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Methods Used in WARP3d, a Three-Dimensional PIC/Accelerator Code

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Abstract. WARP3d(1,2), a three-dimensional PIC/accelerator code, has been developed over several years and has played a major role in the design and analysis of space-charge dominated beam experiments being carried out by the heavy-ion fusion programs at LLNL and LBNL. Major features of the code will be reviewed, including: residence corrections which allow large timesteps to be taken, electrostatic field solution with subgrid scale resolution of internal conductor boundaries, and a bent beam algorithm. Emphasis will be placed on new features and capabilities of the code, which include: a port to parallel processing environments, space-charge limited injection, and the linking of runs covering different sections of an accelerator. Representative applications in which the new features and capabilities are used will be presented along with the important results.

INTRODUCTION

Heavy-ion-fusion (HIF) requires low temperature, or emittance, beams so that they can be focused on to a small fusion target. The presence of non-linear self-fields and applied fields can lead to an increase in emittance and make a self-consistent model necessary. Since the space-charge-dominated beams in an induction accelerator are effectively non-neutral plasmas, analysis of the beams can be carried out with computational modeling techniques related to those used in plasma physics. Particle-in-cell (PIC) simulation techniques are especially effective and have proved valuable in the design and analysis of both ongoing experiments and future machines, as well as in the study of basic physics issues of intense beams.

The three-dimensional electrostatic PIC simulation code, WARP3d, was developed for HIF to study beam behavior from first principles in realistic geometries. Here, we present an overview of the WARP3d code, describing in detail some of the major features which in combination make WARP3d a versatile beam simulation tool. We also present applications of the code that demonstrate the use of these features of WARP3d and highlight important results.

OVERVIEW OF WARP3D

WARP3d is part of a larger code, WARP, which includes different levels of high-current beam modeling, including WARPrz, a two-dimensional, axisymmetric PIC code, and a simple envelope equation solver which is primarily used to obtain an initial beam state well-matched to the accelerator. The code is built atop the Basis code development and run-time system, which affords a flexible and powerful interpretive user interface.

The WARP3d code combines PIC with a description of the "lattice" of accelerator elements. The fields affecting the beam particles include both the self-fields of the beam and the external fields from the lattice. The self-fields are assumed to be electrostatic and are calculated in the beam frame by solving Poisson's equation on a Cartesian grid which moves with the beam. The electrostatic solution is valid since, with the high mass of the beam ions, the beam is nonrelativistic throughout most of the accelerator. The Poisson solvers can optionally include any conductor geometry self-consistently in the field solution.

The lattice is a general set of finite-length accelerator elements, including focusing, bending, accelerating gaps, elements with arbitrary transverse multipole components, and curved accelerator sections (described in reference 1). The field from the lattice elements can be specified at one of several levels of detail which are described below.

METHODS USED IN WARP3D

A number of features and capabilities have been implemented in WARP3d to make possible simulation of a broader class of accelerators, both by way of inclusion of the relevant physics, and by optimization of the code to allow simulation of larger scale problems. The most important and novel of these are described.

Lattice Description

The lowest level of description of lattice elements is a hard-edged, axially uniform field. As the particles enter and exit such an element, "residence corrections" are used; the force applied on the particles is scaled by the fraction of the time-step spent inside the element. These residence corrections allow use of larger time-steps by ensuring that the particles receive approximately the correct impulse from the element independent of the time-step size. The applied field can be a sum of arbitrary multipole components.

At a higher level of detail, fields which vary axially can be applied. The coefficients of the multipole components are stored as tabulated data along the axial direction and are interpolated to the particles. This allows application of realistic fields, including for example fringe fields and more rapidly varying higher order multipole moments associated with a quadrupole focusing element.

The highest level of detail is specification of the field via a three dimensional grid. This allows application of fields more efficiently than a multipole description for an element with many multipole components. The field can be calculated in a different code, for example using TOSCA(3) to calculate the magnetic fields.

FIGURE 1. A curved conductor is shown on a grid. Poisson's equation at the circled points outside of the conductor is modified to explicitly include the location of the conductor surface by replacing the term which would use the squared points inside.

With electric elements, the field can be calculated self-consistently with WARP3d by inclusion of the electrodes in the field solution, thereby obtaining the realistic fields and image affects from the electrodes on the beam.

Subgrid-Scale Conductor Boundary Resolution

To allow more accurate modeling of electrodes for a given grid cell size and to avoid problems associated with the jaggedness of representing tilted or curved electrodes on a Cartesian grid, the iterative SOR field solver allows subgrid-scale resolution of the conducting boundary locations. Referring to Figure 1, this can be explained as follows. For grid points just outside the surface of a conductor, the form of Poisson's equation is changed to explicitly include the location of the surface. The potential at points inside the conductor, which is normally used in the evaluation of Poisson's equation at the points outside, is replaced by a value which is extrapolated from the potential at the conductor surface and at the grid point outside the surface. The method is similar to one used in EGUN(4), extended to three dimensions and time dependence.

