AN IMPLEMENTATION OF THE FAST MULTIPOLE METHOD FOR HIGH ACCURACY PARTICLE TRACKING OF INTENSE BEAMS

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Abstract

We implement a single level version of the fast multipole method in the software package COSY Infinity. This algorithm has been used in other physics fields to determine high accuracy electrostatic potentials, and is implemented here for charged particle beams. The method scales like NlogN with the particle number and has a priori error estimates, which can be reduced to essentially machine precision if multipole expansions of high enough order are employed, resulting in a highly accurate algorithm for simulation of intense beams without averaging such as encountered in PIC methods. In order to further speed up the algorithm we use COSY Infinity's innate differential algebraic methods to help with the expansions inherent in this system. Differential Algebras allow for fast and exact numerical differentiations of functions that carries through any mathematical transformations performed, and can be used to quickly create the expansions used in the fast multipole method. This can then be combined with moment method techniques to extract transfer maps which include space charge within distributions that are difficult to approximate.

INTRODUCTION

When examining the dynamics of intense beams the effects of space charge cannot be ignored, and a number of methods exist for determining how space charge can affect various quantities of interest in a charged particle beam. We use the computer code COSY Infinity 9.0 to perform our simulations, and have developed our own method to add the effects of space charge. COSY Infinity is a map based code that uses differential algebras to determine exact numerical derivatives which are used to create transfer maps to arbitrary order [1]. These differential algebraic vectors act as objects which carry through algebraic operations, thus it is possible to construct a transfer map by simply integrating the path of the reference particle with the differential algebraic vectors representing offsets from the position of the reference particle.

We have developed a method to add the effects of space charge to a transfer map using these differential algebras as well as the statistical moments of the test particles to create a Taylor series of the distribution, and compose each coefficient with pre-calculated potential integrals [2]. This method allows us to determine the transfer map of a beam element with space charge in a self consistent manner, as well as advance the particles through the machine using the map. Under certain circumstances not all of the particles can be accurately transferred using this moment method. If the beam is extremely flat, its distribution is not easily determined using a Taylor series; or it has a wide, diffuse halo there will be divergence issues. In fig 1 we see an example where a distribution with diffuse edges runs into difficulty using the moment method. In order to still advance the particles and generate the map accurately we have implemented a version of the fast multipole method.

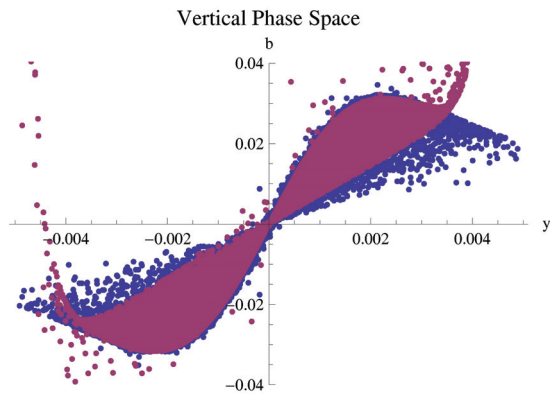

Figure 1: This is a phase space plot of the kicks given to a Gaussian distribution. The blue points indicate the particles as calculated with the fast multipole method, while the purple particles are the same ones advanced using the moment method.

In the first section we will be looking at the way a fast multipole method is normally applied. In the second section we look at the changes that we have made to the algorithm. Finally, in the third section we look at how the new method performs.

FMM BASICS

The fast multipole method is a fast way to get accurate electrostatic fields for a large number of particles without averaging the charges or the fields [3]. The method works by first separating the particles into boxes on a grid. The boxes then have their multipole expansions calculated,

$$\phi(z) \quad = \quad Qlog(z) + \sum_{k=1}^{\infty} \frac{a_k}{z^k}, \tag{1}$$

where,

$$Q = \sum_{i=1}^{m} q_i \quad and \quad a_k = \sum_{i=1}^{m} \frac{-q_i z_i^k}{k}, \tag{2}$$

with $z = x + iy$, and q_i,z_i is the charge and complex position of each test particle. The expansion is truncated at

order m. Then, for each box a local expansion is calculated from the sum of the multipole expansions of the boxes that do not have direct contact with the box in question, see Fig. 2,

