SMOOTH FAST MULTIPOLE METHOD FOR SPACE CHARGE TRACKING: AN ALTERNATE TO PARTICLE-IN-CELL

A. Gee*,1 and B. Erdelyi†,1,2

[1]Physics Department, Northern Illinois University, DeKalb, IL 60115, USA
[2]Physics Division, Argonne National Laboratory, Argonne, IL 60439 , USA

Abstract

The fast multipole method (FMM) algorithm was developed by Greengard and Rokhlin in 1987 [1]. As one of the top ten algorithms of the 20th century, it has been applied in a wide range of fields. The FMM complexity is $O(N)$, where N is the number of particles, allowing for large-scale simulations. However, it includes all the two-body collisional forces, in contrast to other methods such as the popular particle in-cell (PIC) methods. While collisionality can be very important, many applications require only the mean field effects. PIC is frequently used in this regime. Due to recent concerns of unphysical effects of grids, interpolation and other approximations in PIC codes, an alternative based on different underlying assumptions would prove enlightening. For these cases, a smoothed or softened FMM using a Plummer-like smoothing parameter holds much promise. Unfortunately, the original FMM algorithm based on analytic expansions of the $\frac{1}{r}$-like potentials does not allow for Plummer softening. We present our new soft-FMM employing differential algebras (DA) to obtain the modified expansions. We also compare the performance of the smoothed DA-FMM with examples from PIC simulations.

INTRODUCTION

Algorithms to solve the N-body problem have advanced greatly in recent years. With increasing interest in high intensity beams, tracking codes must efficiently simulate collective effects, particularly space charge. Particle in-cell (PIC) is the standard class of methods for the accelerator and beam community. Since all PIC methods share the basic assumptions [2], comparing PIC codes would not distinguish unphysical behavior, which are well-known to exist due to numerical noise, interpolation errors, grid heating, etc. An alternative method based on completely different assumptions would prove insightful.

Of recently developed methods, the fast multipole method (FMM) shows great promise. We present the smoothed FMM as an alternative to PIC. Previously, we implemented the FMM using a differential algebraic (DA) framework. With the DA method, we reformulated the FMM in real Cartesian space and made it kernel independent. However, while PIC estimates the mean fields, the FMM includes all collisional effects. Since close encounters lead to strong collisions, unphysical in this context, we introduced Plummer-like smoothing or softening into the FMM. This technique could not be done with the original FMM, but the kernel independence based on the DA framework allows computational cost in the smooth FMM to be near the same as the original FMM. With appropriate softening parameter, the FMM can estimate the mean fields to be used for space charge tracking. This paper illustrates the behavior of the smoothed FMM for transverse space charge and compares it to theory, the method of statistical moments (MoM) [3], and a widely-used representative PIC code.

* agee1@niu.edu
† berdelyi@niu.edu

SMOOTHED DA-FMM IN CARTESIAN FORM

The smoothed 2D Coulomb potential at (x, y) due to a source at (x_0, y_0) of unit charge with smoothing parameter λ is given by (1), or alternatively by (2). (1) and its derivative are used for particle-particle interactions.

$$\Phi(x, y, \lambda) = -\frac{1}{2}\log\left((x - x_0)^2 + (y - y_0)^2 + \lambda^2\right) \quad (1)$$

$$= -\frac{1}{2}\left\{\log\left(x^2 + y^2 + \lambda^2\right) + \log\left[1 + \frac{x_0^2 + y_0^2}{x^2 + y^2 + \lambda^2} - 2\frac{x x_0 + y y_0}{x^2 + y^2 + \lambda^2}\right]\right\} \quad (2)$$

Far multipole expansion

We can separate (2) as $\Phi(x, y, \lambda) = \Phi_T + \Phi_M$, where Φ_T only depends on the target position. We expand Φ_M in (2) from the origin. Let $r^2 \equiv x^2 + y^2 + \lambda^2$. We define DA variables, $d_x = \frac{x}{r^2}$, $d_y = \frac{y}{r^2}$, $d_\lambda = \frac{\lambda}{r^2}$, and $d_r^2 = \frac{1}{r^2} = d_x^2 + d_y^2 + d_\lambda^2$. Substituting these into the second log term of (2), we have the form for the smooth multipole expansion Φ_M, given in (3).