Beam Injection

Several models of particle beam injection are used, all of which can model emission from planar or curved surfaces. Beside injection at a preset current, two space-charge limited injection methods have been implemented where the injected current is calculated self-consistently from the conditions near the emitting surface. To calculate the emitted current, the first model uses the Child-Langmuir relation in a region in front of the emitting surface, the length of which is small compared to the length of the diode. In the second model, the surface charge required to produce the desired zero normal electric field on the surface is calculated assuming an infinite conducting plane. The amount of charge injected into a grid cell is that surface charge integrated over the grid cell, subtracting the charge already in the grid cell from earlier times.

FIGURE 2. A simulation of an ion gun is linked to the following transport channel. With the simulation regions overlapping, data is saved in simulation 1 at the interface to simulation 2 and used as initial conditions in simulation 2.

For both self-consistent models, the normal electric field is obtained by calculating the potential at a point far enough in front of the emitting surface so that the grid points from which interpolation is done are all in front of the emitting surface. This avoids the problem of estimating a potential behind the emitting surface. The normal electric field is used both in the calculation of the injected current and as the field applied to particles near the emitting surface.

With space-charge limited injection, WARP3d can be run in an efficient iterative manner which captures only the steady state behavior. The algorithm is similar to that used in the two-dimensional electron gun design code EGUN(4). It should be pointed out that this capability was added to the code entirely through the Basis interpreter and required no modification of the existing code.

Linking of Simulations

For efficiency, sections of the accelerator often need to be simulated separately, linking from one to the next. For example, in simulating an ion gun followed by a transport channel, a much larger transverse grid is needed in the diode, to include the Pierce electrode, than is needed in the channel with a small pipe radius as shown in Figure 2. Other examples are the transition from a straight to a bent lattice where different symmetries should be used, and the transition from electric focusing to magnetic focusing, which have different boundary conditions and usually need different field solvers.

To link the simulations, the region covered by the first overlaps into that covered by the second, and data is saved from the first and is used as the initial conditions in the second. At each time step in the first simulation, the position and velocity of particles which pass the transition plane are saved, as well as the potential at the transition plane and the plane one grid cell to the left. In the second simulation, at each time step the particles previously saved are "injected" and the two planes of potential are loaded onto the field grid as a Dirichlet boundary condition. Two planes of potential are needed for the correct evaluation of the finite difference to obtain the electric field for particles near the transition plane. The overlap must be large enough so the fields in the region of the transition are calculated accurately.

FIGURE 3. The timings of WARP3d on the massively parallel Cray T3D show nearly linear speed-up with increasing number of processors. The squares give the timings of the field solver and the circles the timing of the particles. The gray line is the ideal linear speed-up. On the right are the actual timings, nanoseconds per grid cell per field solve and nanoseconds per particle per timestep.

Parallel Processing

WARP3d was originally designed to run on vector supercomputers and on workstations. With the present trend toward massively parallel processing, WARP3d was ported to a parallel environment. WARP3d now can run on the CRAY T3D, using both the PVM(5) message passing library and the native shared memory library, and on multi-workstation clusters using PVM.

Domain decomposition is done only along the axial dimension, which is generally longer than the transverse dimensions. With the FFT field solver, the field grid is divided evenly among the processors who share one grid cell with adjacent processors. A transpose is done for the axial FFT. The number of processors and number of grid cells both must be powers of two. With the SOR field solver, an overlap of 2 grid cells is needed so that a plane which is calculated by one processor can be passed to its neighbor to be used as a Dirichlet boundary condition. The data is passed on each iteration in the field solve. The particles are divided into same regions as the field grid. This is not ideal since the beam may not fill entire axial extent of the grid leaving some processors with fewer or no particles.

An effort was made to keep the same user interface for the parallel code as for the serial code. The effort was complicated by the fact that the Basis interpreter does not run on the parallel machine. The parallel code is run through the Basis interpreter on a serial machine, allowing same structured input decks as the serial code. The processes on the parallel machine are then spawned via PVM and the initial data is passed down to them. The user can then issue commands, which are passed to the parallel code, allowing the user to run the simulation, set or access variables, and retrieve grid, particle, diagnostic, or time history data.

