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Comparison of the Fast Multipole and Ewald methods for the evaluation of the magnetodipolar field in disordered systems

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Abstract

In this contribution, we present the comparative analysis of the simple Ewald, lattice-based Ewald and Fast Multipole (FMM) methods for the evaluation of the long-range dipolar field in disordered systems. We show that the FMM method with the optimally chosen hierarchical structure and the improved lattice version of the Ewald algorithm are superior with respect to original Ewald method starting from the particle number $N\sim10^4$. FMM and lattice Ewald versions demonstrate comparable performance for systems up to $N\sim4\times10^4$ particles.

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The problem of the dipolar field evaluation is especially difficult in disordered systems, where usage of the fast Fourier transformation (FFT) is impossible due to the absence of the translational symmetry of particle positions. In such systems one can either apply the Fast Multipole method (FMM) [1] or map the initial system onto a regular lattice, where the interaction field can be computed using the lattice-based Ewald method and then mapped back to initial particle positions. For systems with 1/r-interaction (gravitational and Coulomb forces) such methods are well known [2,3].

In our previous work [4] we have developed a FMM-version for the direct treatment of the dipolar interaction. Here we complete the comparative analysis of various methods for the dipolar field evaluation presenting the optimized particle-mesh Ewald algorithm based on our version of the Ewald method for dipolar lattices [5].

First we recall that the original Ewald method [2] was invented for computing conditionally converging lattice sums for Coulomb interaction in ionic crystals and is now a de facto standard for handling long-range interactions in systems with periodic boundary conditions (PBC). In such systems one has to use the Fourier expansion over the reciprocal lattice vectors $\mathbf{k}$ corresponding to the infinitely repeated simulation cell. For the point field sources the Fourier components of this expansion decay relatively slowly (or may not decay at all) with increasing k. For simulations we have to our disposal only a finite number of wave vectors. Due to the abovementioned slow decay of the Fourier components the cut-off of the Fourier spectrum of our long-range interaction at any maximal finite value k_{max} is sharp. This leads to large artificial oscillations of the interaction potential when transformed back to the real space.

The Ewald method applied to dipolar systems cures the problem by adding and subtracting a Gaussian dipole at each location of a point dipole $\boldsymbol{\mu}_i$ in the initial system. This corresponds to adding and subtracting the charge distribution

$$\rho_i^G(\mathbf{r}) = -\frac{(\mathbf{r}-\mathbf{r}_i,\boldsymbol{\mu}_i)}{(2\pi)^{3/2}\sigma^5}\exp\left[-\frac{(\mathbf{r}-\mathbf{r}_i)^2}{2\sigma^2}\right]. \quad (1)$$

The field $\mathbf{H}^{dip}$ is then calculated as the sum of contributions $\mathbf{H}^{dip}=\mathbf{H}_A^{dip}+\mathbf{H}_B^{dip}$ of subsystems A and B: the first consisting of Gaussian dipoles (1) and the second one composed of the original point dipoles minus these Gaussian

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dipoles:

$$\rho_B(\mathbf{r}) = -\sum_i^N \left[\boldsymbol{\mu}_i \cdot \nabla\delta(\mathbf{r}-\mathbf{r}_i) - \rho_i^G(\mathbf{r}-\mathbf{r}_i)\right], \quad (2)$$

where the first term in square brackets represents the charge density of a point dipole located at $\mathbf{r}_i$.

The field of a charge distribution in square brackets is [5]

$$H^\alpha_{B,i}(\mathbf{r}-\mathbf{r}_i) = \left[\frac{3(\alpha-\alpha_i)(\boldsymbol{\mu}_i\Delta\mathbf{r}_i)}{(\Delta r_i)^5} - \frac{\mu_i^\alpha}{(\Delta r_i)^3}\right] f_G(\Delta r_i) + \sqrt{\frac{2}{\pi}}\frac{(\alpha-\alpha_i)(\boldsymbol{\mu}_i\Delta\mathbf{r}_i)}{(\Delta r_i)^5}\exp\left[-\frac{(\Delta r_i)^2}{2\sigma^2}\right], \quad (3)$$

where $\alpha = x, y, z$ and $f_G(r)$ decays with distance as $\exp(-r^2)$:

$$f_G(r) = 1 - \mathrm{erf}(r/\sigma\sqrt{2}) + \sqrt{2/\pi}(r/a) \times \exp(-r^2/2\sigma^2). \quad (4)$$

After this decomposition of the original point dipole system, the field (3) from the subsystem B is short-ranged, because each point dipole is screened by a Gaussian dipole with the same total moment but the opposite sign. Hence its computation takes $\sim N$ operations for the system of N particles. Contribution from part A can be safely calculated using the Fourier expansion, because the Fourier components of the smooth Gaussian charge distribution (1) decay rapidly with k [5], thus allowing a cut-off of the Fourier spectrum at large k.

