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Cross-Check Methods in Protein Simulations

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The aim of this work[1,2] is to study the behavior of three advanced Monte Carlo methods in protein simulations employing a realistic ECEPP/3-based all-atom model[3]. The implementation is based on the open source package SMMP[4]. The techniques applied were Wang-Landau sampling[2], parallel tempering[6,7] and random tempering. All three techniques show very good agreement in the outcome, a cross-check of the simulation results is possible.

1 Introduction

We started from the question which present algorithm is the best. First we used parallel tempering and Wang-Landau sampling. After our first simulations[2] we found that both algorithms had nearly the same strength. Therefore, we moved to the question if the results correspond for all algorithms. This provides the opportunity to have a cross-check for your simulation data.

2 Model

The SMMP[4] package we applied uses the well-known ECEPP/3 Potential[3]

$$E_{\text{tot}} = E_{\text{LJ}} + E_{\text{el}} + E_{\text{hb}} + E_{\text{tors}} \; .$$

3 Methods

3.1 Wang-Landau Sampling

This method is a combination of the Wang-Landau algorithm[8] and the multicanonical algorithm[5]. First we use the Wang-Landau algorithm to evaluate the multicanonical weights $W_{\text{Muca}}(E)$ from the given estimator of the density of states $\Omega(E)$. The second step was a normal multicanonical simulation with fixed weights.

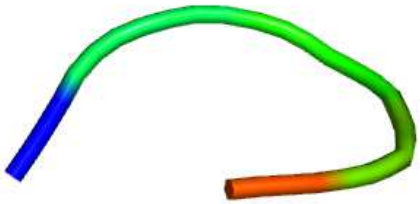

Figure 1. Backbone of the vacuum ground state of Met-enkephalin

3.2 Parallel Tempering

We also used the well known parallel tempering technique, which is a multi Markov chain process that provides the local updates at fixed temperature and global exchange updates between different temperatures.

3.3 Random Tempering

The latest method we studied was a uncommon type of simulated tempering[9]. We used the Wang-Landau algorithm[8] to estimate the temperature depending weights for the global update which changes the temperature.

4 Object of study

We used the pentapeptide Met-enkephalin (see Fig. 1)

Tye-Gly-Gly-Phe-Met

with a ground state energy at -12.43 kcal/mol. Because of its simplicity this peptide becomes a check point for every new algorithm.

5 Results

As Fig. 2 shows the mean value of the energy is sampled very good for all algorithms. The normalized specific heat shows small variation (see Fig. 3).

6 Conclusion

All techniques, parallel tempering, Wang-Landau sampling and random tempering allow to obtain information over a large temperature range from a single simulation. All are at least two orders of magnitude faster than a canonical simulation at a low temperature of $T = 100$ K.

Hence, choice between the algorithms will depend on the equipment available and the personal preferences of the researcher. As all three techniques are numerically different a cross-check of the simulation results in protein studies is possible.

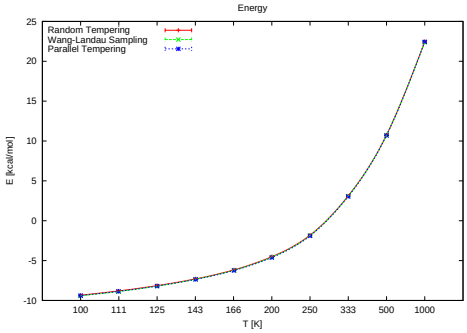

Figure 2. Averages of energy simulated with different methods show very good agreement.

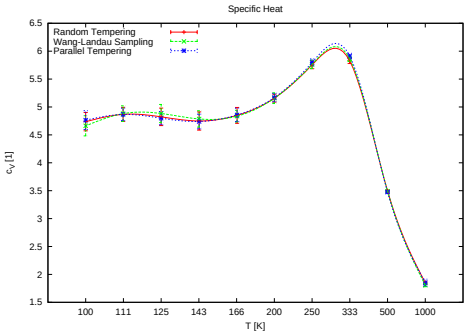

Figure 3. Specific heat simulated with different methods show small variations, but still good agreement.

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