

A NOVEL CODE WITH HIGH-ORDER ADAPTIVE DYNAMICS TO SOLVE THE N-BODY PROBLEM

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Abstract

Although there are several publicly available algorithms to model the behavior of natural systems such as the N-body system, limited computing power hinders the attempt to simulate them efficiently. With the improvement of high performance computing, scientists will be able to run simulations at an unprecedented scale in the future. Therefore, it is necessary to develop new algorithms and data structures to harness the power of high performance computing. In this paper we show a newly developed code, particles' high order adaptive dynamics (PHAD), to serve future computing demands. We use Fast Multipole Method (FMM) to calculate the interactions among charged particles. We use the Strang splitting technique to reduce the number of FMM calls and enhance the efficiency. Picard iterations-based novel integrators are employed to achieve very high accuracies. Electron cooling in the proposed Electron Ion Collider (EIC) has been identified as a potential testing environment for PHAD.

INTRODUCTION

Computer simulations are heavily used in designing particle accelerators and the efficiency and accuracy of them can be improved with ever changing computational power. Clearly, this demands dramatic improvements on existing code for beam dynamics. In this paper we present a new code developed using novel ideas to significantly divert the existing trend and electron cooling will be one of the potential candidates of its application.

The densely packed particles in a beam, which can be considered as our N-body system, experience two types of forces, long range and short range. The long-range forces are the Coulomb forces and the short-range forces are Coulomb collisions. Also, the motion of the particles in the beam should be taken into consideration for precise modeling and simulation of the beam. Therefore, our code enables to calculate Coulomb interactions and study the changes in the particle configuration with time.

ALGORITHM

In an N-body system each object continuously interacts with every other object in the system. The direct computation or pairwise calculation of such interactions gives the exact results and needs a computational complexity in the order of N^2 . For very large N , this method quickly becomes untenable. Using some approximate methods, such as the basis function methods, particle-mesh methods, and hierarchical subdivision methods, can circumvent this drawback. The challenge is to mitigate the approximation artifacts. The

hierarchical (or recursive) subdivision method has three distinct flavors: tree, cluster and fast multipole method and the algorithm used to develop our code belongs to the hierarchical fast multipole method (FMM). In FMM particles are confined to spatially bound cells and the interaction between cells are computed. Therefore, the force experienced by any particle inside a cell can be approximated to the addition of Taylor expansions calculated from the multipole expansion of the far away cells. Also, FMM can calculate interactions among N- bodies while retaining accuracy because its computational time typically grows linearly with the number of bodies.

Again, FMM has different versions and they vary with the dimensionality and the type of particle distribution. The code described in this paper uses the 3D adaptive FMM; it is well suited for any arbitrary distribution [1,2]. Even though FMM is considered as an approximation to get the solution of the Poisson equation, its accuracy can be set a priori and can be tuned to get even more accurate results than the direct summation method.

In order to study the beam propagation as time progresses, we need to split the total time into smaller steps and examine the beam dynamics after each small time step. A fixed time step size is not a good choice to study the behavior of the beam. For example, to study the close encounters of particles the step size should be adjustable. Hence, we used a variable order Picard iteration-based integrator. It is an integrator with dense output and flexible for automatic adjustment of the optimal order and time step to achieve a prescribed accuracy with a minimum computational cost.

The implementation of the automatic step size and order selection is not yet completed. Therefore, our code is tested only for the variable order with the fixed time step size [3,4].

To further enhance the computational throughput, we use Strang splitting [5]. Strang splitting is a second order accurate operator splitting method. This method splits a complicated problem into a few simpler parts and solves them separately and composes all solutions to get the final solution of the problem. Two types of forces—strong forces that change rapidly and smooth forces that vary slowly, act upon each particle in a beam. When the particles get closer they experience a very strong force and undergo rapid changes. This type of behavior occurs in the nearby region or the neighborhood of an evaluation point. Therefore, small time steps are needed to model the strong forces and it is possible each particle in the close encounter to have its own time step size. The influence caused by the far away particles can be considered as the mean force exerted by them and

it varies slowly. In this simulation we work on three time scales. The first time scale is the total time, or the entire simulation time. The second scale is created by dividing the first to equal step sizes and used to study the motion of particles due to slowly varying forces. The third scale is the subdivision of the second and as explained above it can vary from particle to particle. Since the FMM is the most time consuming process we need to minimize number of FMM calls. This led us to call FMM only in the second time scale, i.e. in the case of slowly varying forces.

