Three Dimensional PIC Simulation of Heavy Ion Fusion Beams: Recent Improvements to and Applications of WARP *

David P. Grote and Alex Friedman
Lawrence Livermore National Laboratory
P.O. Box 808, Livermore CA, 94550-0808 USA
and Irving Haber
Naval Research Laboratory
Washington D.C. 20375 USA

Abstract

The multi-dimensional particle simulation code WARP is used to study the transport and acceleration of space-charge dominated ion beams in present-day and near-term experiments, and in fusion drivers. The algorithms employed in the 3d package and a number of applications have recently been described.[1] In this paper we review the general features and major applications of the code. We then present recent developments in both code capabilities and applications. Most notable is modeling of the planned ESQ injector for ILSE, which uses the code's newest features, including subgrid-scale placement of internal conductor boundaries.

I. Introduction

Heavy-ion particle accelerators are attractive candidates for inertial fusion drivers.[2] The required beams have high current and must have a low transverse emittance, so the beam can be focused down onto a small (few mm) spot at the fusion target. Nonlinearities of the self-fields of the beam, as well as manipulations of the beam, can lead to emittance growth. A self-consistent description of the space-charge fields is thus needed: the particle-in-cell method is well suited to such simulations. The WARP3d code is being developed to study the transport and acceleration of space-charge dominated heavy ion beams; it combines features of particle-in-cell simulation with those of an accelerator code.

II. Code Overview

The code's accelerator "lattice" consists of a fully general set of focusing and bending elements. These elements are described in the laboratory frame and can be periodic. The description includes the strengths of the fields, location of the elements, and other properties specific to the types of elements. For flexibility, each multipole component is specified separately- this allows the possibility of overlapping elements. The lattice fields are calculated in the local lab frame for each particle at each time step. These fields, along with the self-consistently calculated self-fields, are used in the Lorentz force law to advance the particles at each time step. For efficiency, the lattice information is loaded onto a one-dimensional local grid which moves with the beam at the beginning of each time step. This avoids having to search the master list to find the information for each particle.

The code's particle-in-cell sections calculate particle trajectories and self-consistent electrostatic fields from the particles' positions. The particle trajectories are calculated with the leapfrog advance, using either full steps for efficiency or split steps to have the particle's velocity and position synchronized in time for diagnostics. Residence corrections are used to account for differing number of steps through sharp-edged elements; without residence corrections, particles landing inside an element more times or fewer times would receive dramatically different impulses. The self-potential ϕ is calculated via a Poisson solver on a co-moving mesh that is only large enough to hold the beam. The electric fields are applied by directly differencing ϕ for each particle.

In a bend, each particle is described in its own Cartesian frame; as the particle advances around the bend, the frame changes. Assuming a small inverse-aspect-ratio, an approximate algorithm is used. The dipole or bend field is augmented with a "pseudo-gyrofrequency" that accounts for the rate of change of the velocity angle due to the frame transformation. The algorithm is inexact since it does not account for the changes in beam position and velocity during the time step. The self-potential is calculated assuming a gentle bend. It is first calculated in Cartesian coordinates and then modified through iterations to include the non-Cartesian terms.[1]

Additional features include a full set of RMS particle moment calculations, including emittance, in both the beam frame and the lab frame. A multitude of phase space plots can also be generated.

III. Applications

A. *Drift Compression in a Misaligned Lattice*

Current amplification from drift compression can lead to emittance growth, especially in the presence of misaligned

*Work performed under the auspices of the U.S. DOE by LLNL under contract W-7405-ENG-48, and by the Naval Research Laboratory under contract numbers DE-AI05-92ER54177 and DE-AI05-83ER40112

0-7803-1203-1/93$03.00 © 1993 IEEE

quadrupoles. With the side-to-side oscillations from the misalignments and fattening of the beam from the compression, particles will sample more non-linear fields from the focusing structure and from the images on the surrounding pipe. In one case, with 1 mm (RMS) random misalignments and a square surrounding pipe, the beam experienced an increase in emittance of 25%. When the walls were moved out farther (from 7 cm to 9 cm), the emittance growth went away almost completely.

