\omega\) were fixed at the value \(180^\circ\) for simplicity, which leaves 19 angles \(\phi_i, \psi_i,\) and \(\chi_i\) as independent variables.

Parallel tempering simulations with 7 copies were performed. The corresponding temperatures were \(T_1 = 1000\) K, \(T_2 = 500\) K, \(T_3 = 330\) K, \(T_4 = 250\) K, \(T_5 = 170\) K, \(T_6 = 100\) K and \(T_7 = 50\) K. The simulation consists of 144,000 sweeps for each copy where in every sweep each of the 19 angles is updated once. After one sweep for each copy an exchange of conformations between pairs of copies at neighboring temperatures was tried simultaneously for each of the three pairs. Hence, the total number of updates in the parallel tempering simulation was \((19 + 3) \times 7 \times 144,000 = 22,176,000\). This large number was chosen to ensure high statistics and is similar to the 1,000,000 sweeps (= 19,000,000 updates) used in earlier work where also Met-enkephalin was used to compare the effectiveness of various numerical algorithms \(^{[11]}\). For the above number of updates 15 hour CPU time were needed on a Silicon Graphics Indigo 2 workstation. While parallel tempering is best suited for parallel computers the workstation was used because it was easier accessible than the parallel machine at IMS computer center.

The results of the parallel tempering simulation was compared with that of a multicanonical simulation and canonical simulations keeping the number of updates constant (preliminary runs had shown that all methods need roughly the same amount of CPU time for a fixed number of updates). In the case of the multicanonical simulation this number includes the 100,000 sweeps (1,900,000 MC updates) necessary to obtain the weights by the iterative procedure described in Ref. \(^{[7]}\). The canonical simulations were performed at the same 7 temperatures as used in the parallel tempering method and each temperature was simulated with same number of updates (3,168,000 MC updates).

To compare the performance of the various algorithms the potential energy and the overlap with the (known) ground state was measured. The latter quantity indicates how \(^2\)The program SMC was written by Dr. Frank Eisenmenger (eisenmenger@rz.hu-berlin.de)
much a given configuration differs from the ground state and is given by

\[ O(t) = 1 - \frac{1}{90 n_F} \sum_{i=1}^{n_F} |\alpha_i^{(t)} - \alpha_i^{(GS)}| , \]  
(19)

where \( \alpha_i^{(t)} \) and \( \alpha_i^{(GS)} \) (in degrees) stand for the \( n_F \) dihedral angles of the conformation at \( t \)-th Monte Carlo sweep and the ground-state conformation, respectively. Symmetries for the side-chain angles were taken into account and the difference \( \alpha_i^{(t)} - \alpha_i^{(GS)} \) was always projected into the interval \([-180^\circ, 180^\circ]\). The above definition guarantees that one has

\[ 0 \leq < O >_T \leq 1 , \]  
(20)

with the limiting values

\[
\begin{align*}
\left\{ \begin{array}{ll}
< O(t) >_T & \to 1 , \quad T \to 0 , \\
< O(t) >_T & \to 0 , \quad T \to \infty .
\end{array} \right.
\]  
(21)

I start presenting my results by showing in Fig. 1 the histogram of energies as obtained from the parallel tempering simulation with Monte Carlo updates. Note the overlap between the Boltzmann distributions which correspond to neighboring temperatures. The energies where the two histograms have a common overlap are the ones where the transition probabilities of Eq. 9 are large enough to allow for an exchange of configurations. The larger the overlap of histograms the higher is the probability for an exchange of conformations. Hence, the temperatures \( T_i \) of the copies have to be chosen such that there is sufficient overlap between Boltzmann distributions which correspond to neighboring temperatures.

To demonstrate the time evolution of states in the parallel tempering algorithm the start configurations of each of the seven copies were marked by a label. The labeled configurations were called “replicas” and their evolution through the whole parallel tempering simulation was followed. Note that the “replicas” are independent from each other. Through the exchange moves of parallel tempering the seven “replicas” are shuffled between the seven temperatures (copies), however, these moves do not introduce any correlation between them. In Fig. 2a it is shown for one of the “replicas” how the seven
different temperatures are visited in the course of the simulation. Due to this random walk in temperatures the replica changes dramatically between ground state like conformers and random coils. This can be seen from the corresponding “time series” of the overlap of the studied replica with the ground state in Fig. 2b. The overlap varies through the simulation between $O \ll 1$ (disordered states) and $O \approx 1$ (ordered state). Note that the values of overlap in Fig. 2b and temperature in Fig. 2a are correlated. Ground state like conformations ($O$ close to 1) were observed when the “replica” stayed at low temperatures, while disordered structures (small values of $O$) appeared together with high temperatures.