There are two types of frames involved in this problem: the lab frame and the beam frame. In fact, under the influence of self-fields the motion of the particles in the beam frame is nonrelativistic and therefore the forces are electrostatic. The external electric and magnetic fields are given in the lab frame. Since the Lorentz force due to the external fields and the self-fields determine the beam dynamics, we need to consider the collective effects of the fields. There are two choices: calculate the forces due to self-fields and convert them into the lab frame or calculate the forces due to the external fields and convert them to the beam frame. As the intention is to study the particles' behavior in the lab frame, the straightforward approach is to transform the fields from the beam frame to the lab frame, and solve the equations of the motion in the lab frame.

The immediate testing environment of this code is the electron cooling section in the proposed Electron Ion Collider (EIC). Therefore, our code should work for the design parameters suggested in the Electron Ion Collider accelerator design [6]. The cooling device will be installed in the pre-booster ring and the collider ring of the EIC and each part of the collider carries ions with distinct energy ranges. The kinetic energy of the ions injected into the pre-booster ring is about 280 MeV and they are accelerated to 3 GeV, while the kinetic energy of ions during the collision in the collider ring varies from 60 to 100 GeV. The lowest gamma value in the pre-booster is about 1.3. In the collider ring the corresponding gamma values vary from 60 to 107.

PERFORMANCE ANALYSIS

In a previous paper [7], using the same particle distribution for both source points and target points, we have shown that the results produced from PHAD and N-body (SA) codes are in good agreement. We obtained those results for the case where points are normally distributed and they move with nonrelativistic speeds. Hence, the initial momenta, p_x , p_y , p_z , are all near-zero. In this paper we introduce relativistic corrections to both our codes, PHAD and SA. For details on these codes, please see [7]. The relativistic gamma value is reflected in the initial momentum in the z direction, p_z , by assigning the corresponding momentum value to p_z while p_x and p_y are still near-zero.

As indicated in the introduction, we have identified that the lowest gamma value is 1.3 and the highest is 100. We tested our code for three specific gamma values, 1.3, 60 and 1000. Figure 1 shows the comparison of trajectories of

PHAD with those of the N-body code for gamma value 1.3 when each particle carries a unit positive charge and a unit mass. The total time is 0.05 with time step size of 0.001.

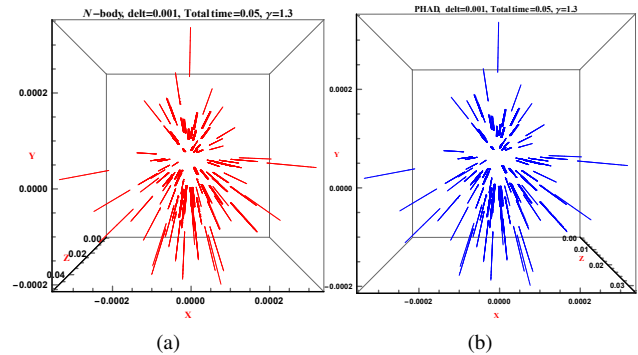


Figure 1: Trajectories of N-body and PHAD for the particles with unit mass and $\gamma=1.3$.

Figure 2 shows the comparison of trajectories of PHAD with those of N-body code for gamma value of 1.3 when each particle carries a unit positive charge and different masses ranging from 2 to 99. The total time is 0.05 with time step size of 0.001.

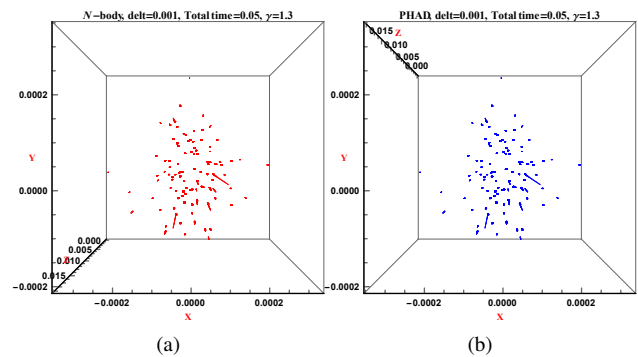


Figure 2: Trajectories of N-body and PHAD for the particles with different masses and $\gamma=1.3$.

