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Multilevel summation and Monte Carlo simulations

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The energy U of a system of N point particles is given by

$$U_N = \frac{1}{2}\sum_{i\neq j}^{N} q_i \cdot G\left(|\vec{r_i}-\vec{r_j}|\right)\cdot q_j, \tag{1}$$

where q_i is the "charge" (electrostatic charge, mass, etc.) and $\vec{r_i}$ is the location of the i-th particle. The interparticle interactions are defined by the kernel $G\left(|\vec{r_i}-\vec{r_j}|\right)$. The kernel usually is singular at the origin and becomes smoother as the distance between the two particles grows; such kernels are called asymptotically smooth [1]. A "softening" of such kernel can be obtained by its splitting into two parts

$$G(r) = G_{\text{loc}}(r) + G_{\text{smooth}}(r), \tag{2}$$

where the local part of the kernel is defined to be zero beyond some cutoff radius r_{cut}

$$G_{\text{loc}}(r) = \begin{cases} G(r) - G_{\text{smooth}}(r), & r \le r_{\text{cut}} \\ 0, & r > r_{\text{cut}} \end{cases}. \tag{3}$$

A suitable choice for the smooth part of the kernel is given by

$$G_{\text{smooth}}(r) = \begin{cases} P_m(r), & r \le r_{\text{cut}} \\ G(r), & r > r_{\text{cut}} \end{cases}, \tag{4}$$

where the function $P_m(r) = \sum_{i=0}^{m} a_i \cdot (r)^{2i}$ is a polynomial of order $2m$. Sufficient smoothness of $G_{\text{smooth}}(r)$ can be guaranteed by the condition that this function and its first m derivatives are continuous at the point $r=r_{\text{cut}}$. From this condition we get a system of equations for the unknown coefficients a_i (for the kernel $G(r)=1/r$ the values of these coefficients are given in Gloskovskaya and Ilyin [2]).

Taking into account that the kernel is separated into local and smooth parts, the interaction energy (1) can also be split into two parts

$$U_N = U_{\text{loc}} + U_{\text{smooth}}, \tag{5}$$

where the contribution to the potential energy of the local, short range interactions is defined by

$$U_{\text{loc}} = \frac{1}{2}\sum_{i\neq j}^{N} q_i \cdot G_{\text{loc}}\left(|\vec{r_i}-\vec{r_j}|\right)\cdot q_j. \tag{6}$$

If r_{cut} is chosen comparable to the average inter-particle distance, a direct summation in (6) is not computationally expensive.

Unlike the local kernel, the smooth part (4) is nonsingular at $r=0$. Therefore, the last term in (5) can be written as

$$\begin{aligned} U_{\text{smooth}} &= \frac{1}{2}\sum_{i,j}^{N} q_i \cdot G_{\text{smooth}}\left(|\vec{r_i}-\vec{r_j}|\right)\cdot q_j - \frac{1}{2}\cdot a(0)\cdot\sum_{i=1}^{N} q_i^2 \\ &= U^s_{\text{smooth}} + U_{\text{self}}, \end{aligned} \tag{7}$$

where U_{self} is independent of particle locations and can be calculated once for all as the self-interaction energy.

The main idea of the Multilevel Summation [1] consists in the interpolation of $G_{\text{smooth}}(r)$ from some grid. The space is covered by a uniform grid which is defined by a set of gridpoints $\{R_{\mathbf{I}}\}_I$, the mesh size being h. The value of the smooth part of the kernel for given locations of particles i and j can be interpolated from that grid

$$\begin{aligned} &G_{\text{smooth}}\left(|\vec{r_i}-\vec{r_j}|\right) \\ &\quad = \sum_{\mathbf{I}\in\sigma_{\mathbf{i}}}\sum_{\mathbf{J}\in\sigma_{\mathbf{j}}} \varpi_{\mathbf{I}}(\vec{r_i})\cdot G_{\text{smooth}}\left(|R_{\mathbf{I}}-R_{\mathbf{J}}|\right)\cdot\varpi_{\mathbf{J}}(\vec{r_j}) + O(\varepsilon) \end{aligned} \tag{8}$$

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where $\varpi_{\mathbf{I}}(\vec{r}_i)$ are the interpolation coefficients, ε is the error of the interpolation and σ_i is a neighborhood of the point $\vec{r}_i$.

Substitution of (8) in (7) yields after change of the summation order

$$U^s_{\text{smooth}} = \frac{1}{2}\sum_{\mathbf{I},\mathbf{J}}^{N} Q_{\mathbf{I}} \cdot G_{\text{smooth}}(|R_{\mathbf{I}} - R_{\mathbf{J}}|) \cdot Q_{\mathbf{J}}, \tag{9}$$

where the set of "*super charges*" $\{Q_{\mathbf{I}}\}$ is defined at the coarse level gridpoints by

$$Q_{\mathbf{I}} = \sum_{i \text{ such that } \mathbf{I} \in \sigma_{\mathbf{i}}} \varpi_{\mathbf{I}}(\vec{r}_i) \cdot q_i \tag{10}$$

The fine-to-coarse transfer (10), which is the adjoint of interpolation, is called *anterpolation*.

