# A NEW PARADIGM FOR MODELING, SIMULATIONS AND ANALYSIS OF INTENSE BEAMS

E. Nissen, B. Erdelyi, Department of Physics, Northern Illinois University, Dekalb, IL 60115, USA

# Abstract

Currently when the effects of space charge on a beam line are calculated the problem is solved using a particle in cell method to advance a large number of macroparticles. If quantities such as space charge induced tune shifts are desired it is difficult to determine which of the many variables that make up the beam is the cause. The new method presented here adds the effects of space charge to a nonlinear transfer map, this allows us to use normal form methods to directly measure quantities like the tune. This was done using the code COSY Infinity which makes use of differential algebras, which allow the direct calculation of how the tune depends on the beam current. The method involves finding the high order statistical moments of the particles, determining the distribution function, and finally the potential. In order to advance the particles as accurately as possible a fast multipole method algorithm is used. In this talk we present the new methods and how they allow us to follow the time evolution of an intense beam and extract its nonlinear dynamics. We will also discuss how these methods can improve the design and operation of current and future high intensity facilities.

# **INTRODUCTION**

The purpose of this study is to create a method whereby the effects of space charge in a particle beam are included in the transfer map of the machine the beam is passing through. Currently the transfer map governs the motion of single particles in the machine, which is useful for steering, bare tunes, dynamic apertures, and many other quantities of interest governing the motion of single particles. Creating this new space charge added map will allow for the analysis of the effects of space charge on quantities that are directly extracted from the map using normal form methods such as tunes and chromaticities.

The calculation of the space charge effect involves first creating a distribution of particles which will serve as proxies for the beam. These are used to calculate the distribution function throughout the beam pipe, the distribution function is then integrated with an appropriate Green's function to determine the potential. The potential is used to find the electric fields, which are used to create an electric field map which is applied to the map of the element using Strang splitting. We will begin with an overview of the process before examining some results.

# SOFTWARE ENVIRONMENT

The software being used is COSY Infinity 9.0 [1]; this package uses differential algebras to perform exact numerical differentiation as well as to create Taylor models of the elements in question. Differential algebras work by creating vectors with their elementary mathematical operations redefined in such a way that they retain the derivatives of each quantity as they move through an algorithm. This allows for not only non-linear Taylor maps, but for coordinate transforms to normal form coordinates that retain any variable dependances that the original map had. These Taylor models allow for high order transfer maps, as well as non-linear normal form transformations. The easy inclusion of non-linearity in the transfer maps, which allows outside calculation using differential algebras makes the task of adding space charge to the transfer map significantly less cumbersome than a traditional code.

# **DISTRIBUTION CALCULATION**

In order to create a map of the effects of space charge in a region, the distribution must be calculated within that region. We use a set of discrete test particles as proxies for the distribution which can be used to calculate the Taylor series.

The particles are formed into a Taylor series using their statistical moments. If two distributions have the same moments, mathematically they are identical [2]. The moments are calculated by,

$$M_{nm} = \sum_{i=1}^{N_{particles}} x_i^n y_i^m.$$
(1)

If we assume that the distribution is a Taylor series of the form,  $\rho(x, y) = \sum_{i} \sum_{j} C_{ij} x^{i} y^{j}$ , then the moments can be connected to the coefficients with the equation,

$$M_{nm} = \sum_{i} \sum_{j} \int_{-x_r}^{x_r} \int_{-y_r}^{y_r} C_{ij} x^{n+i} y^{m+j} dx dy, (2)$$

where  $x_r$  and  $y_r$  are the x and y boundarys. This is trivially integrated, forming a matrix equation. This matrix is inverted using truncated single value decomposition, which gives the proper values for the Taylor series coefficients. This is the same way that the coefficients are found for three dimensions.