$$\Phi_M(x, y, d_x, d_y, \lambda, d_\lambda) = -\frac{1}{2}\log[1 + (x_0^2 + y_0^2)d_r^2 - 2(x_0 d_x + y_0 d_y)] \quad (3)$$

The DA framework allows efficient expansion of Φ_M in terms of the DA variables. Thus, we will get a Taylor series in d_x, d_y, d_λ describing the multipole expansion, which we may evaluate using the DA variables defined earlier.

Multipole-to-multipole translation

To remap (3) to a new multipole center, (x_m, y_m), we redefine the DA variables as $d_{x_2} = \frac{x_2}{r_2^2}$, $d_{y_2} = \frac{y_2}{r_2^2}$, $d_{\lambda_2} = \frac{\lambda}{r_2^2}$,

ISBN 978-3-95450-168-7

and $d_{r_2}^2 = d_{x_2}^2 + d_{y_2}^2 + d_\lambda^2$ with $x_2 = x - x_m$, $y_2 = y - y_m$. Let $R_2 \equiv \frac{r_2^2}{r^2}$. Thus, the map of the translation between the multipole centers is given by (4) with Φ_{M_2} being the translated multipole expansion.

$$\left.\begin{aligned} d_x &= \frac{x}{r^2} = R_2(d_{x_2} + x_m d_{r_2}^2) \\ d_y &= \frac{y}{r^2} = R_2(d_{y_2} + y_m d_{r_2}^2) \\ d_\lambda &= \frac{\lambda}{r^2} = R_2 d_{\lambda_2} \end{aligned}\right\} \equiv M_2 \tag{4}$$

$$R_2 = \frac{1}{1 + (x_m^2 + y_m^2)d_{r_2}^2 + 2(x_m d_{x_2} + y_m d_{y_2})}$$

$$\Rightarrow \Phi_{M_2} = \Phi_M \circ M_2$$

Multipole-to-local translation

Similarly, to translate (3) to a local point (x_l, y_l) near (x, y), we redefine the DA variables as $d_{x_3} = x - x_l$, $d_{y_3} = y - y_l$, and $d_{\lambda_3} = \lambda$. Since $d_{\lambda_3} = \lambda$, we may evaluate it and eliminate the third DA variable before translation. Let $R_3 \equiv \frac{1}{r^2}$. So the map for translation is now given by (5). The potential is thus given by $\Phi = \Phi_T(d_{x_3} + x_l, d_{y_3} + y_l, \lambda) + \Phi_L(d_{x_3}, d_{y_3}, \lambda)$.

$$\left.\begin{aligned} d_x &= R_3(x_l + d_{x_3}) \\ d_y &= R_3(y_l + d_{y_3}) \\ d_\lambda &= R_3\lambda \end{aligned}\right\} \equiv M_3 \tag{5}$$

$$R_3 = \frac{1}{(x_l + d_{x_3})^2 + (y_l + d_{y_3})^2 + \lambda^2}$$

$$\Rightarrow \Phi_L = \Phi_M \circ M_3$$

Local-to-local translation

At this point, d_λ is no longer needed. For local-to-local translation, the new DA variables simply require a shift similar to d_{x_3}, d_{y_3}.

