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Fast Multipole Method Using Cartesian Tensor in Beam Dynamic Simulation

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Abstract. The fast multipole method (FMM) using traceless totally symmetric Cartesian tensor to calculate the Coulomb interaction between charged particles will be presented. The Cartesian tensor based FMM can be generalized to treat other non-oscillating interactions with the help of the differential algebra or the truncated power series algebra. Issues on implementation of the FMM in beam dynamic simulations are also discussed.

INTRODUCTION

Collective effects are very important in modern accelerators. Numerical simulation is inevitable to study strong and highly nonlinear collective effects. Most current simulation codes use the Particle-in-cell (PIC) method [1]. The grid in the PIC method could be inconvenient in some scenarios. For example, it may be difficult to generate an efficient grid for a system with strongly nonuniform charge distribution and/or complex geometry. If the charged area is much smaller than the boundary, redundant computation is unavoidable, due to the grid that covers the whole domain. In a highly correlated system, it is difficult to accurately calculate the local interaction to simulate the fine structures by the PIC method without using a very fine grid, which greatly increases the computation cost. In such cases, the grid-free fast multipole method (FMM) [2] may be preferred.

The FMM method takes advantage of the fact that the long-range Coulomb field decreases quickly as the distance between the charges increases, so that the field contributed from the particles far away from the observer can be represented by multipole expansions, while the near region interaction is calculated using the theoretical formula. The total field is the summation of the near region field and the far region field. The area with no charges is ignored in the computation. The grid-free property allows the FMM to treat systems with any charge distribution and any geometry efficiently. And since the local interactions are calculated accurately without any approximation, the FMM has the ability to keep the fine structures of a strongly correlated system. For any non-oscillating interactions between N particles, including the Coulomb interaction, the FMM has an efficiency that scales $O(N)$.

THE GRID-FREE FAST MULTIPOLE METHOD

A Brief Description of the Fast Multipole Method

In the FMM, the whole charged domain is divided into boxes of different sizes, according to the charge density, and the amount of particles inside each box is kept roughly equal. The hierarchical structure of the boxes forms a partial tree with empty boxes discarded. A 2D example is shown in Fig. 1. The 3D FMM is in principle the same. The field contribution from one box to its far region can be represented by a multipole expansion. The multipole expansion of a childless box, a leaf in the tree, is calculated from the particles inside the box. The multipole expansion of a parent box is calculated by shifting and adding up the multipole expansions of its child boxes. The field contribution from the far region of one box to the domain inside the box can be represented by a local expansion around the box center. The local

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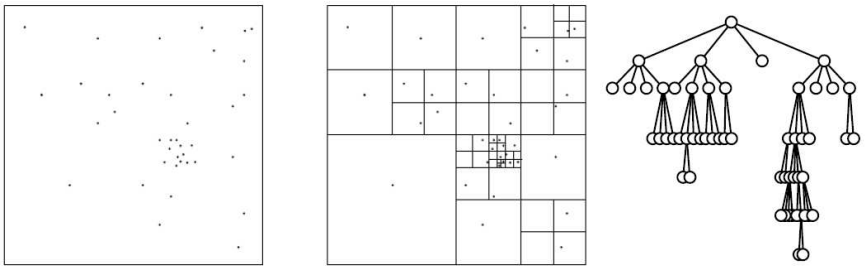

FIGURE 1. Decomposition of the charged domain for FMM.

expansion is calculated from the multipole expansions of the far region boxes or from the charges of the far region boxes. The child boxes inherit the local expansion from their ancestor boxes. The field on a particle is only calculated inside the childless box, and it composes two parts: the far region field calculated by expansions, and the near region field calculated by the theoretical formula. The FMM can be summarized as the following steps. (1) Decompose the whole domain into small boxes and build up the hierarchical tree structure of boxes. (2) Going upward, from the finest level to the coarsest level, calculate the multipole expansion for each box. (3) Going downward, from the coarsest level to the finest level, calculate the local expansion for each box. (4) Inside each childless box, calculate the far region field from the expansions, calculate the near region field by the theoretical formula, and take the summation of them. The detailed description of the algorithm can be found in [3].

Fast Multipole Method Using Cartesian Tensor

Besides the construction of the hierarchical tree of boxes, the FMM includes the following operations: (i) Calculate the multipole expansion from the source particles (P2M), (ii) translate the multipole expansions from the child boxes to their parent box (M2M), (iii) convert the multipole expansions into the local expansions (M2L), (iv) translate the local expansions from a parent box into its child boxes (L2L), (v) calculate the local expansions from the source particles (P2L), (vi) calculate the potential/field on the observer particles from the local expansions (L2P), (vii) calculate the potential/field on the observer particles from the multipole expansions (M2P), and (viii) calculate the potential/field on the observer particles due to the source particles nearby using the pairwise theoretical formula (P2P).

