Abstract

In the early design stages it is customary to work with a highly simplified analytic model to describe a beamline. Dipoles and quadrupoles are often based on hard-edged approximations. This is not only unrealistic, it also significantly slows down time-domain spacecharge tracking codes such as the General Particle Tracer (GPT) code. The underlying reason for the poor performance is that, despite the fact that the simple hard-edged field equations are fast to evaluate, they force the integration process to use excessively small step sizes near the field discontinuities in order to achieve the desired accuracy. In other words, the apparently simple equations turn out to be the most difficult ones to evaluate numerically. An obvious solution is to switch to field-maps, but this is not practical in the early design stages. In this contribution we show a new solution implemented in the GPT code based on analytical expressions for the fringes where the transverse size of the magnet is properly taken into account. In addition to producing more realistic results, the smooth fields increase tracking speed by an order of magnitude for typical cases.

INTRODUCTION

Time domain simulations codes such as GPT [1, 2], PARMELA and ASTRA are essential tools for the design and understanding of high-brightness charged particle accelerators. The physics included in these codes is a particularly good match for injector / RF-photogun simulations producing pulsed, high-brightness, high-charge beams. The way the simulation codes operate is by tracking a large number of sample particles through the superposition of external fields and spacecharge fields. At each step in the simulation the codes maintain a collection of sample particles, where all particles are stored at the same time. This ensures self-consistent results for Coulomb interactions, even when the beam shape changes on relatively short time-scales. A simulation step involves the calculation of all electromagnetic fields due to external beamline components at the position of all sample particles, in addition to calculating the fields due to space charge. These fields are fed into an Ordinary Differential Equation (ODE) solver to solve the relativistic equations of motion, thereby advancing the entire population in time.

Regardless of the exact integration scheme, it is important to have the correct timestep length. On the one hand, a very small timestep gives accurate results at the costs of excessive CPU time. On the other hand, a very large timestep gives incorrect results. The best operating mode is arguably with the largest timestep possible, giving results which are 'barely good enough'. Finding the right balance is difficult, and this is further complicated by the fact that the optimal timestep varies greatly along the beamline. Very small steps must be taken during the emission process and in beamline components with large gradients, whereas very large steps can be taken in relatively constant or zero field regions.

Problems arise when part of the beamline is modelled with hard-edge approximations. It might be that the fringes capture relevant physics, and with ever brighter sources these effects become increasingly important. Furthermore, tiny integration steps need to be taken during the crossing of the interface to maintain sufficient accuracy. For just one particle this could be acceptable, but all particles have to be tracked together to get self-consistent results. Consequently, a timestep reduction for one particle crossing the interface of a hard-edged beamline component implies in a timestep reduction for all other particles as well. This significantly slows down simulation speed, especially for long bunches where there is always some particle crossing some interface. This is the problem we address in this paper, in particular for quadrupoles.

One solution to the problem of requiring small time-steps crossing a hard-edge interface is to split the trajectory in two halves at the interface: Neither half contains any discontinuities, and the simulation speed is restored. However, this solution misses relevant physics captured in the fringe fields, it requires non-trivial interpolation of the spacecharge fields to a set of intermediate timesteps, and it involves extra bookkeeping that makes misaligning beamline components in 3D prohibitively difficult. Another solution is to use realistic field maps, not containing these discontinuities. This restores the missing physics, it solves the problems arising from discontinuities, but it is often rather unpractical in the early design stages when fast parameter scans are required. Furthermore, field-maps are intrinsically based on interpolations causing a whole list of potential problems of their own.

The conceptually easiest and arguably best solution that solves all issues mentioned above is to track through a simple continuously differentiable equation for the fields, Maxwell compatible, including the fringes. Inspired by the analytical fringe fields of dipoles [3], we show in the next section how such expressions can be derived for higher order multipoles. The subsequent section presents the results of a GPT implementation of these expressions for the case of quadrupoles. Although the equations are far more complicated than the hard-edge counterparts, we will show that the overall GPT simulation speed is significantly improved.
QUADRUPOLE FIELDS

We summarise below the results described in [3], we start by writing Maxwell’s equations for three-dimensional fields in a simple form and define the following new variables:

\[ u = \frac{1}{\sqrt{2}}(x + iy), \]
\[ v = \frac{1}{\sqrt{2}}(x - iy), \]
\[ \zeta = \sqrt{2}z. \]

We express the magnetic field in terms of components:

\[ B_u = \frac{1}{\sqrt{2}}(B_x + iB_y), \]
\[ B_v = \frac{1}{\sqrt{2}}(B_x - iB_y), \]
\[ B_\zeta = \frac{1}{\sqrt{2}}B_z. \]

In terms of the new variables, Maxwell’s equations can now be written as:

\[ \partial_u B_u + \partial_\zeta B_\zeta = 0, \]
\[ \partial_v B_v + \partial_\zeta B_\zeta = 0, \]
\[ \partial_\zeta B_u - \partial_u B_\zeta = 0, \]
\[ \partial_\zeta B_v - \partial_v B_\zeta = 0. \]

From (1) and (2), one can see immediately that, in the absence of any fringe fields, the general solution of Maxwell’s equations for any magnet is given by:

\[ B_u = f(v), \]
\[ B_v = h(u), \]

for any functions \( f(v) \) and \( h(u) \). The case of a multipole of order \( n \) (\( n = 1 \) for a quadrupole, \( n = 2 \) for a sextupole, and so on) is given by:

\[ B_u = iv^n, \]
\[ B_v = -iu^n, \]
\[ B_\zeta = 0. \]

