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Computational Methods in the Warp Code Framework for Kinetic Simulations of Particle Beams and Plasmas

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Invited Paper

Abstract—The Warp code (and its framework of associated tools) was initially developed for Particle-in-Cell simulations of space-charge-dominated ion beams in accelerators, for heavy-ion-driven inertial fusion energy and related experiments. It has found a broad range of applications, including non-neutral plasmas in traps, stray “electron clouds” in accelerators, laser-based acceleration, and the focusing of ion beams produced when short-pulse lasers irradiate foil targets. We summarize novel methods used in Warp, including: time-stepping conducive to diagnosis and particle injection; an interactive Python-Fortran-C structure that enables scripted and interactive user “steering” of runs; a variety of geometries (3-D x,y,z ; 2-D r,z ; 2-D x,y); electrostatic and electromagnetic field solvers; a cut-cell representation for internal boundaries; the use of “warped” coordinates for bent beam lines; Adaptive Mesh Refinement, including a capability for time-dependent space-charge-limited flow from curved surfaces; models for accelerator “lattice elements” (magnetic or electrostatic quadrupole lenses, accelerating gaps, etc.) at user-selectable levels of detail; models for particle interactions with gas and walls; moment/envelope models that support sophisticated particle loading; a “drift-Lorentz” mover for rapid tracking through regions of strong and weak magnetic field; a Lorentz-boosted frame formulation with a Lorentz-invariant modification of the Boris mover; an electromagnetic solver with tunable dispersion and stride-based digital filtering; and a pseudo-spectral electromagnetic solver. Warp has proven useful for a wide range of applications, described very briefly herein. It is available as an open-source code under a BSD license.

This paper describes material presented during the Professor Charles K. (Ned) Birdsall Memorial Session of the 2013 IEEE Pulsed Power and Plasma Science Conference. In addition to our overview of the computational methods used in Warp, we summarize a few aspects of Ned’s contributions to plasma simulation and to the careers of those he mentored.

Index Terms—Plasma, particle beam, laser, numerical simulation, particle-in-cell, Maxwell, computer, algorithms, Ned Birdsall.

I. INTRODUCTION

This paper describes material presented by the lead author during the Professor Charles K. (Ned) Birdsall Memorial Session of the 2013 IEEE Pulsed Power and Plasma Science Conference. Parts of the presentation were devoted to describing Ned’s impact on science and on the careers of the lead author and numerous others. Ned was a friend and mentor to many scientists and engineers. He served as the

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academic advisor or supervisor of many students and post-doctoral researchers, including the lead author; taught many others in courses at U.C. Berkeley and around the world; and authored (with Bruce Langdon) a seminal text on the numerical simulation of plasmas [1], along with important texts on other topics. In this article, along with our overview of the computational methods used in the Warp code, we summarize a few aspects of Ned’s wide-ranging influence and their reflection in the code’s structure and features.

The Warp code was initially developed to meet the needs of the U.S. Heavy Ion Fusion (HIF) research program [2], [3]. The goal of HIF is to apply the principles of inertial confinement fusion to the commercial production of electric power, using ion beams instead of lasers as drivers. Motivations include: the projected efficiency of the induction accelerators chosen as the principal approach of the U.S. HIF program; the compatibility of the beams and targets with a fusion chamber environment based on protection of the chamber walls by neutronically thick liquids (bearing Lithium, to enable Tritium breeding); and the volumetric deposition characteristics of the ion beams. However, the beams are of unusually high density but moderate kinetic energy (of order 5 GeV), and their phase space must be kept compact (small transverse and longitudinal emittances) to enable focusing onto targets. The beams are effectively non-neutral plasmas, and their manipulation and control presents challenges related to those of both accelerator physics and plasma physics.

Warp thus combines elements of plasma particle-in-cell codes and traditional accelerator codes. While borrowing from both fields, we also found it useful to introduce new methods so as to achieve improved versatility, accuracy, and efficiency. Many of these methods have been adopted for use in other codes. This paper presents a brief summary of a number of the methods, with reference to other publications wherein more details may be found. In particular, the reader is directed toward four summary papers that reflect the state of the code as it has developed from its beginnings in the late 1980’s [4]–[7]. Warp is available as an open-source code under a BSD license; details can be found at the Warp web site [8].