To visualize the exchange of conformations by parallel tempering for a single copy (temperature), the label of the “replicas” which is visiting the copy associated with the lowest temperature ($T = 50$ K), is displayed in Fig. 3 as a function of simulation time (in MC sweeps). Since the “replicas” are independent from each other, each change of the “replica”-label indicates that the new conformation is no longer correlated with the previous conformation. Hence, through the exchange of conformations the Markov chain converges much faster to the stationary distribution than it does in the case of a regular canonical simulation with only local Monte Carlo updates. This can be seen in Fig. 4a where the “time series” in energy is displayed for both a regular canonical simulation at $T = 50$ K and for the copy with $T = 50$ K of a parallel tempering simulation. Obviously the regular canonical Monte Carlo got stucked in a local minimum and was not able to thermalize. From previous simulations (see Ref. 5) it is known that even 1,000,000 sweeps are not enough to thermalize Met-enkephalin at $T = 50$ K. On the other hand, with the exchange of configurations by parallel tempering the simulation thermalizes at that temperature in less than 10,000 sweeps. This follows also from Fig. 4b where the “time series” of the overlap function is displayed for both simulations. In the case of parallel tempering at $T = 50K$ most of the conformations are close to the ground state which is consistent with observations from previous simulations 6. On the other hand the regular canonical simulation got stucked in a conformation far from the ground state showing again that the regular Monte Carlo simulation never converged to the true distribution.
Hence, ignoring in the parallel tempering simulation the first 10,000 sweeps necessary for thermalization one can calculate expectation values for average energy and the overlap with the (known) ground state. The obtained values were in all cases within the errorbars identical with the ones obtained by the multicanonical simulation and agree with the results of earlier work \[9, 10\]). On the other hand, the regular canonical simulations yield at low temperatures to different and unreasonable values, since for these temperatures the simulations never thermalized. The data for the two quantities are summarized in Tab. 1 and 2 for all three methods.

An important question is how the effectiveness of new approach compares with other methods and under which conditions it is optimal. To answer this question, further parallel tempering simulations with same number of updates were performed, but where either the local Monte Carlo updates in Eq. 3 were replaced by molecular dynamics trajectories or the canonical weights for the copies in Eq. 2 by the the generalized ensemble weights of Eq. 13. The molecular dynamic updates were performed in dihedral space. The trajectories followed for each copy consisted of 19 leap frog steps with time step $\Delta t = 0.005$ (in arbitrary units). As an example for a combination of parallel tempering with generalized ensemble techniques, a simulation was done where for the 3 lowest temperatures ($T = 50, 100$ and 170 K) the weights of Eq. 13 were used and Boltzmann weights for the higher temperatures. The generalized ensemble weights for the three lowest temperatures were chosen such that the resulting deviation from a canonical distribution would be small. This was ensured by choosing $m = 5 \times n_F = 95$ (with $n_F$ the number of degrees of freedom) and an arbitrary value $E_0 = -20.72$ kcal/mol.

In each case expectation values for physical quantities were obtained which were within the errorbars the same as the one given in Tab. 1 and 2. However, the transition probabilities varied. It did not depend on whether Monte Carlo or molecular dynamics techniques were used as local updates, but only on the chosen weights. This can be seen in Tab. 3 where these transition probabilities are summarized. As one can see the probabilities for exchange of conformations between copies can be enhanced by choosing suitable non-canonical weights like the ones defined in Eq. 13 and used here. To measure the effectiveness of parallel tempering and to compare it with other sophisticated methods like the
multicanonical algorithm the number of “tunneling events” was measured. This quantity gives a lower bound for the number of independent ground state conformers found in the simulation. A tunneling event is defined as a random walk between a ground state like conformer (defined by the condition that the overlap $O \geq 0.9$ and that the potential energy is not more than 1 kcal/mol above the ground state energy $E_{GS} = -10.72$ kcal/mol) and a coil conformer ($O \leq 0.3$). Using Monte Carlo updates, only two tunneling events (at $T = 250$ K) were observed for all seven canonical simulations but 22 events in the case of parallel tempering. This number should be compared with that of a multicanonical run of same statistics where 26 tunneling events were found. Hence, one can conclude that both parallel tempering and multicanonical algorithms are of similar efficiency and much better than regular canonical Monte Carlo with solely local updates. The effectiveness of parallel tempering can be improved by choosing suitable generalized ensemble weights. With the generalized ensemble weights used here the number of tunneling events could be increased by a factor 1.5 to 34 events (reflecting the increased transition probabilities between the copies, see Tab. 3). However, a drawback of such a combination with generalized ensemble methods is that the weights are no longer $a$ priori given for parallel tempering. The gained improvement requires careful choice of additional parameters and may not always be worth the additional effort. For some other combinations of the exponent $m$ and the constant $E_0$ in Eq. 13 it was found that the efficiency became even worse than for the case where canonical weights were assigned to all copies (data not shown). Hence, by assigning generalized ensemble weights to all or only some copies, the effectiveness of parallel tempering can be increased, but whether such approach is useful or not, may depend on the molecule under investigation.

