Multilevel summation methods for N-body interactions[1]

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Outlined are the main ideas of some multilevel methods for the fast calculation of energies and forces for pairwise interactions in classical molecular mechanics. The common principle that underlies these methods is described, as is the fundamental difference between multigrid methods and tree methods. Also discussed are Ewald sum methods for periodic boundary conditions.

The electrostatic energy arising from N particles with positions $\vec{r}_i$ and charges q_i is proportional to $\frac{1}{2}\sum'_{i,j} q_i q_j |\vec{r}_j - \vec{r}_i|^{-1}$ where the prime denotes omission of $j = i$ (as well as covalently bonded atom pairs). Forces are (best) calculated from derivatives of the multilevel approximation to the energy. Periodic boundary conditions are often imposed. Alternatively, there may be walls or no boundaries at all. The purpose of this calculation may be Monte Carlo simulation, energy minimization, or molecular dynamics. In addition to wanting small errors it is desirable that the energy approximation have a certain degree of smoothness and possibly that the forces satisfy Newton's third law.

In an abstract sense the problem is one of calculating $\frac{1}{2}q^{\mathrm{T}}Gq$ where q is the collection of all charges and G is a matrix of reciprocal distances. The major part of this calculation is that of the matrix–vector product $e = Gq$, which are electric potentials. The first step of a multilevel method is to partition the computational domain by a sequence of successively finer lattices, each lattice defining either a grid or a set of cells. The matrix G of particle-level interactions is approximated by a sum

$$G \approx \hat{G} + I_h^* G_h I_*^h,$$

where the first term contains only interactions between particles within a certain distance and the second term approximates long-scale interactions that can be well resolved on the finest lattice. The matrix G_h represents interactions at the level of the finest lattice and its dimension is only a fraction of that of G. The other three matrices have only $O(N)$ nonzero elements in them. In a similar way, the matrix G_h is approximated using a second level matrix, $G_h \approx \hat{G}_h + I_{2h}^h G_{2h} I_h^{2h}$, and so on. This leads to a nested approximation to G. The process of forming $e = Gq$ is described by a V-cycle:

$$\begin{array}{ccccccc}
q & - & - & - & - & \rightarrow & e \\
& \searrow & & & & \nearrow & \\
& q_h & - & - & \rightarrow & e_h & \\
& & \searrow & & \nearrow & & \\
& & \cdots & \cdots & \cdots & & \\
& & \searrow & & \nearrow & & \\
& & & q_{Mh} \rightarrow e_{Mh} & & &
\end{array}$$

For each level a set of charges and a set of potentials is calculated. Each arrow represent multiplication by a matrix having $O(1)$ entries per row, and the junction of two arrows represents an addition. The total number of operation is $O(N)$ if enough levels are used. (There are $O(N \log N)$ methods [3], for which only charges are represented at each level.)

In multigrid methods [5] the separation into short scale and long scale is based on a splitting $r^{-1} = (r^{-1} - g_a(x)) + g_a(x)$ where $r^{-1} - g_a(x)$ vanishes for $r > a$ and where $g_a(x)$ is sufficiently smooth that it can be approximated accurately on the finest grid. The quantity $g_a(|\vec{r}\,' - \vec{r}|)$ is then approximated as a linear combination of products of basis functions of $\vec{r}\,'$ and of $\vec{r}$. Each basis function is nonzero on some region containing only $O(1)$ gridpoints. This idea is repeated for the interactions between gridpoints on the first level grid in order to transfer the calculation to a higher level.

Tree methods, such as the fast multipole method (FMM) [11], use an oct-tree decomposition of the domain into cells. For each cell one constructs a compressed representation of the charges in it and of the potentials due to distant charges. The separation into spatial scales is done on a pair by pair basis depending on the octree structure. The approximation needed to represent the charges or potentials in a cell is based on a Taylor expansion of $|\vec{r}\,' - \vec{r}|$ in terms of $\vec{r}\,'$ about the centers of source cells and of $\vec{r}$ about the centers of destination cells. A reduction in the number of terms is achieved by expressing the expansion as a series in the set of harmonic polynomials of three variables. The calculations of the coefficients involve multipole expansions containing negative powers of cell-to-cell distances. Alternatives to multipoles are possible [2, 17, 15].

The primary advantage of the tree methods is their ability to exploit the harmonicity of r^{-1} in 3D. But this advantage does not generalize easily to other nonbonded potentials such as Lennard-Jones. Also, a truncated Taylor expansion is significantly less accurate for the same amount of data than is centered piecewise polynomial interpolation, which can be used by a multigrid method. Moreover, for a multigrid method it is easy to ensure continuity of derivatives, which is important for stable dynamics [4]. In addition, the separation of spatial scales effected by multigrid is smoothly changing and hence can be exploited by multiple time stepping. Finally, the relative simplicity of multigrid is a definite advantage.

For periodic boundaries the energy is not well defined even if the net charge is zero. The meaning is usually made precise by a limiting process which approximates a massive spherical collection of periodic boxes surrounded by a specified dielectric [1]. The calculation of this energy is commonly achieved by an $Ewald\ sum$. Specifically, the r^{-1} interaction is split into a short-ranged part and a smooth part. The energy for the short-ranged part is (in practice at least) a finite summation. The energy for the smooth part can be transformed into a rapidly converging Fourier series. An optimal splitting leads to an algorithm of complexity $O(N^{3/2})$. The particle–mesh Ewald method [7, 9] reduces this to $O(N \log N)$ by interpolating the trigonometric functions in the Fourier series onto a grid so that an FFT can be applied. Periodic boundaries can also be handled by FMM by doing an Ewald sum at the highest level. There are good reviews [8, 16] of these and other methods.

A method not yet mentioned is P3M [12], which also does a splitting into short-ranged parts and smooth parts. It handles the smooth part using a fast Poisson solver. Also not mentioned are adaptive methods [6], the reaction field method [14, 1], and the generalization to the case of implicit solvents and ions modeled by the Poisson-Boltzmann equation [13]. The literature on the calculation of N-body interactions is extensive. A source of many references is [10].

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