Multiple-time-stepping Hybrid Monte Carlo Methods

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Design of numerical algorithms, which accelerate molecular dynamics simulations by making use of the multi-scale nature of the macromolecular systems, has been the area of intense focus for over two decades. Multiple-time-stepping (MTS) methods are among the most popular approaches of this type. The prototypical algorithm is the Verlet-I/r-RESPA/Impulse integrator (Grubmüller et al., 1991; Humphreys et al., 1994), which divides the forces into fast (short-range) and slow (long-range) components, and then evaluates the slow forces less frequently than their fast counterparts. However, the method suffers from severe instabilities that limit the largest possible time-step (Ma et al., 2003; Izaguirre et al., 2001). These step-size limitations have been partially overcome by the mollified MTS methods of García-Archilla et al. (1998) and Izaguirre et al. (1999, 2001).

Another problem is that the common time-stepping methods do not accurately sample from the target temperature even if the simulations are stable and are subject to a thermostat (Pastor et al., 1988; Bond and Leimkuhler, 2007). This error can be controlled by increasing the frequency of updating slow forces with a loss of computational efficiency.

The aim of this report is to further improve MTS methods by making advantage of recent advances in generalized hybrid Monte Carlo (GHMC) techniques (Akhmatskaya et al., 2009; Kennedy and Pendleton, 2001; Horowitz, 1991). More specifically, we present two novel multiple-time-stepping generalized hybrid Monte Carlo methods for constant temperature molecular simulation of large biomolecular systems. The proposed MTS-GHMC / GSHMC methods resolve the sampling problem and ensure correct sampling from the canonical ensemble. Moreover, the methods allow for nearly twice as large step-size ratios than those permitted for Langevin stabilized MTS methods (Izaguirre et al., 2001).

References:

1. Grubmüller, H., Heller, H., Windemuth, A. and Schulten, K., Generalized Verlet algorithm for efficient molecular dynamics simulations with long-range interactions (**1991**), Mol. Sim., 6: 121-142
2. Humphreys, D., Friesner, R. and Berne, B., A multiple-time-step molecular dynamics algorithm for macromolecules (**1994**), J. Phys. Chem., 98 [27]: 6685-6892
3. Ma, Q., Izaguirre, J. and Skeel, R., Verlet-I/R-Respa/Impulse is limited by nonlinear instabilities (**2003**), SIAM J. Sci. Comput., 24 [6]: 1951-1973
4. Izaguirre, J., Catarello, D., Wozniak, J. and Skeel, R., Langevin stabilization of molecular dynamics (**2001**), J. Chem. Phys., 114: 2090-2098
5. B. García-Archilla, G. M. Sanz-Serna, R. D. Skeel, Long-time-step methods for oscillatory differential equations (**1998**), SIAM J. Sci. Comput., 20[3]: 930-963
6. Izaguirre, J., Reich, S. and Skeel, R., Longer time steps for molecular dynamics (**1999**), J. Chem. Phys., 110: 9853-9864
7. Pastor, R., Brooks, B. and Szabo, A., An analysis of the accuracy of Langevin and molecular dynamics algorithms (**1988**), Mol. Phys., 65: 1409-1419
8. Bond, S. and Leimkuhler, B., Molecular dynamics and the accuracy of numerically computed averages (**2007**), Acta Numerica ,16: 1–65
9. Akhmatskaya, E., Bou-Rabee, N. and Reich, S., Generalized hybrid Monte Carlo methods without momentum flip (**2009**), J. Comput. Phys., 228: 2256–2265
10. Horowitz, A., A generalized guided Monte Carlo algorithm (**1991**), Phys. Lett. B, 268: 247-252
11. Kennedy, A. and Pendleton, B., Cost of the generalized hybrid Monte Carlo algorithm for free field theory (**2001**), Nucl. Phys.B, 607: 456-510