FAST MULTIPOLE APPROXIMATION OF 3D SELF FIELDS EFFECT IN HIGH BRIGHTNESS ELECTRON BEAMS

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Abstract

A tree-code approach for the computation of space charge effects between N mutually interacting bodies is presented in the context of electron beam dynamics in high brilliance photo-injectors. Computational effort in simulations of such "dense" systems is usually dominated by evaluation of self-interaction effects. The method described here is based on a hierarchy of cubic cells incorporating a fraction of the total charge, which can be made to mutually interact by first computing fields from a distant cell at another cell center of mass by means of a multipole approximation of some type followed by a local expansion to actual positions of macroparticles therein. It has been shown such an approach to reduce the complexity of the problem to $\mathcal{O}(N)$.

INTRODUCTION

High brilliance, coherent X-ray sources require the generation of high current/low emittance electron beams. Numerical codes devoted to the simulation of such "dense" systems must account for beam self-interaction. A variety of methods have been devised to solve this problem. In this contribution a tree-code[1] algorithm is discussed. These methods are based on sorting of macroparticles in a hyerarchical tree of cubic cells, whose charge multipole moments are precomputed and stored. At any other particle's position, the field from the charges of a given cell are evaluated by a suitable multipole expansion[2] if the particle is well separated from the cell; otherwise the fields from the cell's children are summed, in an iterative branching process bound to cease when all the cells host at most one particle. It has been shown that the number of interactions per particle inherent to such an approach is $\mathcal{O}(\log N)$, so that the overall complexity is $\mathcal{O}(N \log N)$. Insofar, these methods have been used to atomic physics, electromagnetics[3] fluid [4] and stellar([5, 6] dynamics and extended to three dimensions[7]. In this contribution a cartesian formulation of the type described in ref. [6] has been implemented in the context of simulation code TREDI[8], a 3D Monte-Carlo devoted to simulation of non axi-symmetric beam dynamics in RF photo-injectors featuring a covariant smoothing technique to suppress numerical artifacts in electromagnetic self-fields[9].

APPROXIMATION OF VELOCITY (COULOMB) FIELDS

The electrostatic potential of a N-body discrete charge distribution generated at all charge positions $\boldsymbol{r}_i$ by the other $N-1$ particles writes

$$\Phi(\mathbf{r_i}) = \sum_{j \neq i} q_j G(\boldsymbol{r}_i - \boldsymbol{r}_j) \tag{1}$$

where q_i is the charge of i^{th} particle and

$$G(\boldsymbol{r}_i - \boldsymbol{r}_j) = \frac{1}{\|\boldsymbol{r}_i - \boldsymbol{r}_j\|} \tag{2}$$

The value of Green function (2) for a generic argument $\boldsymbol{\xi}$ can be Taylor expanded around a given position $\boldsymbol{\Delta}$ is the

$$G(\boldsymbol{\xi}) \approx \sum_{k=0}^{p} \frac{1}{k!} (\boldsymbol{\xi} - \boldsymbol{\Delta})^{(k)} \odot \nabla^{(k)} G(\boldsymbol{\Delta}) \tag{3}$$

up to a given truncation order p. The notation follows Warren and Salmon [4] by using a shorthand in which $\boldsymbol{x}^{(n)}$ indicates the n-fold outer product of the vector $\boldsymbol{x}$ by itself (in d dimension, a d^n-component symmetric tensor) and the symbol $\odot$ the (tensor) inner product. For example, assuming that in (2) particle "i" belongs to cell A and particle "j" to cell B (see fig. 1 for details), $G(\boldsymbol{\xi})$ (with $\boldsymbol{\xi} = \boldsymbol{r}_i - \boldsymbol{r}_j$) can be expanded around cell separation $\boldsymbol{\Delta} = \mathbf{r}_A - \mathbf{r}_B$ ($\boldsymbol{r}_A$ and $\boldsymbol{r}_B$ are the weighted mean positions of charges contained in cells A and B, respectively). In general, for any $\boldsymbol{\xi} = \boldsymbol{x} - \boldsymbol{y}$ with $\boldsymbol{x} \in \mathrm{A}, \boldsymbol{y} \in \mathrm{B}$ one can further expand $(\boldsymbol{\xi} - \boldsymbol{\Delta})^{(k)}$ in $\boldsymbol{x}$ around $\boldsymbol{r}_A$ and in $\boldsymbol{y}$ around $\boldsymbol{r}_B$:

$$\begin{aligned} (\boldsymbol{\xi} - \boldsymbol{\Delta})^{(k)} &= [(\boldsymbol{x} - \boldsymbol{r}_A) + (\boldsymbol{r}_B - \boldsymbol{y})]^{(k)} \\ &= \sum_{m=0}^{p} \binom{k}{m} (\boldsymbol{x} - \mathbf{r}_A)^{(m)} \odot (\mathbf{r}_B - \boldsymbol{y})^{(k-m)} \end{aligned} \tag{4}$$

for any $p \geq k$. Substituting back in (3) and re-ordering sums yields:

$$\begin{aligned} G(\boldsymbol{\xi}) &\approx \sum_{k=0}^{p} \frac{1}{k!} \sum_{m=0}^{p} \binom{k}{m} (\mathbf{x} - \mathbf{r}_A)^{(m)} \\ &\quad \odot (\mathbf{r}_B - \boldsymbol{y})^{(k-m)} \odot \boldsymbol{\nabla}^{(k)} G(\boldsymbol{\Delta}) \\ &= \sum_{m=0}^{p} \frac{(\mathbf{x} - \mathbf{r}_A)^{(m)}}{m!} \odot \boldsymbol{\Gamma}_{\boldsymbol{B}}^{(\boldsymbol{m})}(\boldsymbol{y}, \boldsymbol{\Delta}) \end{aligned} \tag{5}$$

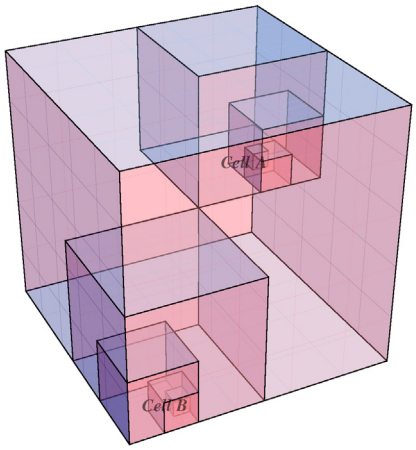

Figure 1: A tree hierarchy of cubic cells.

where

$$\boldsymbol{\Gamma}_{\boldsymbol{B}}^{\boldsymbol{m}}\left(\boldsymbol{y},\boldsymbol{\Delta}\right) = \sum_{n=0}^{p-m}\frac{\left(\boldsymbol{y}-\boldsymbol{r}_{B}\right)^{(n)}}{n!}\odot\boldsymbol{\nabla}^{(n+m)}G\left(\boldsymbol{\Delta}\right) \tag{6}$$

Putting (5) in (1) yields the final expression for the potential at a generic position $\boldsymbol{x}$ in cell A (e.g. $\boldsymbol{x}=\boldsymbol{r}_{i}$) from charges in cell B:

$$\Phi_{BA}\left(\boldsymbol{x}\right)\approx\sum_{m=0}^{p}\frac{1}{m!}\left(\boldsymbol{x}-\mathbf{r}_{A}\right)^{(m)}\odot C_{B}^{(m)}\left(\mathbf{r}_{A}-\mathbf{r}_{B}\right) \tag{7}$$

with

$$\boldsymbol{C}_{\boldsymbol{B}}^{(\boldsymbol{m})}\left(\boldsymbol{\Delta}\right)=\boldsymbol{Q}_{B}\cdot\sum_{n=0}^{p-m}\frac{(-1)^{n}}{n!}\boldsymbol{\nabla}^{(n+m)}G\left(\boldsymbol{\Delta}\right)\odot\boldsymbol{Q}_{B}^{(n)} \tag{8}$$

