

Lattice Cutoff Computation For Multilevel Summation

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Introduction

The simulation of biomolecules (molecular dynamics) requires computing the pairwise forces between atoms over millions of time steps. The multilevel summation method provides a fast approximation to the electrostatic interactions between all pairs of atoms, with a total amount of work that increases linearly with the number of atoms, rather than quadratically. This method enables simulations on larger systems for longer timescales. An added benefit of multilevel summation over alternative methods is that it can be used, essentially unchanged, with either nonperiodic or periodic boundary conditions.

Description

Multilevel summation approximates the $q_i q_j (|r_i - r_j|)^{-1}$ electrostatic potential and corresponding forces between atoms by splitting the potential into a short-range part, evaluated exactly, and a smooth, slowly varying long-range part that is interpolated from a hierarchy of grids. The short-range part involves calculating a pairwise potential between atoms that are within a given cutoff distance from each other. The long-range part involves performing a similar cutoff calculation between pairs of grid points on a 3D lattice, and then interpolating these results back to the atoms.

For the long-range part, the regularity of working on a lattice permits the cutoff computation to be described as a sequence of 3D convolutions. A potential is computed at a grid point by taking a weighted sum of the sphere (or cube by padding the corners with zero weight) of charges surrounding that point. The weights are a function of the distance to each charge, and since these relative distances are the same around every grid point, this lattice of weights can be computed once and reused at every grid point. The lattice cutoff computation can be expressed mathematically as an inner product (or convolution) of the fixed lattice of weights with a sub-lattice of charges centered at each grid point.

Objective

The project is to implement the lattice cutoff computation described above. It should be possible to produce a highly optimized implementation within the time allotted. The implementation will be benchmarked with different sized lattices of charge (ranging from 30^3 to 150^3 grid points, not necessarily cubic) and different sized cutoffs (resulting in the cubic lattice of weights ranging from 15^3 to 25^3 grid points), with a report made on limitations of the hardware for this application. Both nonperiodic and periodic versions should be implemented. The nonperiodic case truncates the lattice of weights to fit the edges of the charge grid, whereas the periodic case applies the entire lattice of weights at each grid point by wrapping around the edges of the charge grid.

Background

No specialized knowledge is necessary to work on the application, since the algorithm to be implemented is straightforward. Having some background in linear algebra and basic physics is helpful to better appreciate the problem. Programming expertise is assumed.

Resources

Algorithm references, papers, and sample code will be made available online:
<http://www.ks.uiuc.edu/Research/vmd/projects/ece498/>

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