Table 1: Spread in x, y, z after 50 Time Steps of Size 100

γ	Spread in x	Spread in y	Spread in z
1.3	1.07×10^{-2}	1.07×10^{-2}	3194.85
1000	6.69×10^{-4}	5.67×10^{-4}	5000.00

After a single time step of 100 the coordinates of points (y vs x and z vs x) with relativistic gamma values 1.3 and 1000 are shown in Figures 3 and 4, respectively. Each point carries a unit charge and a unit mass. We choose $\gamma=1000$ due to the fact that in the ultra-relativistic limit the space charge effect vanishes, so it is a straightforward sanity check of our codes. After 50 time steps of step size 100, the spread in x, y, and z are shown in Table 1. The particles with the high gamma value of 1000 are displaced more along the z

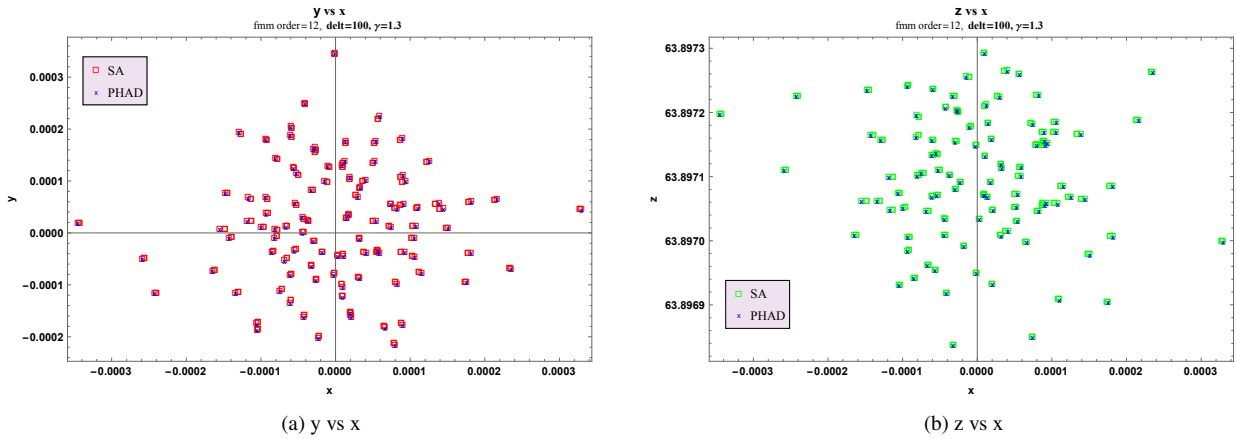


Figure 3: $\gamma=1.3$

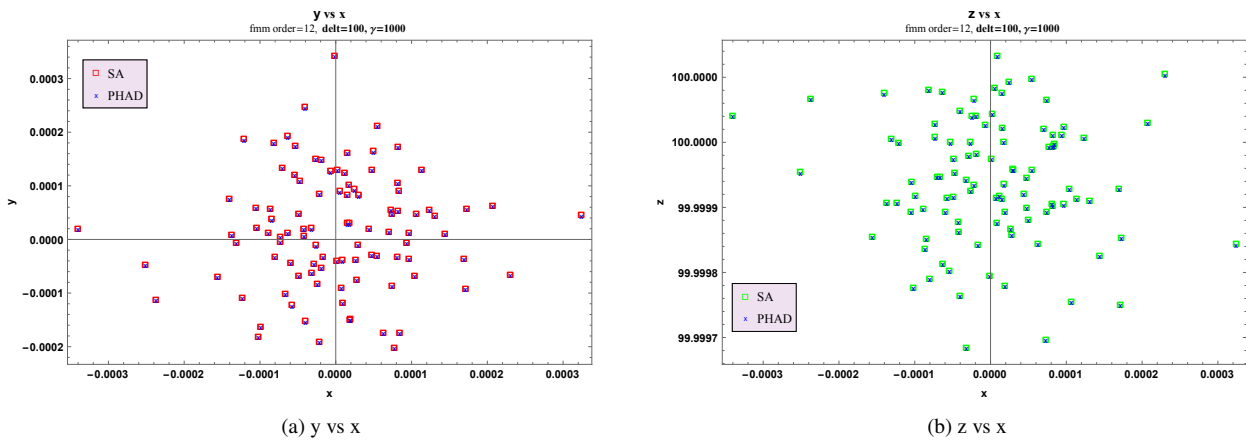


Figure 4: $\gamma=1000$

direction than those with low gamma value of 1.3. This is can be attributed to the fact that our initial configuration has a low/high momentum corresponding to a low/high gamma value. As expected, the space charge effect diminishes at higher energies (or higher gamma), and when $\gamma=1000$ points get closer to each other compared to those for $\gamma=1.3$. The values in Table 1 shows that both x and y spread become smaller for $\gamma=1000$.

We are still investigating if the discrepancies observed in the transverse momentum figure (Figure 5) are within the expected numerical errors or a still uncovered coding bug. The data structuring part of the code is implemented in C++. Picard iteration based integrator and calculations of Coulomb interactions are implemented in COSY INFINITY [8].

SUMMARY

In order to achieve highly accurate results efficiently we have to exploit the high processing power of computers through new approaches of modelling and simulations of N-body systems. In this paper we presented a new code developed to model and simulate a particle beam efficiently while maintaining high accuracy. Three key measures are