B. *Beam Equilibria*

The code allows us to follow beams over long distances. Beams have been followed for as long as 175 strong-focusing lattice periods, or 210 meters in 10500 time steps. The bulk of the beam remained quiescent over this time. The ends of the beam did show some emittance growth because the initial state was not a true equilibrium. Other runs show equilibration between transverse and longitudinal temperature ($T_{x,y}$ and T_z). When T_z is much less than $T_{x,y}$, there is (over a certain range of physical parameters) a rapid, collective process that equilibrates the two temperatures. Equilibrium in the other direction ($T_{x,y} < T_z$) is observed to proceed more slowly, on a collisional timescale.

C. *MBE-4 Experiment*

Drift compression experiments on the MBE-4 facility at LBL showed anomalous emittance growth.[6] Simulations show that the growth, in large part, results from the dodecapole components of the focusing fields. As the beam compresses and grows fatter, the particles experience more of the non-linear dodecapole field.

D. *Bent Beams in an ILSE Lattice*

The transport of beams through bent lattices is being studied. Simulations have shown that beams that are axially cold do not exhibit any emittance growth during a bend, whereas beams that are axially hot ($T_{x,y} \sim T_z$) do show emittance growth. We believe this growth arises as a result of dispersion in the bend; this has been described in more detail in reference [1].

IV. Recent Additions

A. *Injection*

A simple model of injection has been added to WARP3d. At each time step, a preset number of particles are injected from the plane of injection. The injection is not space-charge-limited. The region into which the particles are injected extends from the plane of injection to the axial distance traveled in one time step. That distance includes acceleration from any potential gradients along the beam axis. The particles are distributed as if they were injected uniformly in time and accelerated along a uniform electric field given by the ratio of the potential across the region of injection to the length of the region.

B. *SOR Field Solver With Internal Conductors*

In order to simulate the transport of beams through complex conducting structures, the field solver must be able to include those conductors in the field solution self-consistently. For that purpose, a successive overrelaxation (SOR) iterative Poisson solver was added to the code. SOR was chosen because of its simplicity, ease of use, and flexibility in dealing with internal conductors. The seven point finite-difference form of Poisson's equation is used with the three-dimensional extension of red-black ordering. The potential of the conductors internal to the field mesh is enforced by setting the grid points inside the conductors to the appropriate potential before each iteration. For more accuracy, a scheme for allowing subgrid-scale placement of boundaries was implemented.

Subgrid-Scale Placement of Boundaries: The conductors that produce the quadrupole focusing fields consist of round, cylindrical rods, but the field mesh is a rectangular Cartesian grid. The round rods would be represented by stacks of rectangular blocks or "legos." This leads to inaccuracy of the fields. With space-charge dominated beams, the focusing fields need to be accurate in order to produce the correct beam envelope. A scheme was developed to solve for the potential near conducting surfaces that are not aligned with the computational grid.

The finite-difference form of Poisson's equation near conducting surfaces is changed to explicitly include the location of the boundary. In the finite-difference equation, one (or several) of the points will be inside a conductor, so ϕ at these points can be used as a free parameter. In one dimension, the potential at the surface of the conductor is given by linear interpolation from the two surrounding points, one outside the conductor, the other inside.

$$\phi_{\text{surface}} = (1-\delta)\phi_{\text{outside}} + \delta\phi_{\text{inside}} \qquad (1)$$

where δ is the distance between the surface and the point outside. This is rearranged to give an expression for ϕ_{inside} which is put into the finite-difference equation. The resulting expression is rearranged to make it fully explicit. The altered equation is used to calculate ϕ_{outside} in the iteration in place of the finite-difference equation used for the bulk. This process is done for all points near conducting surfaces. With multiple dimensions, several nearby points may be inside a conductor. Each point is handled separately as above. The linear interpolations for ϕ_{surface} in each direction are used to give separate equations for the ϕ_{inside}. These are all place into the seven point finite-difference equation which is then rearranged to be fully explicit.

V. ESQ Injector

The electrostatic quadrupole injector that is being designed for ILSE uses ESQ's for both focusing and acceleration. The quadrupoles are arranged to give a net acceleration along the axis while maintaining alternating gradient focusing. A major issue of concern is emittance growth from both the nonlinear multipole components of the focusing fields and the "energy effect". The cause of this effect are the focusing potentials, which are a large fraction of the particle's energy. Particles which are off axis

have a significantly different axial velocity than those on axis and are focused differently, causing beam distortion. Note that this effect is present in all electrostatic focusing systems but is generally insignificant, since the focusing potentials are a small fraction of the beam energy.

