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

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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 $\phi$ 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 differentiating $\phi$ 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
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 equilibrium 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 decapole 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 ∼ 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 "lego." 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 there 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.

\[ \phi_{\text{surface}} = (1 - \delta)\phi_{\text{outside}} + \delta\phi_{\text{inside}} \]

where \( \delta \) is the distance between the surface and the point outside. This is rearranged to give an expression for \( \phi_{\text{inside}} \), 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 \( \phi_{\text{outside}} \) 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 \( \phi_{\text{surface}} \) in each direction are used to give separate equations for the \( \phi_{\text{inside}} \). These are all placed 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 50x50 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 typ-
ically 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 se-
lectively canceling various multipole components, it was
found that about half of the emittance growth was the re-
sult 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 inter-
action of the difference in kinetic energy between particles
on axis and off axis and the quadrupole field. By analyt-
ically 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 emit-
tance 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 alter-
nating 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 main-
taining 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 increas-
ing 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 be-
tween experiment and simulation. Scans, varying the diode
energy, were made with both WARP3d and the experi-
ment. 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.

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