where

$$\boldsymbol{Q}_{B}^{(n)}=\frac{1}{Q_{B}}\sum_{j\in B}q_{j}\left(\boldsymbol{r}_{j}-\boldsymbol{r}_{B}\right)^{(n)} \tag{9}$$

is the (normalized) n^{th}-order charge multipole moment and Q_{B} the total charge in cell B. Since is clear that

$$\boldsymbol{C}_{\boldsymbol{B}}^{(\boldsymbol{m}+\mathbf{1})}\left(\boldsymbol{\Delta}\right)=\boldsymbol{\nabla}\boldsymbol{C}_{\boldsymbol{B}}^{(\boldsymbol{m})}\left(\boldsymbol{\Delta}\right)$$

it follows that the $\boldsymbol{C}$'s can be Taylor expanded as follows

$$\boldsymbol{C}_{\boldsymbol{B}}^{(\boldsymbol{m})}\left(\boldsymbol{\Delta}+\boldsymbol{\epsilon}\right)=\sum_{n=0}^{p-m}\frac{1}{n!}\boldsymbol{\epsilon}^{(n)}\odot\boldsymbol{C}_{\boldsymbol{B}}^{(\boldsymbol{m}+\boldsymbol{n})}\left(\boldsymbol{\Delta}\right)$$

Electric field is

$$\boldsymbol{E}_{BA}\left(\boldsymbol{x}\right)\approx-\sum_{m=0}^{p}\frac{1}{m!}\left(\boldsymbol{x}-\mathbf{r}_{A}\right)^{(m)}\odot\boldsymbol{C}_{B}^{(m+1)}\left(\mathbf{r}_{A}-\mathbf{r}_{B}\right) \tag{10}$$

In particular

$$\boldsymbol{E}_{BA}\left(\boldsymbol{r}_{A}\right)=-\boldsymbol{C}_{B}^{(1)}\left(\mathbf{r}_{A}-\mathbf{r}_{B}\right) \tag{11}$$

For a newtonian ($G=r^{-1}$) potential the explicit form for the first few coefficients $\boldsymbol{C}$ is

$$\begin{aligned}
\boldsymbol{C}_{\boldsymbol{B}}^{(\mathbf{0})} &= \boldsymbol{Q}_{B}\left[D^{(0)}+\frac{1}{2}D^{(1)}\boldsymbol{Q}_{B,mm}^{(2)}\right.\\
&\quad\left.+\frac{1}{2}D^{(2)}\boldsymbol{\Delta}_{m}\cdot\boldsymbol{Q}_{B,mn}^{(2)}\cdot\boldsymbol{\Delta}_{n}+\ldots\right]\\
\boldsymbol{C}_{\boldsymbol{B},\boldsymbol{i}}^{(\mathbf{1})} &= \boldsymbol{Q}_{B}\left[\left(D^{(1)}+\frac{1}{2}D^{(2)}\boldsymbol{Q}_{B,mm}^{(2)}+\right.\right.\\
&\quad\left.\left.+\frac{1}{2}D^{(3)}\boldsymbol{\Delta}_{m}\cdot\boldsymbol{Q}_{B,mn}^{(2)}\cdot\boldsymbol{\Delta}_{n}+\ldots\right)\boldsymbol{\Delta}_{i}+\right.\\
&\quad\left.+D^{2}\boldsymbol{Q}_{B,im}^{(2)}\cdot\boldsymbol{\Delta}_{m}+\ldots\right]\\
\boldsymbol{C}_{B,ij}^{(2)} &= \boldsymbol{Q}_{B}\left[\left(D^{(1)}\delta_{ij}+D^{(2)}\boldsymbol{\Delta}_{i}\boldsymbol{\Delta}_{j}+\ldots\right)\right]\\
\boldsymbol{C}_{B,ijk}^{(3)} &= \boldsymbol{Q}_{B}\left[D^{(2)}\left(\delta_{ij}\boldsymbol{\Delta}_{k}+\delta_{jk}\boldsymbol{\Delta}_{i}+\delta_{ki}\boldsymbol{\Delta}_{j}\right)\right.\\
&\quad\left.+D^{(2)}\boldsymbol{\Delta}_{i}\boldsymbol{\Delta}_{j}\boldsymbol{\Delta}_{k}+\ldots\right]
\end{aligned} \tag{12}$$