$$\phi(z) = \sum_{\ell=0}^{\infty} b_\ell z^\ell. \quad (3)$$

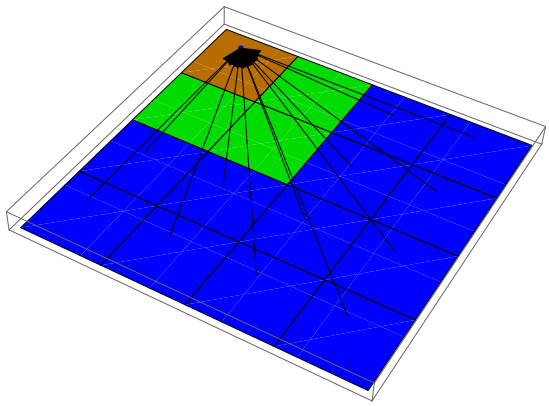

Figure 2: The region containing the particles is subdivided into boxes. In this instance it is a two dimensional region divided into sixteen boxes. The orange box denotes the region containing the particles in question, the green boxes are the nearest neighbors, and the blue boxes are the distant boxes. The distant boxes all contribute their multipole expansions to the local expansion in the orange box.

Finally, for each particle in the box the potential is calculated as the sum of the potential from the local expansion, and the particle to particle interactions of the box they are contained in, and the boxes touching it, see Figure 3.

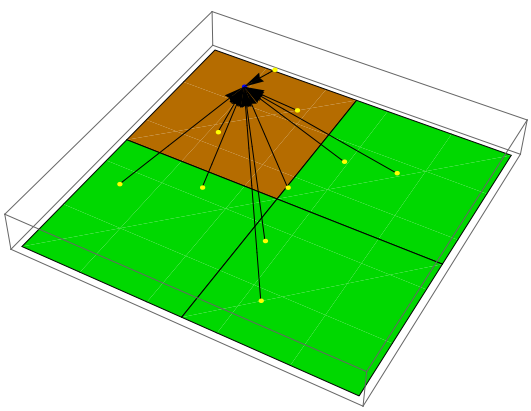

Figure 3: This is a closeup of the box in question and its nearest neighbors. The potential is determined by the local expansion and, as is shown here, the point to point coulomb interactions of the particles in the box and their nearest neighbors.

THE NEW METHOD

In the two dimensional algorithm, as currently practiced, the local expansion as seen in (3) is calculated from the multipole expansion coefficients in (2) using the relations,

$$b_0 = a_0 log(-z_0) + \sum_{k=1}^{\infty} \frac{a_k}{z_0^k}(-1)^k, \quad (4)$$

whereas for $\ell \geq 1$,

$$b_\ell = -\frac{a_0}{\ell z_0^\ell} + \frac{1}{z_0^\ell}\sum_{k=1}^{\infty} \frac{a_k}{z_0^k}\binom{\ell+k-1}{k-1}(-1)^k. \quad (5)$$

This is a time consuming method that requires first creating a multipole expansion and then creating a local expansion. The method we have developed skips this step. When creating the multipole expansions, we use differential algebras while finding the potential at the center of each box with the multipole expansion.

$$\phi(z+dz) = Q\log(z+dz) + \sum_{k=1}^{\infty} \frac{a_k}{(z+dz)^k}, \quad (6)$$

where dz is the differential algebraic vector $(dx + idy)$. COSY Infinity can then insert the positions of the points within the box into dz and thus directly extract the potential from the multipole expansion. Furthermore, using the original method, two separate sums needed to be calculated to find the electric fields of each particle, while with the differential algebraic method this is done directly on the differential algebraic vector.

As can be seen in fig 4, for the regions we are interested in there is significant time savings with the differential algebraic methods we have developed.

THE METHOD IN PRACTICE

The FMM was benchmarked against a series of both analytical results, and other codes and shown to be accurate. In fig 5 we see that the accuracy becomes saturated at and above fifth order.

The timing of the code has been measured using quantities such as number of particles, multipole order and number of boxes. As can be seen in fig 6, the time required to advance the particles scales between N, N^2, and $N \log N$. The experiment shown in Fig. 6 uses a fixed order and box number with a varying number of particles. The results show that for a small number of particles the timing scales with N^2; this occurs when the number of particles in a given box are small, and it becomes more time consuming to make a local expansion than to simply expand each particle. At a certain point, in this case 20000 particles, the expansion is no longer more trouble than it's worth and the rate of growth slows down, until as the number rises it becomes $N \log N$, asymptotically.