RADIAL SPREAD DUE TO SPACE CHARGE IN A DRIFT

Space charge in a drift is the simplest solvable case. For a zero-emittance beam, the radial spread is purely from space charge. From Reiser [4], the equation of motion is given by (6) where r_0 is initial beam radius, I is the current, $I_0 = {}^{4\pi\epsilon_0 m c^3}/_q$ is the characteristic current, and K is the generalized perveance with no charge neutralization.

$$\frac{\partial^2 R}{\partial z^2} = \frac{K}{r_0^2 R}; \quad R \equiv \frac{r(z)}{r_0}; \quad K = \frac{I}{I_0}\frac{2}{\beta^3\gamma^3} \tag{6}$$

Solving (6), we get an integral equation (7) for a zero-emittance electron beam or an approximate solution (8) as described in [4].

$$\frac{z}{r_0} = \left(\frac{2}{K}\right)^{\frac{1}{2}} \int_0^{\sqrt{\ln R}} e^{R'^2}\, \mathrm{d}R' \tag{7}$$

$$\Rightarrow R \approx 1 + 5.87 \times 10^{-5} \left(\frac{z}{r_0}\right)^2 \tag{8}$$

$$\tag{9}$$

We limited ourselves to this regime to maintain the paraxial approximation. This led to the beam parameters in Table 1.

BEAM PARAMETERS AND SIMULATION CONDITIONS

Table 1: Beam and System Parameters

Species	Electron
Energy	100 keV
Current	1 A
Spatial distribution	Uniform circular
Initial radius	1 cm
Initial emittance	0 m·rad
Drift length	0.5 m
Radial spread (Theory)	1.521

We set up the simulation to calculate a single space charge kick at order 12 with optimal FMM parameters. We chose IMPACT-T [5] to represent PIC for this paper. For PIC, we set the time step such that we could compare the FMM with a single time step, analogous with a single space charge kick, and after the PIC behavior converges, choosing around 300 time steps. For other parameters, see Table 2.

The beam radius is calculated simply using the maximum particle distance from the origin. Collisional effects in the FMM could cause particles at the edge of the distribution to jump significantly, leading to outliers. Thus, the outliers will inflate results from the beam radius calculation.

Table 2: PIC Simulation Conditions

Code	IMPACT-T
No. particles	300000
Bunch length	1.03 m
No. slices (transverse)	64
No. slices (longitudinal)	32
i^{th} Z-slices picked	16-17
Total travel time in drift	3.1 ns
Convergent time step	0.01 ns

RESULTS

Full smoothing

We started by testing the behavior of the FMM with equal smoothing in the particle-particle interactions and multipole expansions. We compared the predicted radial spread of the same distribution, as described by Table 1, using the FMM,

PIC after convergence, PIC with 1 time step, the MoM, and (8). Figure 1 shows the theoretical crossover point. The MoM at order 12 nearly matches the theoretical result as expected from previous work [3]. Inspection of the final distribution showed the radial spread from the FMM was inflated by some outliers. The clear beam edge showed $R = 1.63$. For this setup, we expect theory to be most accurate without collisions. With collisions, R will be slightly larger than given by (8). We see this behavior in the range of moderate smoothing, where the outliers match the beam edge.

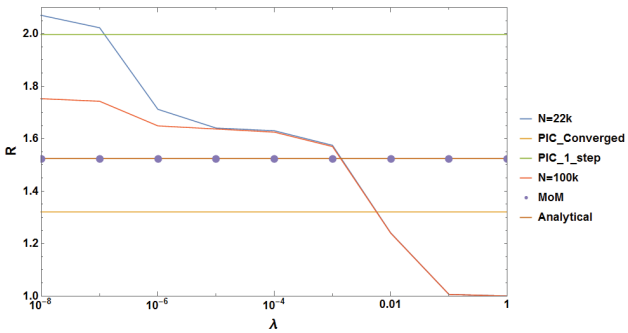

Figure 1: Smoothed DA-FMM vs. PIC, MoM, and theoretical radial spread along $\lambda_{PP} = \lambda_{Mult}$. The two FMM cases converge around $\lambda = 10^{-3}$ with a slight difference for moderate smoothing, $10^{-6} \leq \lambda_{P\text{-}P} \leq 10^{-4}$. The FMM equals the theoretical radial spread around $\lambda = 1.4 \times 10^{-3}$.

