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Adaptation and performance of the fast multipole method for dipolar systems

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Abstract

We have developed a new specialized version of the fast multipole method (FMM) for dipolar systems. For this purpose we have derived general expressions of the multipole expansion coefficients (in spherical coordinates) for a system of point dipoles with the potential $\varphi_{\text{dip}} \sim 1/r^2$. Our version is especially useful for simulations of fine magnetic particle systems (magnetic nanocomposites, ferrofluids), molecular dipolar fluids or electric dipolar glasses.

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Keywords: Fast multipole method; Dipolar system

1. Introduction and motivation

The fast multipole method (FMM) allows for a certain class of matrices to perform the matrix-vector multiplication in $O(N)$ instead of $O(N^2)$ operations with any desired accuracy. Since the constant prefactor in this $O(N)$-dependence is quite large, the FMM is practically suitable only for large-scale simulations. It has been proved to be very useful by simulation of systems with long-range interactions (molecular fluid dynamics, electrostatics, astrophysics etc.) as well as for numerical solution of partial differential equations (acoustics). By the simulation of dipolar systems, however, this method has been barely used probably due to the following two reasons.

(A) The standard FMM-technique [1] is based on the well-known series expansion of the function $1/r$ and so can be applied to the evaluation of corresponding potentials and/or forces (electrostatics or gravity). The potential of a magnetic dipole decays, however, as $\sim 1/r^2$ and so the analytical derivation of its multipole expansion is not straightforward; up to our knowledge the corresponding general expression was not derived up to now. The only relevant attempt to use FMM for dipolar systems was made by Kutteh et al. [2], where a few first multipole expansion coefficients for dipolar systems were calculated *manually* (in Cartesian coordinates), which obviously imposes a strong limitation on the expansion order and limits the accuracy of simulations.

(B) As an alternative to FMM a quite powerful method for simulation of dipolar systems—the Ewald method (EwM) exists (see, e.g., Ref. [3]). Its standard version is very time consuming ($O(N^2)$), but some time ago new versions with the operation count $\sim O(N^{3/2})$ (3/2-EwM) or even $\sim O(N \log N)$ were developed [3].

In this article we present the *analytical* expression of multipole coefficients for magnetic potential and compare the computational costs of the FMM and the 3/2-EwM. We have found that the FMM is comparable with 3/2-EwM even for moderate systems ($\sim 10^4$ particles) and is definitely faster than 3/2-EwM for large-scale simulation ($N > 3 \times 10^4$).

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2. Analytical expression for the multipole coefficients of the dipolar magnetic potential

To demonstrate how to evaluate multipole coefficients for the dipolar potential, let us first consider a system of N charges q_i located at the points $Q_i = (\rho_i, \alpha_i, \beta_i)$, $i = 1 \ldots N$. We can evaluate the electrostatic potential of such system at the point $P = (r, \theta, \varphi)$, $r > \rho_i$, using the well-known series expansion

$$\frac{1}{r_i'} = \sum_{n=0}^{\infty} \frac{\rho_i^n}{r^{n+1}} P_n(\cos\gamma_i),$$

where $\mathbf{r}_i' = \mathbf{r} - \rho_i$, γ_i is the angle between the vectors $\mathbf{r}$ and $\boldsymbol{\rho}_i$, P_n are Legendre polynomials. The resulting expansion of the potential is

$$\Phi(P) = \sum_{i=1}^{N} q_i \sum_{n=0}^{\infty} \frac{\rho_i^n}{r^{n+1}} P_n(\cos\gamma_i) = \sum_{n=0}^{\infty} \sum_{k=-n}^{n} M_n^k \frac{Y_n^k(\theta,\ \phi)}{r^{n+1}},$$

where

$$M_n^k = \sum_{i=1}^{N} q_i \rho_i^n Y_n^{-k}(\alpha_i,\ \beta_i)$$

are multipole coefficients and Y_n^k denote spherical functions. The FMM uses these coefficients for calculation of a far-field contribution to the potential (the near-field part is evaluated by the direct summation). Our aim is to evaluate these coefficients for a system of dipoles. Afterwards they will be used in the dipolar FMM-version in the same way as in electrostatics.

We consider now a system of N magnetic dipoles $\boldsymbol{\mu}_i$ at the points $Q_i = (\rho_i, \alpha_i, \beta_i)$, $i = 1 \ldots N$. We build each dipole as a limit of the following standard construction: two charges $q_i^+ = q_i$ and $q_i^- = -q_i$ are located at points $Q_i^+ = (\rho_i^+, \alpha_i^+, \beta_i^+)$ and $Q_i^- = (\rho_i^-, \alpha_i^-, \beta_i^-)$ connected via the vector $2\mathbf{d}_i$ (so that $\boldsymbol{\rho}_i^+ = \boldsymbol{\rho}_i + \mathbf{d}_i$ and $\boldsymbol{\rho}_i^- = \boldsymbol{\rho}_i - \mathbf{d}_i$). The length $d_i \to 0$ and the charge magnitudes $q_i \to \infty$ so that the product $2\mathbf{d}_i q_i = \boldsymbol{\mu}_i$ $\boldsymbol{\rho}_i - \mathbf{d}_i$ remains constant. Next we write down the potential in the same way as in electrostatics and expand the corresponding expression at the points Q_i over small parameters d_i and pairs of angles appearing due to the introducing of small vectors $\mathbf{d}_i$. After tedious but straightforward calculations we obtain the final expression for multipole coefficients:

$$M_n^k = \sum_{i=1}^{N} n(\boldsymbol{\mu}_i, \boldsymbol{\rho}_i) \rho_i^{n-2} Y_n^{-k}(\alpha_i, \beta_i) + \sum_{i=1}^{N} (\boldsymbol{\mu}_i,\ \mathbf{H}_{i,n}^{-k}) \rho_i^{n-1}$$

with

$$\mathbf{H}_{i,n}^k = \begin{pmatrix} \cos\alpha_i \cos\beta_i \dfrac{\partial Y_n^k(\alpha_i,\ \beta_i)}{\partial \alpha_i} - \dfrac{\sin\beta_i}{\sin\alpha_i} \dfrac{\partial Y_n^k(\alpha_i,\ \beta_i)}{\partial \beta_i} \\ \cos\alpha_i \sin\beta_i \dfrac{\partial Y_n^k(\alpha_i,\ \beta_i)}{\partial \alpha_i} + \dfrac{\cos\beta_i}{\sin\alpha_i} \dfrac{\partial Y_n^k(\alpha_i,\ \beta_i)}{\partial \beta_i} \\ -\sin\alpha_i \dfrac{\partial Y_n^k(\alpha_i,\ \beta_i)}{\partial \alpha_i} \end{pmatrix}.$$

Here we would like to discuss briefly the convergence of the multipole expansion series. In electrostatics taking p moments ($\Phi(P) \approx \sum_{n=0}^{p} \sum_{k=-n}^{n} M_n^k Y_n^k(\theta,\ \phi)/r^{n+1}$), we achieve the accuracy of the order $(a/r)^{p+1}$, where a is the radius of the sphere which includes all charges. Using the same technique as by evaluation of M_n^k one can derive the corresponding error for the magnetic potential which is of order $p^2(a/r)^{p+1}$. This rate is slightly worth than in electrostatics, but it does not lead to any complications.

3. Implementation and speed comparisons

The expression for multipole coefficients of magnetic dipolar potential should be utilized in exactly the same way as its counterpart from electrostatics. So one can use for his simulation an arbitrary FMM-algorithm from the numerous ones developed for other areas of physics. We have implemented a quite optimal (with tabulations of the most time consuming calculations) version of the original Greengard–Rokhlin method [1]. We have performed our simulations taking $p = 3$, 4 and 5 multipole moments what corresponds to the accuracy

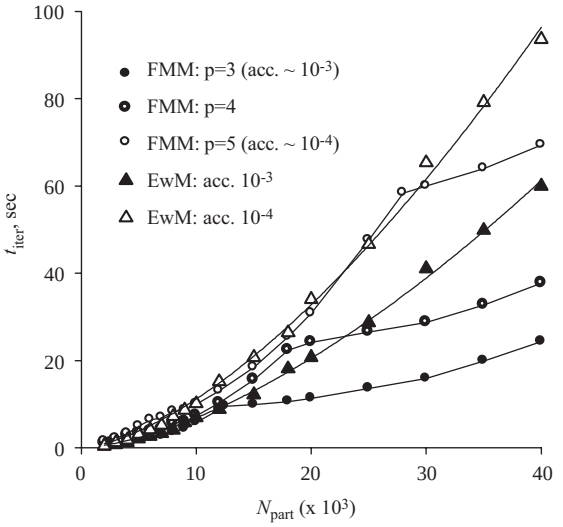

Fig. 1. Comparison of times necessary for one evaluation of the dipolar field on all particles using various methods (see legend) on the particle number (simulations performed on an Athlon 2.7 GHz PC with 1 GB RAM).

region 10^{-3}–10^{-4}. For the speed comparison we have used a standard implementation of the 3/2-EwM (we thank Dr. D. Stock for providing the corresponding routine) and performed the simulation with the same fixed accuracy as by the FMM algorithm.

Simulations were performed for periodic boundary conditions (PBC); the improved version of FMM (reduced interaction list) for PBC based on those given in Ref. [4] was used. Comparing simulation times presented in Fig. 1 one can clearly see that depending on the required accuracy our FMM-version for dipolar systems becomes superior to the 3/2-EwM starting from a few tens of thousands particles $N \sim (20-30) \times 10^3$.

Results of simulation of the ferrofluid dynamics based on the FMM-version for dipolar systems described above will be reported in future publications.

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