Section II presents an overview of the Warp code’s basic architecture, including the synergistic use of both interpreted (Python) and compiled (Fortran and C) components, and the prescription used for time-advancement. Section III describes the available “geometries” and coordinate system, including the use of “warped” coordinates and of “cut cells” for subgrid-scale placement of conducting boundaries. Section IV includes a description of the “drift-Lorentz” mover developed to efficiently compute orbits that pass through regions with

strong magnetic fields, when the gyro-phase is unimportant in those regions; a key application is to problems involving stray “electron clouds.” Many of the physical processes involved in “e-cloud” problems are included in Warp. In Section V, we describe the mesh-refinement capabilities of Warp, for both electrostatic and electromagnetic problems. Section VI describes developments that enable more accurate and efficient computation of relativistic systems, including use of a Lorentz-boosted frame of references, a modified “Boris” advance for particles that preserves frame invariance, and options for advancing the EM field, including non-standard finite-difference and -spectral methods. In Section VII, we describe selected applications of Warp, including the Neutralized Drift Compression Experiment-II (NDCX-II) at Berkeley Lab, and the University of Maryland Electron Ring (UMER). Finally, we offer a few concluding remarks in Section VIII.

II. BASIC ARCHITECTURE

Warp combines efficient Fortran routines for large-scale numerical operations with a modern, object-oriented Python upper layer and user interface. To this end we developed a system, “Forthon” [9], which establishes a linkage between the two levels. It allows all major code quantities to be accessible to both Fortran and Python code, and that compiled subroutines can be called from Python code. Forthon includes a facility for a dynamic run-time database, so that arrays accessible at both levels can be dynamically allocated and deallocated. For more details see [7].

Python offers a flexible and powerful user interface, rapid prototyping, a rich set of capabilities, and a large scientific user community. Input files to Warp are Python programs (some are thousands of lines long). Users often build on established Python functionality to develop their own diagnostics, which can then be applied by others. The boundary between input specification and program is not a sharp one, and, in a sense, Warp may be thought of as a set of “physics extensions to Python.” See Fig. 1. This structure empowers users, help reduce their dependence upon the code’s developers, and minimizes the need to frequently recompile Warp.

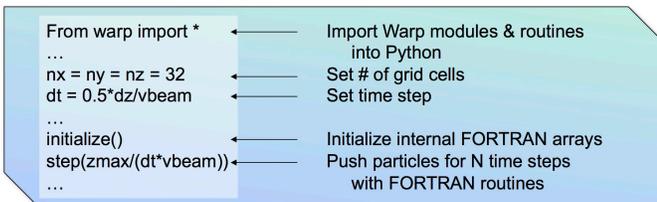


Fig. 1. An excerpt from a Python script used as input to Warp.

This architecture facilitates linking independently written codes so that they can readily communicate with each other, typically (but not necessarily) at the Python level. Python’s flexible handling of name-spaces ensures that conflicts do not arise when the code authors each employ variables with the same name. One of our goals was a robust code with a relatively modest compiled “core” that users generally need not change and that can be maintained by a small developer group, and a rich user-programmable layer that is heavily extended by typical users. Warp is run either interactively from

the terminal or in a batch mode. A graphical user interface (GUI) was developed; it offers ease-of-use and complements the flexibility of invoking user-written scripts while running Warp, but is not currently maintained due to lack of manpower. Also for ease of use and to keep the learning curve minimal, SI units have been adopted throughout, with exceptions as appropriate, *e.g.*, for energies in electron-Volts.

Here it is appropriate to remark that, throughout his career, Ned Birdsall promoted the use of interactive computing as a means of maximizing insights gained and user flexibility. The interactive, user-steerable nature of Warp was in part inspired by Ned’s vision of interactive computing. It also has roots in the long-standing “LLNL model” of interpreted/compiled code, using systems such as Basis [10] (indeed, the earliest versions of Warp employed Basis).

We illustrate the time-advance formalism used in Warp with an electrostatic example. While the approach is straightforward, it did not appear to be in common use when we began writing Warp (and indeed we do not know how commonly it is used today). Our goal was to make it easy for developers and users to write diagnostics, to inject particles, to “dump” particle data, and to change the timestep size dynamically. This requires that, when the calculation is “quiescent,” everything of interest is defined at the same time level. This is most easily accomplished when all key quantities are advanced from one integer time level to the next using an “isochronous” leapfrog advance (Fig. 2), which (in the absence of a magnetic field, or with such a field but correcting for rotation angle) is algebraically equivalent to the usual leapfrog step (Fig. 3(a)).

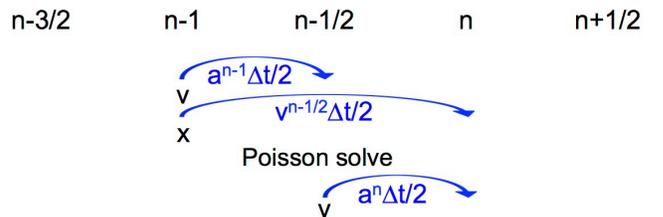


Fig. 2. Isochronous leapfrog particle advance step.