# POTENTIAL INTEGRATION

Now that the distribution function has been determined, the potential must be found. This is accomplished by integrating the distribution function multiplied with the appropriate Green's function over the region of interest. The Green's function takes the form of either  $\frac{1}{|r-r'|}$  or  $\ln(|r-r'|)$  for 3D and 2D distributions respectively. The methods involved for both 2D and 3D are similar, but 2D will be shown in this paper. The integral I which computes the potential at point  $(x_0, y_0)$  due to the distribution function  $\rho(x, y)$  in the domain  $D \in [a, b] \times [c, d]$  is,

$$I = \int_{c}^{d} \int_{a}^{b} \rho(x, y) \ln(\sqrt{(x - x_0)^2 + (y - y_0)^2}) dx dy.$$
 (3)

If our point of interest  $(x_0, y_0)$  is outside of D then standard numerical integration can be performed. However, if the point is within the distribution there will be a singularity at that point where standard numerical integration breaks down. This singularity can be removed using a Duffy transformation[3], which is explained below.

The Duffy transformation is performed by cutting D into four rectangles, which all share a vertex at  $(x_0, y_0)$ , as seen in Fig. 1. This has the effect of splitting the one integral I into four integrals  $I_{ac}$ ,  $I_{ad}$ ,  $I_{bc}$ , and  $I_{bd}$ . These are all integrals of the same form, so we will focus on  $I_{ac}$ . The next part of the transform is to scale the sides so that it is an integral over a unit square,



Figure 1: The integration region is subdivided into four smaller regions with their corners on the expansion point. This moves the singularity from the center to a corner.

$$u_1 = \frac{x - x_0}{a - x_0}; \quad u_2 = \frac{y - y_0}{c - y_0},$$
 (4)

$$dxdy = (a - x_0)(c - y_0)du_2du_1.$$
 (5)

To speed things up we will use  $\lambda_1 = (a - x_0)$  and  $\lambda_2 = (c - y_0)$ . As is shown in Fig. 2, the square is then cut into triangles which will be separately integrated.

$$I_{ac} = \int_0^1 \int_0^{u_1} \lambda_1 \lambda_2 \rho(\lambda_1 u_1 + x_0, \lambda_2 u_2 + y_0) \times$$



Figure 2: This shows how the integration region is further subdivided into triangles.

$$\times \ln(\sqrt{\lambda_1^2 u_1^2 + \lambda_2^2 u_2^2}) du_1 du_2 + \int_0^{u_2} \int_0^1 \lambda_1 \lambda_2 \rho(\lambda_1 u_1 + x_0, \lambda_2 u_2 + y_0) \times \\ \times \ln(\sqrt{\lambda_1^2 u_1^2 + \lambda_2^2 u_2^2}) du_1 du_2.$$
(6)

The final step is to convert the triangles to unit squares with the transformations,

$$u_1 = w_1; \quad u_2 = w_1 w_2,$$
 (7)

and,

 $u_1 = w_1 w_2; \quad u_2 = w_2,$  (8)

which gives the integral in the following form,

$$\begin{aligned} I_{ac} &= \int_{0}^{1} \int_{0}^{1} \lambda_{1} \lambda_{2} \rho(\lambda_{1} w_{1} + x_{0}, \lambda_{2} w_{1} w_{2} + y_{0}) \times \quad (9) \\ &\times (w_{1} \ln(w_{1}) + w_{1} \ln(\sqrt{\lambda_{1}^{2} + \lambda_{2}^{2} w_{2}^{2}})) dw_{1} dw_{2} \\ &+ \int_{0}^{1} \int_{0}^{1} \lambda_{1} \lambda_{2} \rho(\lambda_{1} w_{1} w_{2} + x_{0}, \lambda_{2} w_{2} + y_{0}) \times \\ &\times (w_{2} \ln(w_{2}) + w_{2} \ln(\sqrt{\lambda_{2}^{2} + \lambda_{1}^{2} w_{1}^{2}})) dw_{1} dw_{2}. \quad (10) \end{aligned}$$

Notice that there is now no singularity in the integrand. The 3D version involves cubes and pyramids instead of squares and triangles, but the transformation and the result are similarly effective.

