

Abstracts of Papers to Appear in Special Issue on Computational Molecular Biophysics

MULTIPLE TIME SCALES IN CLASSICAL AND QUANTUM-CLASSICAL MOLECULAR DYNAMICS. Sebastian Reich.
Department of Mathematics and Statistics, University of Surrey, Guildford, Surrey GU2 5XH, United Kingdom. E-mail: s.reich@surrey.ac.uk.

The existence of multiple time scales in molecular dynamics poses interesting and challenging questions from an analytical as well as from a numerical point of view. In this paper, we consider simplified models with two essential time scales and describe how these two time scales interact. The discussion focuses on classical molecular dynamics (CMD) with fast bond stretching and bending modes and the, so-called, quantum-classical molecular dynamics (QCMD) model where the quantum part provides the highly oscillatory solution components. The analytic results on the averaging over fast degrees of motion will also shed new light on the appropriate implementation of multiple-time-stepping (MTS) algorithms for CMD and QCMD.

THE NOSÉ–POINCARÉ METHOD FOR CONSTANT TEMPERATURE MOLECULAR DYNAMICS. Stephen D. Bond,*
Benedict J. Leimkuhler,* and Brian B. Laird.† **Department of Mathematics, and †Department of Chemistry,*
University of Kansas, Lawrence, Kansas 66045.

We present a new extended phase space method for constant temperature (canonical ensemble) molecular dynamics. Our starting point is the extended Hamiltonian introduced by Nosé to generate trajectories corresponding to configurations in the canonical ensemble. Using a Poincaré time-transformation, we construct a Hamiltonian system with the correct intrinsic time scale and show that it generates trajectories in the canonical ensemble. Our approach corrects a serious deficiency of the standard change of variables (Nosé–Hoover dynamics), which yields a time-reversible system but simultaneously destroys the Hamiltonian structure. A symplectic discretization method is presented for solving the Nosé–Poincaré equations. The method is explicit and preserves the time-reversal symmetry. In numerical experiments, it is shown that the new method exhibits enhanced stability when the temperature fluctuation is large. Extensions are presented for Nosé chains, holonomic constraints, and rigid bodies.

A FAST ADAPTIVE MULTIPOLE ALGORITHM FOR CALCULATING SCREENED COULOMB (YUKAWA) INTERACTIONS.
Alexander H. Boschitsch,* Marcia O. Fenley,* † and Wilma K. Olson.† **Continuum Dynamics, Inc., P.O.*
Box 3073, Princeton, New Jersey 08543; and †Department of Chemistry, Rutgers University, Wright and
Rieman Laboratories, 610 Taylor Road, Piscataway, New Jersey 08854-8087.

The screened Coulomb (Yukawa or Debye–Hückel) potential, $\Phi = \exp(-\kappa r)/r$, where r is the separation distance and κ is the Debye–Hückel screening parameter, gives a good description of the electrostatic interactions in a variety of biologically and physically important charged systems. It is well known that the direct calculation of the energy and forces due to a collection of N charged particles involves the pairwise summation of all charged particle interactions and exhibits an $O(N^2)$ computational complexity which severely restricts maximum problem size. This has prompted the development of fast summation algorithms that allow the electrostatic energy and forces to be obtained in only $O(N \log N)$ operations. To date however, practically all such implementations have been limited exclusively to pure Coulombic potentials ($\kappa = 0$), and the central contribution of the present method is to extend this capability to the entire range of the inverse Debye length, $\kappa \geq 0$. The basic formulation and

computational implementation of the spherical modified Bessel function-based multipole expansions appropriate for the screened Coulomb kernel are first presented. Next, a simple model system consisting of a single source charged particle is studied to show that the maximum electrostatic energy error incurred by an M -order multipole expansion for the Yukawa potential is bounded above by the error of the equivalent multipole expansion for the Coulombic potential. Finally, timing and accuracy studies are presented for a variety of charged systems including polyelectrolyte chains, random distributions of charges inside a cube, and face-centered-cubic (FCC) lattice charge configurations containing up to 103,823 charges.

ALGORITHMIC CHALLENGES IN COMPUTATIONAL MOLECULAR BIOPHYSICS. Tamar Schlick,* Robert D. Skeel,† Axel T. Brünger,‡ Laxmikant V. Kale,† John A. Board, Jr.,§ Jan Hermans,¶ and Klaus Schulten.† **Department of Chemistry and Courant Institute of Mathematical Sciences, New York University and The Howard Hughes Medical Institute, 251 Mercer Street, New York, New York 10012*; †*Beckman Institute, University of Illinois at Urbana-Champaign, 405 North Mathews, Urbana, Illinois 61801-2987*; ‡*Department of Molecular Biophysics and Biochemistry, Yale University and The Howard Hughes Medical Institute, 266 Whitney Avenue, Bass Center, Room 434, New Haven, Connecticut 06520*; §*Department of Electrical and Computer Engineering, Duke University, School of Engineering, Durham, North Carolina 27708*; and ¶*Department of Biochemistry and Biophysics, University of North Carolina, Chapel Hill, North Carolina 27599-7260*. E-mail: schlick@nyu.edu, skeel@cs.uiuc.edu, kale@cs.uiuc.edu, kschulte@uiuc.edu, brunger@laplace.csb.yale.edu, jab@ee.duke.edu, hermans@med.unc.edu.

A perspective of biomolecular simulations today is given, with illustrative applications and an emphasis on algorithmic challenges, as reflected by the work of a multidisciplinary team of investigators from five institutions. Included are overviews and recent descriptions of algorithmic work in long-time integration for molecular dynamics, fast electrostatic evaluation, crystallographic refinement approaches, and implementation of large, computer-intensive programs on modern architectures. Expected future developments of the field are also discussed.

KIRKWOOD–BUFF THERMODYNAMICS DERIVED FROM GRAND CANONICAL MOLECULAR DYNAMICS AND DRISM CALCULATIONS. Gillian C. Lynch, John S. Perkyns, and B. Montgomery Pettitt. *Department of Chemistry, University of Houston, Houston, Texas 77204-5641*. E-mail: glynch@uh.edu, jperkyns@uh.edu, pettitt@uh.edu.

The Grand Canonical Ensemble techniques have become very popular in recent years, both Monte Carlo and molecular dynamics, but no direct link between the number fluctuation results from these simulation methods and a Kirkwood–Buff theory has been established. In this article we will look at Kirkwood–Buff integrals computed using thermodynamic averages derived from Grand Canonical Ensemble molecular dynamics (GCMD) simulations and compare them to similar quantities derived from the Dielectrically Consistent Reference Interaction Site Model (DRISM) many-body theory. These calculations will be carried out for three different water models, SPC, SPC/E, and TIP3P.