Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Local algorithms for Coulomb's law in molecular dynamics JOERG ROTTLER, University of British Columbia — The computation of Coulombic interactions still forms one of the major bottlenecks in molecular dynamics simulations of soft and biologial materials. Most current fast Coulomb techniques rely on Fourier methods, but their parallel efficiency on standard compute clusters is not always ideal. In addition, they have difficulty dealing with inhomogeneous dielectric environments that one might like to treat in implicit solvent models. We discuss an attractive alternative, real-space approach that does not rely on Poisson's equation, but mediates the Coulomb interaction through a thermalized auxiliary field that is dynamically constrained to obey Gauss' law. Instead of globally optimizing the field configuration as in conventional approaches, the algorithm performs a partial integration over the transverse degrees of freedom of the electric field, which requires only local operations. The locality leads directly to linear (i.e. O(N)) scaling with the number of particles, implies excellent parallelizability and generalizes easily to inhomogenenous dielectrics without substantial overhead. We show that recent implementations of this method can yield an accuracy sufficient for atomistic simulations, calibrate its parallel efficiency and compare to standard Fourier methods.

Joerg Rottler
University of British Columbia

Date submitted: 13 Nov 2006 Electronic form version 1.4