The Multigrid N -Body Solver

David J. Hardy

Department of Computer Science, University of Illinois, Urbana, IL, 61801, USA
dhardy@uiuc.edu

Abstract

The multigrid N -body solver is a fast method for approximating the pairwise electrostatic forces due to a system of charged atoms. The electrostatic potential can be expressed as $U(r) = (1/2)q^T G(r)q$ where vector q contains the N charges and $N \times N$ matrix $G(r)$ has an element $C/\|r_j - r_i\|$ in its ij th position whenever there is an interaction between atoms i and j . The multigrid N -body solver uses a matrix splitting along with hierarchical interpolation to approximate the smooth dense $\tilde{G}(r)q$ product in $\mathcal{O}(N)$ time. The advantages of this algorithm are its simplicity, the fact that it maintains continuous forces, and that it enables cheaper multiple time stepping for molecular dynamics through a natural separation of spatial scales. The details of this method will be presented, and experimental results will be shown that compare this method with other popular fast electrostatics methods.