The expansions of the Coulomb potential can be constructed in spherical frame as a series of spherical harmonic functions [4, 5], or in Cartesian frame using the Taylor expansion [6, 7, 8]. In the Cartesian frame, the expansions can be represented as contractions of Cartesian tensors. An n^{th} order Cartesian tensor generally has n^3 elements. A totally symmetric Cartesian tensor, which is used to construct the multipole and the local expansions for an interaction in $r^{-\nu}$ format [7], has $(n+1)(n+2)/2$ independent elements. Specifically, for the Coulomb interaction, the Cartesian tensor is traceless and has only $2n+1$ independent elements. In the following, we list the formulas for Coulomb potential/field using the traceless totally symmetric Cartesian tensor.

- **Particles to multipole expansion (P2M)** Consider a domain $\Omega_s \in \mathbb{R}^3$ that is populated with k sources. The i^{th} source has charge q_i and locates at $\mathbf{r}_i \in \Omega_s$, where $i = 1, \cdots, k$. The total potential due to these k sources at any point $\mathbf{r}$, which is far enough away, is given as

$$\phi(\mathbf{r}) = \sum_{i=1}^{k} \frac{q_i}{\|\mathbf{r} - \mathbf{r}_i\|} = \sum_{n=0}^{\infty} \mathbf{M}^{\{n\}} : \boldsymbol{\nabla}^{\{n\}} \frac{1}{r} \quad \text{with} \quad \mathbf{M}^{\{n\}} = \sum_{i=1}^{k} (-1)^n \frac{q_i}{n!} \mathbf{r}_i^{\{n\}}. \tag{1}$$

  $\mathbf{M}^{\{n\}}$ is the multipole expansion around the origin.
- **Multipole expansion to multipole expansion (M2M)** Given a multipole expansion of k sources around $\mathbf{r}_s$, the multipole expansion around the point $\mathbf{r}_{s'}$ can be expressed as

$$\mathbf{M}'^{\{n\}} = \sum_{m=0}^{n} \sum_{P(m,n)} \frac{m!}{n!} \mathbf{r}_{ss'}^{\{n-m\}} \mathbf{M}^{\{m\}}, \tag{2}$$

  where $\mathbf{r}_{ss'} = \mathbf{r}_{s'} - \mathbf{r}_s$ and $P(n, m)$ is the permutation of all partitions of n into sets $n - m$ and m.

- **Multipole expansion to local expansion (M2L)** Assume that the domains Ω_s and Ω_o are sufficiently separated. If a multipole expansion $\mathbf{M}^{\{n\}}$ is located at $\mathbf{r}_s$, then another expansion $\mathbf{L}^{\{n\}}$ that locates at $\mathbf{r}_o$ and produces the same field $\forall \mathbf{r} \in \Omega_o$ is given by

$$\mathbf{L}^{\{n\}} = -\sum_{m=n}^{\infty} \frac{1}{n!} \mathbf{M}^{\{m-n\}} : \boldsymbol{\nabla}^{\{m\}} \frac{1}{r_{so}}, \tag{3}$$

where $\mathbf{r}_{so} = \mathbf{r}_o - \mathbf{r}_s$. $\mathbf{L}^{\{n\}}$ is called the local expansion since it locates in the observer domain Ω_o, and the potential can be calculated as

$$\phi(\mathbf{r}) = \sum_{n=0}^{\infty} \boldsymbol{\rho}^{\{n\}} : \mathbf{L}^{\{n\}} \quad \text{with} \quad \boldsymbol{\rho} = \mathbf{r} - \mathbf{r}_o \tag{4}$$

- **Particles to local expansion (P2L)** The potential inside a domain Ω_o, centered at $\mathbf{r}_o$, due to k sources that are far away enough can be expressed as

$$\phi(\mathbf{r}) = \sum_{i=1}^{k} \frac{q_i}{\|\boldsymbol{\rho} - \mathbf{r}_i\|} = \sum_{n=0}^{\infty} \boldsymbol{\rho}^{\{n\}} : \mathbf{L}^{\{n\}} \quad \text{with} \quad \mathbf{L}^{\{n\}} = \sum_{i=1}^{k} \frac{q_i}{n!} \boldsymbol{\nabla}^{\{n\}} \frac{1}{r_i}, \tag{5}$$

where $\mathbf{r}_i$ is the vector from the i^{th} source with charge q_i pointing to $\mathbf{r}_o$, and $\boldsymbol{\rho} = \mathbf{r} - \mathbf{r}_o$.