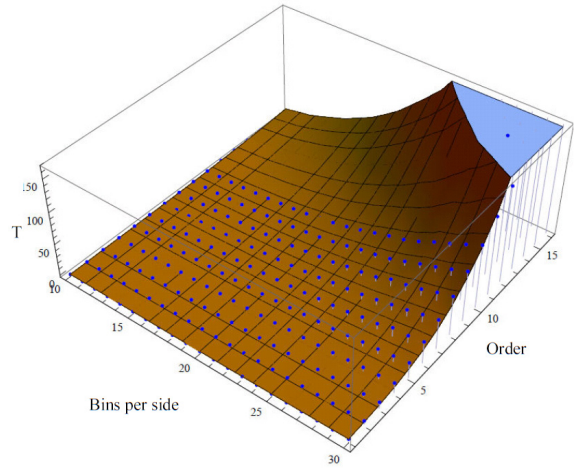

Figure 4: This graph shows a comparison of the amount of time needed to determine the potential of a distribution of 20000 particles. The surface shows the time taken using the differential algebraic method, while the points represent the time taken by the method in the section entitled FMM Basics. As can be seen, the DA method is faster through tenth order.

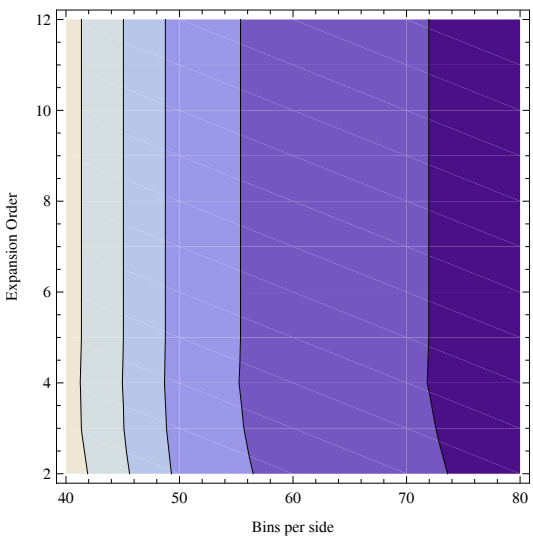

Figure 5: This is a plot of the accuracy of the fast multipole method with different numbers of boxes, and different expansion orders the order value becomes saturated at fifth order.

The DA methods involved are capable, within the larger COSY framework, of applying the fields of the given elements to particles with different masses or energies. This also carries through to the effects of space charge using the FMM. Using this method we are able to simulate a heavy particle beam with multiple isotopes moving through a mass spectrometer, see Fig. 7.

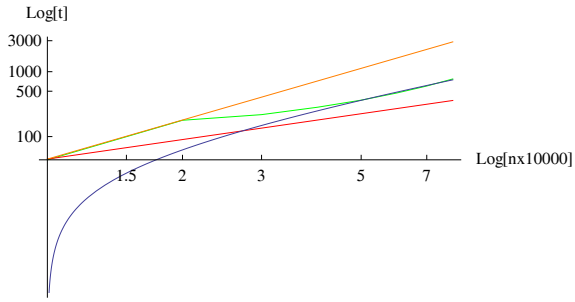

Figure 6: This log-log plot shows in green the measured time of a fixed order, fixed box number distribution as the number of particles are increased. The orange line represents N^2, while the red line represents N, with the blue line representing $N \log N$.

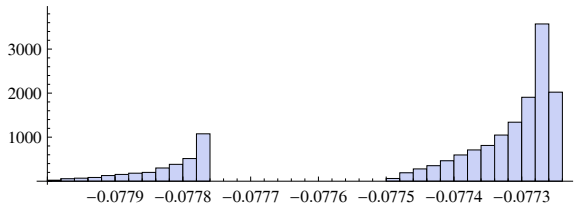

Figure 7: This shows the different angles given to a collection of carbon atoms in the two most common isotopes ionized to one charge.

CONCLUSIONS

We have demonstrated that not only is the fast multipole method useful for determining the effects of space charge, but that it can also be used to help determine the map of a given element with space charge included, even when the distribution function is not easily estimated with polynomials. Furthermore, our use of differential algebras in the calculation of local expansions gives us a faster method for finding the required expansions in the regions of box number and series order in which we are interested. We have confirmed that the timing of the fast multipole method scales as $N \log N$ just as was predicted, and that the method can be adapted to mixed isotope beams.

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