This 'naive' Ewald method, allowing a reliable evaluation of the dipolar field in systems with PBC, has for disordered systems the high operation count $\sim N^2$: particle positions do not form a regular lattice, so that the Fourier expansion for the calculation of the long-range contribution cannot be performed via the FFT. For this reason, several lattice versions of the Ewald method have been developed (see, e.g., [3]), where various mappings of the initial disordered system onto a regular lattice are used. Lacking the space for the comparison of these versions, we would like to justify our choice of the following algorithm.

(i) First we map our dipolar system onto the system of magnetic moments located on points (is the 3-index) using some weighting function $w_{3d}(\mathbf{r})$:

$$\mathbf{m}(\mathbf{r}_p) = \sum_{i=1}^N \boldsymbol{\mu}(\mathbf{r}_i) w_{3d}(|\mathbf{r}_i - \mathbf{r}_p|) = \sum_{i=1}^{M_{nb}} \boldsymbol{\mu}_i \cdot w(|x_i - x_p|) w(|y_i - y_p|) \times w(|z_i - z_p|), \quad (5)$$

(the whole method makes sense only if w is strongly localized, so that the sum over all N dipoles in Eq. (5) is actually restricted to a few nearest neighbors M_{nb} of the lattice node $\mathbf{p}$).

(ii) Then we add and subtract to each point lattice dipole a Gaussian dipole (1), as in the standard Ewald method.

(iii) Next we compute the dipolar field of this lattice system as described above.

(iv) At the last step we map the field obtained this way on the lattice points $\mathbf{r}_p$ onto initial dipole locations $\mathbf{r}_i$ using the same functions w(x) as in Eq. (5).

The advantage of this lattice Ewald version is not only the FFT-usage for computing the long-range part of $\mathbf{H}^{dip}$. Noting that the short-range contribution (3) depends only on the difference $\Delta\mathbf{r}$ between the source and target coordinates and that both source and target points are located on the lattice, we can compute the short-range contribution as a discrete convolution also using FFT. Hence we can increase the number of neighbour shells for the evaluation of the short-range part without additional time cost, thus making the corresponding truncation error arbitrarily small. The FFT-evaluation of the long-range part for the lattice system is exact anyway. Hence the only error source in our algorithm is the mapping of the disordered system onto a lattice. This error can be easily controlled and reduced by choosing the suitable mapping scheme [3]. We have found that for the lattice with the mesh size equal to the particle radius $\Delta x = R$ the 2nd-order mapping

$$w(x) = \begin{cases} 3/4 - x^2, & 0 \leqslant |x| < 1/2, \\ (3/2 - |x|)^2/2, & 1/2 \leqslant |x| < 3/2, \end{cases} \quad (6)$$

($w = 0$ for $|x| > 3/2$) provides by the evaluation of $\mathbf{H}^{dip}$ the relative error $\sim 10^{-4}$, which is small enough for all applications we have studied.

In Fig. 1 we present the speed comparison of the methods discussed above plotting the time for one field evaluation on all N particles as a function of N. All methods were adjusted to obtain the dipolar field with the same relative accuracy $\approx 10^{-3}$. The adjustable parameters are: the number of wave vectors and the real space cut-off radius for the standard Ewald, the number of multipole moments for the FMM and the lattice mesh size for the lattice Ewald version.

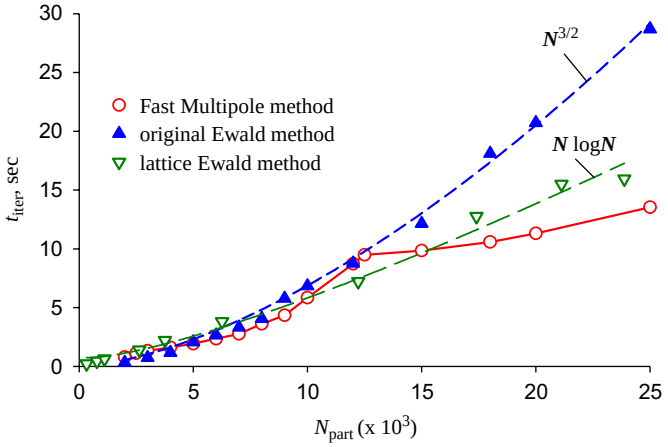

Fig. 1. Performance comparison of various methods used to calculate the dipolar field in systems with PBC (see text for details).

It can be clearly seen that the 'normal' Ewald method (accelerated by us to obtain the operation count $\sim N^{3/2}$) becomes slower than its both competitors starting from $N \sim 10^4$. Our strongly optimized FMM is comparable with the lattice Ewald method already for the same moderate particle numbers $\sim 10^4$ and becomes clearly superior for $N \geqslant 3 \times 10^4$.

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