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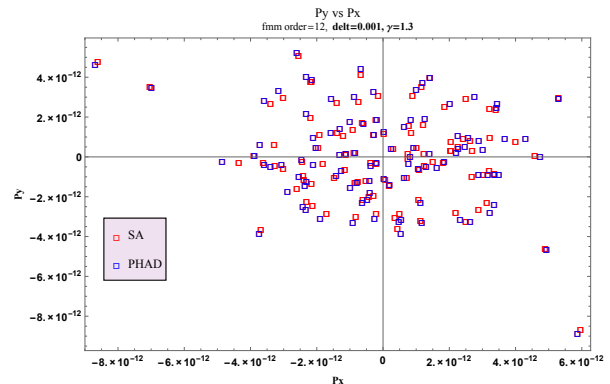


Figure 5: Transverse momenta (p_x and p_y) for $\gamma=1.3$

taken to ameliorate the challenges: Fast multipole method to calculate Coulomb interactions, Picard Integrator with dense output to study close encounters with small time steps, Strang splitting to improve speed up reducing the number of FMM calls.

The approximation errors due to FMM and the estimation errors due to Strang splitting are unavoidable. We showed

that PHAD and SA give similar results and they indicate that influence of the errors incurred is negligible. The drawn conclusions can be extended for any arbitrary distributions, any charge and mass magnitudes and for relativistic or non-relativistic particle motions.

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REFERENCES

- [1] S. Abeyratne, S. Manikonda, B. Erdelyi, "A Novel Differential Algebraic Adaptive Fast Multipole Method", in proceedings of IPAC'13, Shanghai (2013) 1055-1057.
- [2] S. Abeyratne, B. Erdelyi, "Optimization of the Multipole to Local Translation Operator in the Adaptive Fast Multipole Method", in proceedings of NA-PAC'13, Pasadena (2013) 201-203.
- [3] A. al Marzouk, B. Erdelyi, "Numerical Integrator for Coulomb Collisions", in proceedings of NA-PAC'13, Pasadena (2013) 204-206.
- [4] H.N. Schaumburg, B. Erdelyi, "A Picard-Iteration-Based Integrator", in proceedings of NA-PAC'13, Pasadena (2013) 210-212.
- [5] E. Hairer, G. Wanner, C. Lubich, "Geometric Numerical Integration", (New York: Springer Berlin Heidelberg, 2006).
- [6] S. Abeyratne et al., "Science Requirements and Conceptual Design for a Polarized Medium Electron-Ion Collider at Jefferson Lab".
- [7] B. Erdelyi, S. Abeyratne, "A New High-Order Adaptive Dynamics Code with Applications to Electron-Ion Collider", in proceedings of EIC14, Virginia (2014).
- [8] K. Makino and M. Berz, "COSY INFINITY Version 9", Nuclear Instruments and Methods in Research Physics Section A, 558:345-350 December (2005).