Since (9) is a coarse-level version of (1), its summation can be carried out similarly, using a coarser grid, continuing recursively to increasingly coarser grids with level-l mesh size being $h_l = 2^{l-1}h$. Due to the asymptotic smoothness of the kernel $G(r)$, it can be split into local and smooth parts on each level, in the form

$$G^l_{\text{smooth}}(r) = \begin{cases} P^l_m(r), & r \le 2^{l-1} \cdot r_{\text{cut}} \\ G(r), & r > 2^{l-1} \cdot r_{\text{cut}} \end{cases} \qquad (l = 1,2,\ldots). \tag{11}$$

Denoting $G^0 = G$, we recursively define

$$G^l_{\text{loc}}(r) = \begin{cases} G^{l-1}_{\text{smooth}}(r) - G^l_{\text{smooth}}(r), & r \le 2^{l-1} \cdot r_{\text{cut}} \\ 0, & r > 2^{l-1} \cdot r_{\text{cut}} \end{cases}. \tag{12}$$

As a result of the recursion, the potential energy (1), which is estimated at the M coarser levels, can be written as

$$U_N = U_{\text{self}} + \sum_{l=0}^{M-1} U^l_{\text{loc}} + \frac{1}{2}\sum_{\mathbf{I_M},\mathbf{J_M}} Q^M_{\mathbf{I}_M} \cdot G^M_{\text{smooth}}(|R_{\mathbf{I}_M} - R_{\mathbf{J}_M}|) \cdot Q^M_{\mathbf{J}_M}, \tag{13}$$

where M is the number of levels and

$$U^l_{\text{loc}} = \frac{1}{2}\sum_{\mathbf{I}_l,\mathbf{J}_l} Q^l_{\mathbf{I}_l} \cdot G^l_{\text{loc}}(|R_{\mathbf{I}_l} - R_{\mathbf{J}_l}|) \cdot Q^l_{\mathbf{J}_l}. \tag{14}$$

Since the $G^l_{\text{loc}}(r)$ are defined on the uniform grids, their values can be prepared in small precalculated tables. The "super charges" at the grid points of level l are anterpolated from the finer-level grid

$$Q^l_{\mathbf{I}_l} = \sum_{\mathbf{K}_{l-1} \text{ such that } \mathbf{I}_l \in \sigma \mathbf{K}_{l-1}} \varpi^l_{\mathbf{I}_l}(R_{\mathbf{K}_{l-1}}) \cdot Q^{l-1}_{\mathbf{K}_{l-1}}, \qquad l \ge 2. \tag{15}$$

The recursion proceeds until the last term in (13) becomes negligible or its direct calculation does not cost very much.

The Multilevel Summation can easily be extended to systems with dipole interactions. In this case, the energy of N dipoles is defined by

$$U_N = \frac{1}{2}\sum_{i \ne j}^{N} \vec{\mu_i} \cdot \nabla_i \cdot \vec{\mu_j} \cdot \nabla_j \cdot G(|\vec{r_i} - \vec{r_j}|), \tag{16}$$

where $\vec{\mu_i}$ is the dipole moment. For the kernel $G(r) = 1/r$, substituting (2) into (16) yields the energy in the form (5) with

$$U_{\text{loc}} = \frac{1}{2}\sum_{i \ne j, r_{ij} \le r_{cut}}^{N} \left(\frac{1}{r_{ij}} \left[g_1(r_{ij}) \cdot \vec{\mu_i} \cdot \vec{\mu_j} - g_2(r_{ij}) \cdot (\vec{\mu_i} \cdot \vec{e_{ij}}) \cdot (\vec{\mu_j} \cdot \vec{e_{ij}}) \right] \right), \tag{17}$$

where $\vec{r_{ij}} = \vec{r_i} - \vec{r_j}$, $r_{ij} = |\vec{r_{ij}}|$, $\vec{e_{ij}} = \vec{r_{ij}}/r_{ij}$ and

$$g_1(r) = 1 + \frac{P'_m(r)}{r^2}, \quad g_2(r) = 3 - \frac{P''_m(r)}{r} + \frac{P'_m(r)}{r^2}. \tag{18}$$

Calculation of the anisotropic interaction (17) is more involved than (6), but only by a small fixed factor, since the functions $g_1(r)$ and $g_2(r)$ can be interpolated from precalculated tables.

The interpolation (8) of the smooth part of the kernel in (16) gives us the expression (9), except that the set of "super charges" interpolated to the first coarse level is defined by

$$Q_{\mathbf{I}} = \sum_{i \text{ such that } \mathbf{I} \in \sigma_{\mathbf{i}}} \vec{\mu_i} \nabla_i \varpi_{\mathbf{I}}(\vec{r_i}). \tag{19}$$

It follows from (19) that the interpolation maps each dipoles to charges at coarse-level gridpoints in the neighborhood of this dipole. The problem of the summation of anisotropic dipole–dipole interactions is reduced to the estimation of Coulomb interactions that can be performed recursively similar to (9).

The Multilevel Summation method was applied for the calculation of the Madelung constant of ionic crystals and the ground state of the rhombic planar rotator model. It was shown that for $r_{\text{cut}} \ge 3h$ the error is less than 0.1%.

A Monte Carlo method based on separating the potential energy into two parts, one that is less expensive to evaluate and is rapidly varying and another that is slowly varying and evaluated less frequently, was proposed in Hetenyi et al. [3] and Gelb [4]. A very efficient algorithm was developed by evaluating the interaction energy using the Multilevel Summation during this Monte Carlo process. Numerical results for Coulomb and dipole many body systems appear in the Ph.D. theses of I. Suwan and M.Sc. theses of N. Makedonska, which will be published elsewhere.

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