Independent smoothing

Our implementation allows for two separate smoothing parameters, $\lambda_{P\text{-}P}$ for particle-particle interactions and λ_{Mult} for multipole expansions. Figure 2 shows the case for small $\lambda_{P\text{-}P}$. For small λ_{Mult}, we get similar results to Figure 1, but levels off around $R = 1.63$.

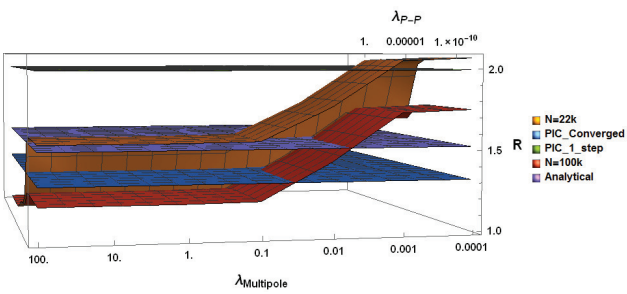

Figure 2: Smoothed DA-FMM vs. PIC, MoM, and theoretical radial spread with small $\lambda_{P\text{-}P}$. Softening the multipole expansions exhibits similar behavior for different N.

With smoothing, we are able to freely adjust the strength of the interactions. Combining the two parameters allows the FMM to match the behavior predicted by the PIC simulation. However, theory and our numerical methods suggest the chosen PIC simulation may underestimate the space charge strength in this regime.

Runtime

The runtime of the unsmoothed and smoothed DA-FMM is nearly the same. Figure 3 shows the runtime vs. N of the smoothed DA-FMM at optimal average bin density, $S = \frac{N}{\text{Bins}}$. The behavior is approximately $O(N)$.

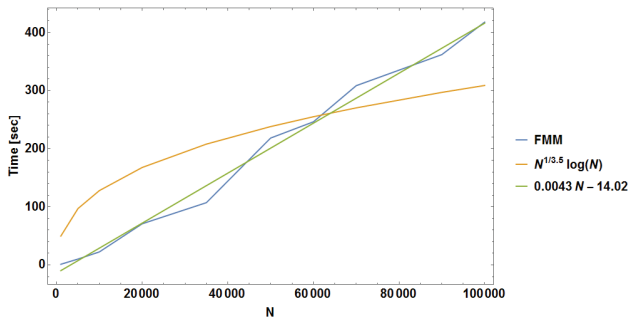

Figure 3: Smoothed DA-FMM runtime vs. N at optimal $S = \frac{N}{\text{Bins}}$ per point. The curve displays near $O(N)$ behavior.

CONCLUSIONS

We implemented a smooth DA-FMM as an alternative to PIC for space charge tracking. The collisional FMM overestimates beam size due to the occasional strong collisions from the low particle numbers used. Our novel smooth FMM, with a softening parameter in the range $10^{-6} \leq \lambda \leq 10^{-4}$, is approximately where the outliers disappear and the beam edge behaves smoothly. Adjusting the smoothing parameter adaptively allows detailed comparisons with PIC. Optimal smoothing parameter ranges will need a systematic study.

ACKNOWLEDGMENT

This work was supported in part by the U.S. Department of Energy, Office of High Energy Physics, under Contract No. DE-SC0011831 with Northern Illinois University.

REFERENCES

[1] L. Greengard and V. Rokhlin. “A fast algorithm for particle simulations", *Journal of computational physics* **73** (1987): 325-348.

[2] R.W. Hockney and J.W. Eastwood. Computer Simulation Using Particles, (1988).

[3] A. Gee and B. Erdelyi, “Study and Comparison of the Method of Moments and the Single Level Fast Multipole Method for 2D Space Charge Tracking”, Conf. Proc., NAPAC 2013, Pasadena, CA, USA.

[4] M. Reiser. Theory and Design of Charged Particle Beams, (1994).

[5] J. Qiang. IMPACT-T User Document Version 1.6. Lawrence Berkeley National Laboratory: Lawrence Berkeley National Laboratory. LBNL-62326, 2007. http://escholarship.org/uc/item/2sw7g9c3

ISBN 978-3-95450-168-7