where

$$D^{(n)}=\left(-1\right)^{n}\frac{(2n-1)!!}{\Delta^{2n+1}} \tag{13}$$

In the first term of $\boldsymbol{C}_{\boldsymbol{B}}^{(\mathbf{1})}$ is easily recognizable the monopole approximation $\boldsymbol{E}_{B}\approx\boldsymbol{Q}_{B}D^{(1)}\boldsymbol{\Delta}=-\boldsymbol{Q}_{B}\frac{\boldsymbol{\Delta}}{\Delta^{3}}$. Simulation of space charge effects in accelerators require also magnetic self-interactions to be accounted for. A typical assumption[10] is that a reference frame exists where the beam is at rest and particles interact only through electrostatic forces, determined by means of a Poisson solver. Splitting of the beam in several "slices" mitigates the effect of energy spread[11]. In the approach described in Ref. [9] smoothing of self-fields is based on the long established trick of giving macroparticles a finite size, yet in a covariant fashion that avoids the need of boosting dynamical variables and fields forth and back from the laboratory to the beam frame. Regularization is achieved by scaling the interaction in terms of an effective charge q_{eff} of the source macroparticle (a Lorentz scalar). Electric and magnetic fields are derived consistently with Lienard-Wiechert formula[12], at the price of a lengthy calculation of retarded times for each of the particles involved in the simulation. In most cases, however, a "static", faster approximation based on a simplified, "instantaneous" formulation of the smoothing procedure is almost indistinguishable from the more rigorous treatment. In this case the magnetic field from a macroparticle at a given point is related to the electric field at the same position as follows[13]

$$\boldsymbol{B}=\boldsymbol{\beta}\times\boldsymbol{E} \tag{14}$$

and is usable also in a tree-code for the magnetic part of the field from a cell.

Table 1: Photo injector parameters.

Peak accelerating field	120 MV/m
Frequency	2.856 GHz
Launch Phase (peak current)	32°
Charge	1.1 nC
Laser spot radius (homogeneous)	1.13 mm
Laser pulse length (flat-top)	11.65 ps
Solenoid peak field	2.73 kG

Table 2: CPU time performance ($n_{\mathrm{cpu}} = 4$).

N_{part}	CPU (sec)	Wall clock (sec)	Efficiency (%)
$1 \cdot 10^5$	$7.537 \cdot 10^3$	1989	94.7
$2 \cdot 10^5$	$1.508 \cdot 10^4$	3822	98.6
$4 \cdot 10^5$	$3.021 \cdot 10^4$	7703	98.0
$8 \cdot 10^5$	$6.081 \cdot 10^4$	15501	98.1

PARALLEL IMPLEMENTATION

Parallelism in TREDI is achieved by assigning only a fraction of the "source" particles (the ensemble of charges responsible of self-fields effects) to a given computing node, while sharing a full copy of the "target" beam (an ensemble of positions that source particles act upon) among all the concurrent processes. This approach exhibits a number of advantages: a dramatic reduction of memory requirements (especially in "retarded" mode); ease of load balancing among processors; confinement of blocking data synchronization to a single reduction point at the end of each time step. Conceptual separation into a "target" and a "source" beam facilitates also evaluation of space charge at the vertexes of a regular mesh (2D, 3D, cartesian, cylindrical etc.) represented as a "fake" beam experiencing fields that can be extrapolated at the actual position of real charges.

