Molecular Dynamics III

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Increasing the Performance and Extensibility of Collective Variable Simulations
Giacomo Fiorin1, Jérôme Hénin2.
1Institute for Computational Molecular Science, Temple University, Philadelphia, PA, USA, 2Laboratoire de Biochimie Théorique, IBPC, CNRS, Paris, France.

The collective variables module (Colvars) is a software library that is tightly integrated with molecular simulation and analysis programs (Fiorin et al, Mol Phys, 2013). It is freely available in community programs for molecular dynamics such as NAMD and LAMMPS, and the visualization and analysis program VMD. Colvars implements reusable functions to reduce the dimensionality of complex chemical and biophysical systems, and a set of algorithms for enhanced sampling and statistical analysis. Recent updates have brought performance improvements for large systems and costly methods, a more flexible scripting interface, and the addition of more stable free energy estimators. We illustrate each advance through examples from biophysics, chemistry and materials science.

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Making Classical and Hybrid (QM/MM) Molecular Dynamics Easy and Fast with QwikMD
João V. Ribeiro1, Rafael C. Bernardi1, Till Rudack1, Klaus Schulten1,2.
1Beckman Institute, University of Illinois at Urbana-Champaign, Urbana, IL, USA, 2Department of Physics, University of Illinois at Urbana-Champaign, Urbana, IL, USA.

“Everything that living things do can be understood in terms of jigglings and wigglings of atoms.” Richard Feynman’s remarks in the early 1960’s summarize what is today widely accepted, namely, that molecular processes can be described by the dynamics of biological molecules, therefore connecting protein function with protein dynamics. Molecular dynamics (MD) simulation, in this regard, is the major methodology employed in structural biology to explore the dynamical behavior of macromolecules. Although the use of MD simulations has consistently increased over the last decades, the barrier imposed by the initial learning curve of the MD packages is still high. To assist new users in overcoming this barrier, and to help the more advanced users to speed up tedious preparation steps, we developed QwikMD(1). This user-friendly program connects the widely used molecular graphics program VMD to the widely adopted MD program NAMD. Employing QwikMD, a user is able to setup an MD simulation in just a few minutes, allowing quick studies of point mutations, partial deletions or even atomic force microscopy experiments. Within the different modules of QwikMD, one can adopt a myriad of popular protocols such as molecular dynamic simulations in vacuum to hybrid QM/MM simulations. QwikMD makes it easy for a new user to perform MD simulations, while it also serves as a learning tool. Many “info buttons” provide the theoretical background underlying the MD procedures carried out in modern MD simulations.

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A Flexible, GPU - Powered Fast Multipole Method for Realistic Biomolecular Simulations in Gromacs
Bartosz Kohnke1, R. Thomas Ullmann1, Carsten Kutzen1, Andreas Beckmann1, David Haensel2, Ivo Kabadshow2, Holger Dachsel2, Berk Hess1, Helmut Grubmüller3.
1Department of Theoretical and Computational Biophysics, Max Planck Institute for Biophysical Chemistry, Goettingen, Germany, 2Institute for Advanced Simulation (IAS), Forschungszentrum Jülich GmbH, Jülich, Germany, 3KTH Royal Institute of Technology, Stockholm, Sweden.

The calculation of electrostatic interactions is typically the computational bottleneck of molecular dynamics (MD) simulations and thus decisive for the overall simulation performance. Further, biomolecules typically contain many sites whose electrostatic charge distribution changes over time, e.g. due to uptake and release of protons or tautomersism at protonatable sites, or electron transfer between redox-active cofactors. Besides computational efficiency, a physically accurate electrostatics treatment therefore has to account for this variability, too, thus aggravating the bottleneck. Taking advantage of the computational power of GPUs through innovative algorithms, high-throughput simulations of large systems become feasible. To that aim, we have developed a fast multipole method (FMM) for the rapid computation of the electrostatic interactions that are required for a lambda-dynamics treatment of the interconversion between the different site forms during the simulation. The tree data structure used by the FMM allows to compute additive charge distributions of the different protonation forms without requiring redundant computations. Therefore, our FMM enables efficient computation of electrostatic forces and interaction energies between large numbers of titratable sites with a small, nearly constant computational overhead. For taking full advantage of GPUs, the FMM implementation ensures that the computational work is evenly distributed among the large number of GPU processing units. To this aim, our parallel GPU-implementation optimally matches hardware and algorithmic requirements, resulting in very good scaling properties.