- **Local expansion to local expansion (L2L)** A local expansion $\mathbf{L}^{\{n\}}$ that exists in the domain Ω_o centered around $\mathbf{r}_o$ can be shifted to a subdomain centered at $\mathbf{r}_{o'}$ using

$$\mathbf{L}'^{\{n\}} = \sum_{m=n}^{\infty} \begin{pmatrix} m \\ m-n \end{pmatrix} \mathbf{L}^{\{m\}} : \mathbf{r}_{oo'}^{\{m-n\}} \quad \text{with} \quad \mathbf{r}_{oo'} = \mathbf{r}_{o'} - \mathbf{r}_o \tag{6}$$

- **Potential calculation using multipole expansion (M2P) and local expansion(L2P)** The potential at any point $\mathbf{r}_i$ far away from domain Ω_o centered around $\mathbf{r}_o$ can be obtained using

$$\phi(\mathbf{r}_i) = \sum_{n=0}^{\infty} \mathbf{M}^{\{n\}} : \boldsymbol{\nabla}^{\{n\}} \frac{1}{\rho_i} \quad \text{with} \quad \boldsymbol{\rho}_i = \mathbf{r}_i - \mathbf{r}_o, \tag{7}$$

or the potential at any point $\mathbf{r}_i$ inside domain Ω_o centered around $\mathbf{r}_o$ can be obtained using

$$\phi(\mathbf{r}_i) = \sum_{n=0}^{\infty} \mathbf{L}^{\{n\}} : \boldsymbol{\rho}_i^{\{n\}} \quad \text{with} \quad \boldsymbol{\rho}_i = \mathbf{r}_i - \mathbf{r}_o. \tag{8}$$

The high order gradients of function r^{-1} need to be calculated in Eqs. (3), (5), and (7). The formula in Cartesian coordinates can be derived from Maxwell's expression for solid harmonics [9]. Since the expansions are represented as contractions of Cartesian tensors, the error of the algorithm is determined by the order of the Cartesian tensor. The higher the order, the lower the error. Knowing that the explicit expression for the potential has been derived as a function of the Cartesian coordinates, the field can be easily calculated by taking the derivative of the respective coordinate.

Figure 2 shows the computation time for the Coulomb potential and field among 10,000 to 10,000,000 electrons with a Gaussian distribution. The expansions are calculated up to the sixth order, and the relative error is less than 1.8×10^{-5} and 3.7×10^{-4}, respectively, for the potential and the field. Fitting the data linearly in the logarithm scale plot, the slopes of the straight lines are 1.020 for the potential calculation and 1.006 for the field calculation. Both slopes are very close to one, which means the algorithm does scale linearly with the number of particles.

The FMM is not limited to the calculation of Coulomb interactions. It can be applied to accelerate the computation of other non-oscillating pairwise interactions and still maintain an efficiency of $O(N)$ for N interacting elements. Algorithms that calculate an arbitrary user-defined non-oscillating interaction using the FMM have been developed. The two best-known ones are the kernel-independent FMM [10] and the black box FMM [11]. The Cartesian tensor based FMM can also be generalized for arbitrary non-oscillating interactions, for which one only needs to replace the gradients of r^{-1} in Eqs. (3), (5), and (7) with the gradients of the user-defined function $f(\mathbf{r})$. Symbolic calculation of the gradients for an arbitrary function is very difficult, but it is not necessary. We notice that the gradients needs to be

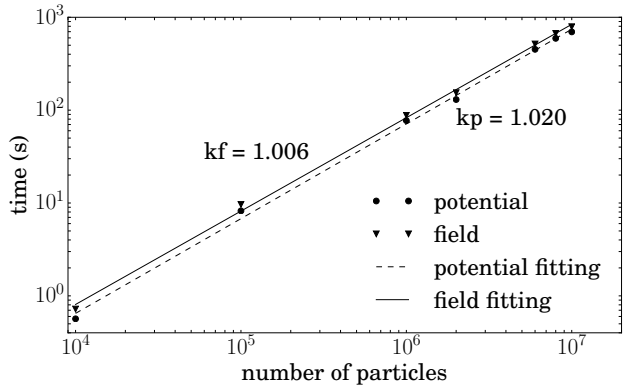

FIGURE 2. Computation time for Coulomb potential and field calculation.