### **ELECTRIC FIELD KICK**

Once the potentials have been calculated, COSY's ability to find exact numerical derivatives comes into play, and is used to find the electric fields for the region in question, which are then added into the map using a technique known as Strang splitting [4]. This is a method of finding a solution to a differential equation that can be thought of as a combination of two differential equations with known solutions,

$$\frac{d\vec{z}}{ds} = \vec{g_1}(\vec{z}, s) \Longrightarrow \vec{f_1}(s), \tag{11}$$

$$\frac{d\vec{z}}{ds} = \vec{g_2}(\vec{z}, s) \Longrightarrow \vec{f_2}(s), \tag{12}$$

Which can be solved in the autonomous case as,

$$\frac{d\vec{z}}{ds} = \vec{g_1}(\vec{z}) + \vec{g_2}(\vec{z}) \Longrightarrow \vec{f_1}(\frac{s}{2}) \circ \vec{f_2}(s) \circ \vec{f_1}(\frac{s}{2}) + \mathcal{O}(s^3).$$
(13)

The space charge kicks are calculated over a region small enough to allow us to assume an autonomous system. Since COSY already contains the maps for the single particle elements, the kick is combined with the pre-existing maps.

## PARTICLE ADVANCEMENT

In cases where the distribution is symmetric and easily modeled using a Taylor series of the desired order then the kickmap that is generated can be used to advance the test particles. In some cases the distribution can be more complex than the Taylor series is capable of advancing. Since quantities such as the space charge induced tune shift affect the reference particle the information is still useful, but a more stable method for advancing the particles is still required. This has been accomplished using a single level instance of the fast multipole method [5].

The method works by subdividing the region of interest into smaller squares. It then calculates the multipole moments of each square up to a desired order. Then a Taylor series for each square is calculated from the multipole expansions of the squares that do not share an edge with the one in question. Finally for each point the potential is calculated using the Taylor series and the individual interactions of each of the particles in the neighboring squares.

#### METHOD EFFECTIVENESS

Now that the method of adding space charge to the map has been derived we need to determine what the optimum conditions are for its use. Since a series of test particles are being used it becomes important to determine how many particles are needed to achieve convergence. If we look at the moments of the distribution when compared to the ideal moments in Fig. 3 we see that there is good convergence at the  $10^6$  particle mark.

Since the Taylor models are given at a particular order as are the moments being used it becomes necessary to determine which orders in the Taylor series or the moment order are ideal. The differences in the potentials over a wide range of the space are averaged to determine how accurate the potential as calculated using the moment method is with respect to a point by point coulomb solver. As can be seen in Fig. 4, the most accurate area is in the region at 17th order in the moment method with the Taylor series order at or above 17 For a uniform distribution.

### **METHOD IN PRACTICE**

A number of tests must be done to see how well this new method works in comparison with systems that can be solved analytically or numerically with high accuracy. First, we compare the expansion of the beam due to space charge as it moves through a drift. Assuming a uniform



Figure 3: This are the moments calculated for a uniform square using an increasing number of test particles, The blue points indicate the moment as calculated, while the purple line indicates the ideal moment.

beam with a diameter of 1 cm with 1 A of current over a drift of 20 cm with an energy of 100 KeV, the relation,

$$\frac{r_m}{r_0} = 1 + 5.87 \times 10^{-5} \frac{I}{(\gamma^2 - 1)^{\frac{3}{2}}} (\frac{z}{r_0})^2, \quad (14)$$

predicts a quadratic increase in radius of 33% [6]. We calculate the increase from the map method in two separate ways; first by placing test particles at the edges of the beginning distribution, the other is by examining the linear map element that compares the initial to the final size of the beam. Projections of the initial and final distribution are shown in Fig. 5 while a comparison of the methods and



Figure 4: This shows the potential of a uniform circular distribution for different integration and moment orders. This was done by creating a grid of the orders. The darker the area the higher the accuracy. The contours show the region between 0 and .002.

sizes are shown in Table 1. A profile of the increase is shown in Fig. 6 which shows the quadratic character of the size growth.



Figure 5: (color) A comparison of the initial and final horizontal and vertical test particle positions in the 20cm drift. Purple indicates the initial points, blue the final.