Although a parallel evaluation of cell-cell interactions is possible, its effective implementation is a non-trivial task, for it is not simple to balance the load among the computing nodes and/or reduce the communication, an issue arising in both shared and distributed memory architectures, at least if one wants to adhere - for sake of simplicity - to a common paradigm to make the algorithm usable on platforms ranging from desktops to large scale facilities. Load balancing, in particular, suffers from the hierarchical structure of the tree, that hinders a homogeneous sharing of the workload among processors at topmost (i.e. closer to the root), more CPU effective, branching levels. The exploited solution is to share source (i.e. "cells") particles among processors, while assigning only a fraction of "target" positions to a given computing node. A drawback of such a method is to make awkward the treatment of the problem in "retarded" mode. A more satisfactory treatment is likely to require a mixed approach, at the price of more frequent communication among processors, sub-optimal work balancing and a substantial programming effort.

Table 1 shows the parameters used for a simulation of the Sparc layout[14] (a S-Band, photo-injector[15] + a focusing solenoid + a drift), aimed at reproducing the well known emittance double minimum located at the end of the drift[16]. The results of the simulations (obtained with many codes) are available in literature and shall not reproduced here. It is more interesting the CPU performance, shown in table 2 for $N = 1, 2, 4, 8 \cdot 10^5$ particles, which exhibits an almost perfect linearity with N which can be explained considering that simulation is dominated by the extrapolation of self-fields to the positions of macroparticles and integration of trajectories (two processes that scale as $\mathcal{O}(N)$). This explains also the higher efficiency for large values of N, for much of time is expended by computed nodes on completely decoupled tasks that not require any data synchronization.

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REFERENCES

[1] A Hierarchical $\mathcal{O}(N \log N)$ force calculation algorithm, *Nature* **324**, 446 (1986).

[2] L. Greengard and V. Rokhlin, A fast algorithm for particle simulations, *J. Comput. Phys.* **73**, 325 (1987).

[3] N. Engheta, W.D. Murphy, V. Rokhlin and M.S. Vassiliou, The fast multipole method (FMM) for electromegnetics scattering problems, *IEEE Trans. Antennas Propag.* **40**, 634 (1992).

[4] M.S. Warren and J.K. Salmon, A portable parallel particle program, *Comput. Phys. Commun.* **87**, 266 (1995).

[5] W. Dehnen, A very fast and momentum conserving tree-code, *Astrophys. J.* **536**, L39 (2000).

[6] W. Dehnen, A Hierarchical $\mathcal{O}(N)$ Force Calculation Algorithm, *J. Comput. Phys.* **179**, 27 (2002).

[7] L. Greengard and V. Rokhlin, A new version of the fast multipole method for the Laplace equation in three dimensions, *Acta Numer.* **6**, 229 (1997).

[8] F. Ciocci, L. Giannessi, A. Marranca, L. Mezi and M. Quattromini, *NIM Phys. Res.* **A393**, 434 (1997);
L. Giannessi, P. Musumeci and M. Quattromini, *Nucl. Inst. Meth.* ***A 436***, 443, (1999).

[9] L. Giannessi and M. Quattromini, *Phys. Rev. ST AB,* **6** 120101 (2003).

[10] L.M. Young, J.H. Billen, Los Alamos National Laboratory, LA-UR-96-1835, 2000.

[11] K. Flottman, http://www.desy.de/~mpyflo/astradokumentation/.

[12] J.D Jackson,, Classical Electrodynamics, 3rd ed., p. 661ff, Wiley & Sons**,** New York (1999).

[13] J.D. Jackson, ibid., p. 558.

[14] SPARC Collaboration, Nucl. Instr. & Meth. A507 (2003) 345-349, see also http://www.sparc.it

[15] AA.VV., LCLS Design Report, SLAC-R-593, April 2002.

[16] M. Ferrario et al., Phys. Rev. Lett. 99, 234801 (2007) and references therein.