Therefore, a quadrupole is described by \( B_u = iv \), \( B_v = -iu \) and \( B_\zeta = 0 \). In strict analogy to the two dimensional case and returning to the initial coordinate system, we find that a particular solution to the three dimensional Maxwell equations may be written as:

\[ B_x = -idf(h + iv\sqrt{2}z) + idg(h - iv\sqrt{2}z), \]
\[ B_y = ef(h + iv\sqrt{2}z) - eg(h - iv\sqrt{2}z), \]
\[ B_z = \sqrt{2}f(h + iv\sqrt{2}z) + \sqrt{2}g(h - iv\sqrt{2}z), \]

where:

\[ d = \frac{1}{\sqrt{2}}\left(\frac{1}{b} + b\right), \]
\[ e = \frac{1}{\sqrt{2}}\left(\frac{1}{b} - b\right), \]
\[ b = \text{constant} \] and \( h \) is expressed as:

\[ h = dx + iey. \]

Now, as far as fringe fields are concerned, it is possible to show that [1] they can always be expressed as appropriate sums of the elementary solutions given by (5), (6) and (7) with different multiplicative constants as well as different values of the constant \( b \) above. The general expected fringe field fall-off is given by the choice of the functions \( f(h + iv\sqrt{2}z) \) and \( g(h - iv\sqrt{2}z) \) which govern the on-axis decay of the field. Further, the constant \( b \) may also be varied and this is found to affect the rapidity of the fall-off as one goes off-axis transversely.

For the purpose of this paper, we take the limit \( b \to 0 \) and we assume a decay of the gradient near the edge of the quadrupole to be given by an Enge function of the form \( 1/(1 + \exp[\alpha(z - z_{\text{edge}})]) \). For \( \alpha = 1 \) and assuming the edge of the magnet is at \( z = 0 \) plane, this results in a magnetostatic field given by:

\[ B_x = \frac{1}{4}\left[y + \arctan\left(-\frac{\sin y}{(e^{-z} + \cos y)}\right) - \frac{y \sinh z}{(\cos x + \cosh z)}\right], \]
\[ B_y = \frac{1}{4}\left[x + \arctan\left(-\frac{\sin y}{(e^{-z} + \cos x)}\right) - \frac{x \sinh z}{(\cos y + \cosh z)}\right], \]
\[ B_z = \frac{-1}{4}\left[\frac{y \sin x}{(\cos x + \cosh z)} + \frac{x \sin y}{(\cos y + \cosh z)}\right]. \]

The field of an entire magnet can be constructed by combining two such profiles, where the distance between the two edges indicates the size of a hard-edge magnet with identical focusing strength, and where \( \pi/\alpha \) is a measure for the bore of the magnet.

This means that we no longer have full control of the fringe field decay as we go off-axis in our quadrupole and the result is no longer general. However, for the purposes of tracking a bunch in a code like GPT, this is not essential and what is far more important is the smoothness of the fall-off and this is ensured thanks to the equations above.

**GPT EXAMPLE**

Implemented in the General Particle Tracer (GPT) code are the fields described in the previous section, for the limiting case \( b = 0 \). The reason for this simplification is that the extra flexibility introduced by this parameter is beyond the scope of this paper. As a test-case, a very simple beamline is investigated using just a quadrupole doublet with a field profile shown in Fig. 1. The doublet is set such that a beam with a Lorentz factor of 100 is focused exactly at \( z = 1 \) m, as shown in the sample trajectories of Fig 2.

The main difference between the hard-edge model and the new analytical model with fringe fields is computational...
In Fig. 3 we see the difference in CPU time for a 10 mm bunch containing 10k sample particles, as function of overall simulation accuracy. It is clear that the result is significant: Whereas the hard-edge model suffers from extreme growth in CPU time as function of accuracy, the new analytical model is much faster over the entire parameter regime and almost independent on accuracy. The reason being that the timesteps need not be reduced to get the desired accuracy. This leads to the main conclusion of this paper: The analytical expressions for quadrupole fields can be used in a time domain tracking code to get physically more realistic results in much faster simulation time.

An additional advantage of the closed form analytical expressions is that they are a perfect match to modern hardware because almost all modern computers have support for Single Instruction Multiple Data (SIMD) vector instructions. Examples are the AVX2 instruction set on Intel CPU's with a vector length of 256 bits, and Graphical Processing Units (GPUs) with far larger vector lengths. This extra computational power is typically very difficult to use, since it requires all elements of the vector to perform the exact same operations. This excludes branches, and consequently all if-based code is extremely difficult to write such that it can tap into these computational resources. The closed form analytical expressions of the quadruple fields however are such that they have the same expression, regardless if evaluated inside or outside the magnet; It is just one smooth branchless transition. Consequently, one single thread of executable can calculate the fields of many particles simultaneously without any addition overhead. On a modern GPU employing thousands of floating point units, this is a potential increase in computational speed of orders of magnitude.

**CONCLUSION**

Analytical expressions for beamline components including fringe fields do not only provide more realistic results, they can simultaneously significantly decrease simulation times for time-domain tracking codes. This has been shown in this paper for the case of quadrupoles, but it is to be expected that the conclusions holds for other beamline components as well. Because the relevance increases with increasing particle numbers and increasing accuracy requirements, analytical expressions including fringe-fields for multipoles and RF-structures are a crucial addition to the next GPT release that can track billions of particles on MPI clusters, including space-charge.

**REFERENCES**