The next set of experiments involves the addition of quadrupoles to the system, we use a drift quad drift quad drift FODO cell system to study how the tune of the system changes with increasing space charge. Both the number of particles and the initial distribution are the same, the only change is in the peak current. In Fig. 7 there is



Figure 6: (color) A profile view of the increase in beam size through a drift.

Table 1: Table of different methods for finding the increase in size from beginning to end in the described problem.

Method	Growth
Edge Point x	35.27 %
Edge Point y	35.30 %
Map Element x	31.21 %
Map Element y	31.34 %

a distinct change in the tune as the current changes, but the quadrupole currents remain constant.

The values that are used in Fig. 7 are directly calculated from the map of the system, which gives direct numbers for the x and y tunes, these values can now be used with a fitting algorithm to solve for a desired set of fractional tunes with space charge included. The results shown in Fig. 8 show that the fitting algorithm was able to frequently determine the quadrupole currents necessary to bring the tune of the system back to the bare tune and counteract the effects of space charge. This new ability to fit a system to desired parameters with space charge as an included quantity provides a deeper understanding of how elements can be adjusted to get desired effects both during the design of new machines and during the evaluation of extant ones.

Finally, another use combines the ability to calculate space charge maps with COSY's ability to create exact numerical derivatives. This involves how the chromaticity of the system is determined by the effects of space charge on the beam. Using the tunes at a different operating point we can see in Fig. 9 that both the tunes and the chromaticities become nonlinear with increasing peak current. This is an excellent example of a system moving from being emittance dominated to being space charge dominated.

## CONCLUSIONS

We developed a method for including the effects of space charge in the transfer map of a system. This method now allows us to calculate how space charge can effect quantities such as tunes and chromaticities using normal form methods. This was accomplished by converting a set of test particles into a distribution function, which could be



Figure 7: (color) The X and Y fractional tunes as calculated through a system with increasing peak beam current.



Figure 8: (color) The X and Y normalized quadrupole currents are shown in the upper diagram with their resultant tunes in the lower diagram.

integrated with a Green's function after a series of coordinate transforms. The resultant potential could then be used to find the electric field and thus apply that to the motion of the particles. This method is a self consistant computation of space charge effects in a transfer map.

The map that we have gained from this method has allowed us to look deeply at what is happening to the dynamics of the beam at the map level. We can calculate how the effects of space charge can alter the tune of the map as well as the chromaticity. Since this method will give a direct numerical value for these quantities in the presence of space charge they can be used to calculate an objective function



Figure 9: (color) The first graph is a tune that initially starts out as a  $90^{\circ}$  phase advance cell, but is subjected to an increased amount of space charge. Below is the chromaticity.

in a fitting algorithm, thus allowing a user to determine directly how to counteract the actions of space-charge in an accelerator. Further work also involves using a fast multipole method to help with the tracking of particles that follow a distribution that is not easily modeled using a Taylor series.

### ACKNOWLEDGEMENTS

This work was supported by the DOE under contract DE-FG02-08ER41532 with Northern Illinois University.

#### REFERENCES

- M. Berz, "Advances in Imaging and Electron Physics vol 108", Academic Press, London, 1999
- [2] M. G. Bulmer, "Principles of Statistics", MIT Press, Cambridge MA, 1967
- [3] M. G. Duffy, "Quadrature Over a Pyramid or Cube of Integrands with a Singularity at a Vertex", Siam J. NUMER. ANAL., Vol. 19, No. 6, Dec. 1982
- [4] E. Hairer et al., "Geometric Numerical Integration: Structure Preserving Algorithms for Ordinary Differential Equations", Springer-Verlag, New York, 2002
- [5] J. Carrier et. al., "A Fast Adaptive Multipole Algorithm for Particle Simulations", Siam J SCI. STAT. COMPU., Vol. 9, No. 4, Jul. 1988
- [6] M. Reiser, "Theory and Design of Charged Particle Beams", Wiley-VCH, Weinheim, 2008