A. *Description of the Computer Runs*

Only steady state phenomena are of interest, so the runs are made in a quasi time dependent fashion. The time step over which the fields are calculated is larger than the time step of the particle advance. This process converges in just over one transit time across the injector, between five and ten field solutions. Transient behavior is lost and only steady-state is obtained. The dimensions of the field grid, including the conductors, are typically 50×50 in the transverse directions and between 200 and 600 in the axial direction, depending on the number of quadrupoles in the system. The lengths of the runs are between 300 and 1000 time steps, again depending on the number of quadrupoles. From 70,000 to 300,000 particles are used. Runs take typically from 3 to 30 minutes on the NERSC Cray C-90. We are effectively able to use WARP3d as a design tool.

B. *Simulation of the ILSE Injector*

The injector is required to supply 1 Amp of 2 MeV singly charged potassium ions at low transverse emittance, less than .5 π-mm-mrad. The initial design was done using an envelope code that does not include the energy effect. The three-dimensional simulations of that design did show significant emittance growth, up to 2 π-mm-mrad. By selectively canceling various multipole components, it was found that about half of the emittance growth was the result of the V_{42} potential component ($\phi_{42} = V_{42} r^4 \cos 2\theta$). The effect of that component is greatest where the beam gets closest to the conductors.

Analysis of single particle motion shows that the energy effect is fourth order ($\phi \sim r^4$) and is the result of the interaction of the difference in kinetic energy between particles on axis and off axis and the quadrupole field. By analytically applying additional fourth order fields, the energy effect can be canceled. Doing this showed that the energy effect accounted for the other half of the emittance growth. When the correction to the energy effect is applied and the V_{42} field is canceled, the beam experiences no emittance growth. This is a favorable result since it shows that the emittance growth is the result of external fields only and not the result of nonlinear space-charge fields. There is confidence, then, that the emittance growth can be greatly reduced or eliminated.

C. *Optimization of Design*

We looked at three ways of optimizing the design to reduce the emittance growth: changing the focusing fields to make the envelope as small as possible, changing the quadrupole structure to reduce the effect of the nonlinear fields, and increasing the beam energy from the source. Decreasing the size of the envelope was simple but of limited help. The envelope reduction is limited by the nature of alternating gradient focusing. Changing the structure was the next most useful. The biggest gain was from moving the focusing rods out and the defocusing rods in. While maintaining the same focusing strength, that moved the rods away from the fattest parts of the beam.

The most effective way of reducing the emittance growth is to increase the beam energy from the source. By increasing the energy before it enters the ESQ, the beam is stiffer and maintains a smaller envelope, reducing the effect of both the nonlinear fields and the energy effect. Also, with a higher beam energy, the energy effect is directly reduced. Simulations show that it is possible to have no emittance growth. Unfortunately, due to experimental constraints, increasing the beam energy at the source is difficult to do in practice.

D. *Comparison With Experiment*

A scaled-down version of the ILSE injector that was tested at LBL was simulated. There was good agreement between experiment and simulation. Scans, varying the diode energy, were made with both WARP3d and the experiment. Comparisons of the final beam phase space show good agreement. The beam's transverse size and velocities agree to within a few percent. Qualitatively, phase space looked the same and both displayed the same distortions that result in emittance growth.

VI. ACKNOWLEDGEMENTS

The authors are pleased to acknowledge the work and help of Simon Yu, and Shmuel Eylon of LBL.

REFERENCES

[1] A. Friedman, D. P. Grote, and I. Haber, "Three-dimensional particle simulation of heavy-ion fusion beams," *Phys. Fluids B* **4**, 2203 (1992).

[2] T. J. Fessenden and A. Friedman, Nucl Fusion, **31**, 1567 (199)

[3] D. P. Grote, A. Friedman, and I. Haber, Bull. Am. Phys. Soc., **36**,2415 (1991)

[4] T. J. Fessenden, Nucl. Instrum. Methods Plasma Res. A **278**,13 (1989)

[5] E. P. Lee, Nucl. Instrum. Methods Plasma Res. A **278**,178 (1989)

[6] Shmuel Eylon et. al.,Proceedings of the Fourteenth Biennial IEEE/APS Particle Accelerator Conference, (1991)