Timings were made, shown in Figure 3, with a model simulation on a Cray T3D

FIGURE 4. The electrostatic quadrupole injector is shown filled with beam. The shading of the beam particles is proportional to the particle's axial velocity relative to the velocity along the axis, lighter being faster. One quadrant is cut away to show the beam.

with up to 32 processors, following a beam through five lattice periods. The field solver showed the slightly superlinear speed-up due to better use of cache with smaller problem size in each processor. The particles showed slightly less than linear speed-up, likely due to small load imbalances.

APPLICATIONS

WARP3d has been used in a wide variety of applications, making use of the methods described above. Several recent applications are described, showing the use of the methods and highlighting important results.

Electrostatic Quadrupole Injector

A HIF driver-scale injector and matching section is being built at LBNL, in collaboration with LLNL, to address beam physics and technology issues(6). The injector uses a sequence of electrostatic quadrupole lenses arranged to obtain a voltage gradient along the axis. The net effect is to both confine the beam transversely and accelerate it. The beam is emitted from a hot-plate source and is accelerated through a diode section into the set of quadrupole lenses. Figure 4 shows an image from a detailed injector simulation. WARP3d was used to understand a major issue in the injector design, namely the increase in emittance caused by the high order multipole components associated with the electrode geometry.

The methods used in the simulations allowed realistic beam injection and mod-

elling of the electric quadrupoles. The beam was formed by space-charge limited injection, using both the EGUN-like iterative mode and time-dependent injection. The subgrid-scale resolution of quadrupole electrode surfaces was used to obtain accurate fields. Four-fold transverse symmetry was used, simulating only one quadrant. Typically, the mesh size used was 40x40x348 with 300,000 particles. The runtime was approximately 30 minutes on a Cray C90, single processor. Code predictions influenced the design geometry, mitigating emittance growth, and good agreement was obtained between the simulation and experimental results.

Bending Experiments

A recirculating heavy-ion induction accelerator, or "recirculator," offers the prospect of reduced cost relative to a conventional linear accelerator because the accelerating and focusing elements are re-used many times per shot(7). A small recirculator is being developed at LLNL to explore the beam dynamics of a HIF driver in a scaled manner; the key dimensionless parameters that characterize the beam are similar to those of a driver-scale ring but the physical scale is much smaller(8).

As a precursor to full recirculator experiments, the beam is being examined in a lattice with an 45 degree bend. The bend experiment will be the first detailed examination of a space-charge dominated heavy-ion beam in a bent, alternating gradient lattice. The experiment consists of a series of electric and then magnetic quadrupoles with 9 degree bends and electric dipoles in the last five half lattice periods. The experiment has been examined with WARP3d. The simulations predict an acceptable emittance growth of about a factor of two, due entirely to the matching of the beam from a straight lattice to a bent lattice.

The beam is initially launched in a simulation of the diode which is then linked to a simulation of the following transport channel. The field from the electric quadrupoles was calculated with WARP3d using the electrode geometry and decomposed into multipole components. The multipole components from the magnetic quadrupoles was calculated analytically. The fields are applied as elements with axially varying multipole components. The electric dipole plates are also modeled in detail using the WARP3d field solver, and the fields are applied to the particles as elements with data on a 3-D grid. The simulation of the bends required the use of the bent lattice algorithm.

Many of the same methods which are used in the simulations of the bent beam experiment are also used in the simulations of the full recirculator experiment. The major difference is that the simulations are carried out over a much longer time, following the beam for hundreds of lattice periods.

Over 15 laps, the simulations show little emittance growth after the initial growth due to the matching of the beam from a straight lattice to a bent lattice. The overall degradation of the beam is acceptable.

AVLIS

An electron gun is used in atomic vapor laser isotope separation (AVLIS) to melt and vaporize the material to be separated. The electron gun has shown anomalous asymmetric beam behavior that cannot be studied with axisymmetric codes. We have begun to use WARP3d to examine the gun. The methods used are space-

charge limited injection of the electrons off the emitter surface and use of magnetic fields calculated by TOSCA and specified on a 3-D grid. The full conductor geometry is simulated using subgrid-scale conductor resolution.

CONCLUSIONS AND FUTURE WORK

Many future code enhancements and applications are planned for WARP3d. Some example enhancements that are envisioned are an interface with a CAD system to input general 3-D conductor shapes, a more advanced field solver which uses an unstructured mesh outside of the beam, and inclusion of beam self-magnetic fields. Also, a number of methods in WARP3d will be further improved. For example, the mechanism for linking simulations can be made more flexible by allowing different grid cell and time step sizes in the linked run.

WARP3d makes use of many different features, all built into one package, which allows it to be applied on a wide variety of beam problems. This makes it a versatile tool is the analysis of the dynamics of space-charge-dominated beams.

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