4. Conclusions

It was shown that a new algorithm, parallel tempering, can be successful applied to simulation of molecules and helps to overcome the multiple minima problem. The new method can be used with both Monte Carlo and molecular dynamics updates. Its effectiveness is comparable to generalized ensemble techniques like the multicanonical algorithm. However, unlike for the case of generalized ensemble techniques, the weights are $a$ priori known for parallel tempering, which makes application of the new method technically
easier than that of generalized ensemble algorithms. Further, the two techniques can be combined which allows to increase their efficiency.

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Tables:

- Tab. 1: Average potential energy $< E >$ as function of temperature.

| $T$  | Canonical | Multicanonical | Parallel Tempering |
|------|-----------|----------------|--------------------|
| 1000 | 17.48 (1) | 17.50 (2)      | 17.51 (6)          |
| 500  | 8.65 (6)  | 8.65 (5)       | 8.75 (8)           |
| 330  | 1.44 (22) | 1.64 (12)      | 1.56 (11)          |
| 250  | -3.23 (76)| -2.85 (15)     | -2.84 (16)         |
| 170  | -4.27 (18)| -6.36 (7)      | -6.27 (4)          |
| 100  | -1.08 (9) | -8.50 (5)      | -8.49 (3)          |
| 50   | -2.54 (5) | -9.69 (3)      | -9.68 (2)          |

- Tab. 2: Average overlap function (defined in Eq. 19) as function of temperature.

| $T$  | Canonical | Multicanonical | Parallel Tempering |
|------|-----------|----------------|--------------------|
| 1000 | 0.29 (1)  | 0.29 (1)       | 0.29 (1)           |
| 500  | 0.34 (1)  | 0.34 (1)       | 0.34 (1)           |
| 330  | 0.48 (3)  | 0.45 (1)       | 0.44 (2)           |
| 250  | 0.62 (2)  | 0.61 (1)       | 0.60 (1)           |
| 170  | 0.10 (1)  | 0.78 (1)       | 0.78 (1)           |
| 100  | 0.34 (1)  | 0.89 (1)       | 0.89 (1)           |
| 50   | 0.42 (1)  | 0.94 (1)       | 0.94 (1)           |

- Tab. 3: Probability for an exchange of configuration between two temperatures for various variants of the parallel tempering method.

|                  | Monte Carlo | Molecular Dynamics | Monte Carlo |
|------------------|-------------|--------------------|-------------|
|                  | Canonical weights | Canonical weights | Generalized Ensemble weights |
| $500 \; K \leftrightarrow 1000 \; K$ | 0.14        | 0.14              | 0.14        |
| $330 \; k \leftrightarrow 500 \; K$ | 0.17        | 0.18              | 0.18        |
| $250 \; k \leftrightarrow 330 \; K$ | 0.31        | 0.28              | 0.29        |
| $170 \; k \leftrightarrow 250 \; K$ | 0.22        | 0.29              | 0.74        |
| $100 \; k \leftrightarrow 170 \; K$ | 0.15        | 0.16              | 0.21        |
| $50 \; k \leftrightarrow 100 \; K$  | 0.10        | 0.10              | 0.31        |
Figure Captions:

- Fig. 1: Histogram of Energies for different temperatures as obtained from a parallel tempering simulation with 7 copies and 144,000 Monte Carlo sweeps for each copy.

- Fig. 2a: “Time series” of temperatures which one of the seven “replicas” encountered over the 144,000 Monte Carlo sweeps in the parallel tempering simulation.

- Fig. 2b: “Time series” of the overlap function, defined in Eq. 19, for one of the seven “replicas” over 144,000 Monte Carlo sweeps in the parallel tempering simulation.

- Fig. 3: “Time series” of “replicas” over 144,000 Monte Carlo sweeps in the parallel tempering simulation as encountered for $T = 50$ K.

- Fig. 4a: “Time series” of energy for $T = 50$ K over 144,000 Monte Carlo sweeps as obtained from the parallel tempering algorithm and a regular canonical simulation.

- Fig. 4b: “Time series” of the overlap function (defined in Eq. 19) for $T = 50$ K over 144,000 Monte Carlo sweeps as obtained from the parallel tempering algorithm and a regular canonical simulation.
HISTOGRAM OF ENERGIES
T=50K

MC SWEEPS

REPLICA
T = 50 K

Regular Canonical MC

Parallel Tempering
T = 50K

Parallel Tempering

Regular Canonical MC

MC SWEEPS

OVERLAP O