calculated in three cases: (1) calculate the multipole expansion from the particles inside a childless box; (2) calculate the local expansion from the particles inside a childless box; and (3) transform a multipole expansion into a local expansion. In all the three cases, when the gradients are calculated, the value of $\mathbf{r}$ is known, and it is either the vector from the center of the childless box to the particle for case (1) and (2), or the vector from the center of the source box holding the multipole expansion to the center of the objective box holding the local expansion. In accelerator physics, the differential algebra (DA) or the truncated power series algebra (TPSA) is widely used to calculate the high order transfer map of a beam transport system. DA and TPSA can be used to calculate the Taylor expansion of a function $f(\mathbf{r})$ at a given value $\mathbf{r}$, even if $f(\mathbf{r})$ has even no explicit expression and can only be numerically calculated by codes. Combining the DA and the FMM using Cartesian tensors, we will be able to generalize the Cartesian-based FMM from Coulomb interaction to any arbitrary non-oscillating interaction. The Cartesian tensor will not be traceless any more, but it is still totally symmetric with $(n+1)(n+2)/2$ independent elements, as long as the derivative of the coordinates are commutable, which is usually satisfied. A prototype code to test the idea has been developed. We calculate the dipole radiation field $\mathbf{E} = \frac{e\mathbf{r}}{4\pi\varepsilon_0 r^3} + \frac{e}{4\pi\varepsilon_0 c^2 r^3}\mathbf{r}\times(\mathbf{r}\times\dot{\mathbf{v}})$ of 16,384 electrons with given positions and accelerations. Table 1 shows the relative errors for different tensor orders. Clearly the error decreases as the order increases, which means the algorithm converges. More work is needed to improve the efficiency of the algorithm.

TABLE 1. Relative error decreases as the Cartesian tensor order increases in the dipole radiation field calculation using Cartesian tensor-based FMM with DA.

Order	2	4	6	8	10
Error	3.93×10^{-2}	1.08×10^{-2}	3.83×10^{-3}	1.48×10^{-3}	6.71×10^{-4}

Issues on Implementing FMM in Beam Dynamic Simulations

The FMM has already been successfully implemented in beam dynamic simulations on the space charge effects [12]. Here we want to discuss three issues related to the simulations: numerical noise, boundary condition, and parallel computation. If a continuous beam is modeled by point charges, when some charges move close to each other, an abrupt increase of potential/field may occur due to the singularity of the Coulomb field at $r = 0$. Such a numerical noise is the result of the point charge model. It can be avoided if the point charges are replaced by small Gaussian electron bunches. The field of a Gaussian bunch reduces to the potential of a point charge when the distance is large enough from the center of the bunch, while the field reduces to zero when the distance goes to zero. Thus the singularity is removed and the field is smooth. In FMM, only the far region field is represented by expansions, so there is no need to change anything in the far-field calculation. Only the point charge field formula for the near region field calculation needs to be replaced by the formula for a Gaussian bunch.

In many beam dynamic simulations, boundary conditions (BC) cannot be ignored, and one needs to solve the boundary value problem (BVP) with Dirichlet BC, Neumann BC, or a mixture of them. The BVP can be solved by the boundary element method (BEM) as follows [13]. First, derive a boundary integral equation (BIE) from the BC

using the Green's function. Converting the problem in the whole domain into the BIE on the boundary, the dimension of the problem is reduced by one. Second, divide the boundary into small elements and discretize the BIE into a linear system. Third, solve the linear system iteratively to get the potential and its derivatives on the boundary. Finally, calculate the potential in the domain using its integral representation. The FMM can be used to accelerate the integral computation on the boundary and/or the whole domain. Details about this method can be found in [13].

Even with a fast algorithm, some complicated simulations are only practical with the power of modern cluster machines. The parallelization of the FMM is very challenging because of the unbalanced partial tree structure, which changes during the simulation with respect to the motion of the particles. But parallel FMM libraries with high parallel efficiency on hybrid CPU-GPU clusters, e.g. ExaFMM [14] and PKIFMM [15], have been developed and successfully implemented to solve scientific problems [16, 17]. Both libraries are open source, which allows researchers to make further development using them. The FMMs for different interactions share the same framework, so that only parts of the code need to be revised for a new interaction, which makes it easier to reuse the existing code.

SUMMARY

The FMM using a traceless totally symmetric Cartesian tensor has been developed. Combining with the DA or TPSA, the Cartesian tensor-based FMM can be generalized to other non-oscillating interactions. The FMM scales linearly with the number of particles for non-oscillating interaction. Due to its gridless property, the FMM catches exactly the charged domain and the boundary for any charge distribution and geometry, and avoids redundant computation in the charge-free space. In the FMM, the near region field is calculated without approximation, which helps to simulate the fine structure of a highly correlated system. The FMM has been successfully implemented in beam dynamic simulations of the space charge effect.

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