However, the isochronous algorithm is inefficient because it requires two separate passes through the particle lists with a field-solving step in the middle. While improvements to this isochronous advance can be made (*e.g.*, by storing the interpolated field on a particle-by-particle basis), we have chosen a hybrid approach that combines leapfrog steps with periodic “special” steps, arranged so that the user and the diagnostic routines never see un-synchronized data. On most steps, perhaps 9 out of 10, the leapfrog advance (labelled internally “Fullv”; see Fig. 3(a)) is used; however, when the next step is to include diagnostics, or is the last step requested by the user in an interactive run, a “Syncv” step (Fig. 3(b)) is used to synchronize x and v . Furthermore, at $t = 0$ or when x and v were synchronized by the previous step, a “Halfv” advance (Fig. 3(c)) (preceded by a Poisson solution if necessary) is used to restart the leapfrog sequence. It is possible to request that “history” quantities be tallied at every step, even leapfrog steps; this is accomplished by (*e.g.*) interpolating v to the integer time level before tallying.

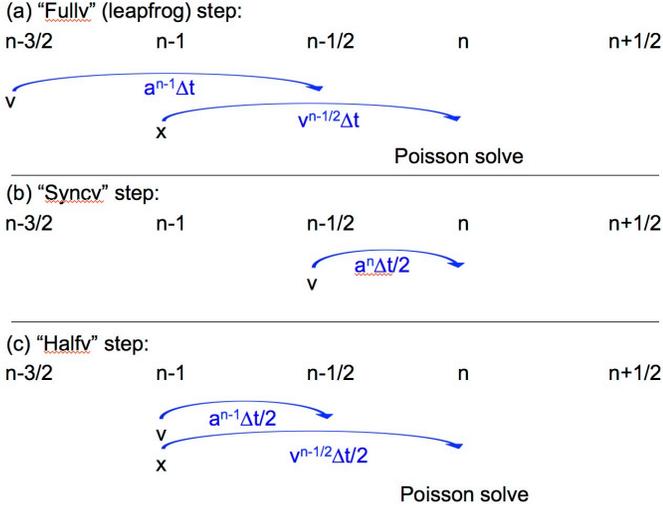


Fig. 3. Time-advance steps for electrostatic problems: (a) “Fully” (leapfrog) particle advance step; (b) “Syncv” step; (c) “Halfv” step.

Another element of the approach to scientific computing promoted by Ned Birdsall was the dictum, “write the diagnostics first.” The rapid-prototyping nature of Warp’s interpreter layer, and the time-stepping formalism whereby key quantities are known at integer time levels, were in part motivated by the desire to make diagnostics easy to write and to modify. As a consequence, Warp gained a rich set of diagnostics very early in its development, and complex applications continue to benefit from these choices.

III. CODE GEOMETRIES, “CUT CELLS”

Warp offers several geometries. These include 3-D Cartesian (x, y, z) with associated momenta, axisymmetric (r, z) with three momentum components, a 2-D (x, z) “sheet beam” model, and a 2-D transverse (x, y) “slice” model with 2 or 3 momentum components. The last of these simulates a steady flow, examined at successive stations along the beam line, and is a good approximation for the central portion of a long, flat-topped beam. The flow is steady in the laboratory frame, but each particle experiences a time-varying field as it moves. When a thermal spread in the axial momenta of the particles is included, or when the beam line is bent, the code uses a unique timestep size for each particle, adjusted so that, at the end of the step, all particles in the slice are at the same axial station. Among other benefits, this enables the code to effectively use a reduced (x, y) model to simulate such effects as beam passage through “transition” in rings.

In addition to the conventional PIC advance with time as the independent coordinate, and the above-mentioned “slice” model with z as the independent coordinate (whereby particles are advanced in time and the timestep size adjusted for the desired step in z), Warp offers two other modes. The first of these is a 3-D or (r, z) “gun” mode, used for designing particle injectors, wherein particle “markers” are tracked along the entire system, their space charge accumulated along their entire trajectories, a field solve carried out, and the process iterated until convergence. The second is a “quasistatic” mode, as used for, *e.g.*, electron cloud studies, whereby a 2-D slab of

electrons is stepped backward through the positively-charged beam, and advanced using the combined beam+self field. The aggregate impulse of these slice fields is applied to the beam, which is then advanced over a relatively long distance to the next electron-containing station. Here, the integration of the Posinst code [19] into Warp enables calculation of the electron secondary emission and buildup. Models are also available for background gas and atomic processes such as ionization.

Warp also includes a novel approach to simulating bent beam lines. While most accelerator codes employ a “paraxial” expansion about a nominal “reference orbit,” and some track particles in a global 3-D space, Warp uses “warped Cartesian” Frenet-Serret coordinates in 3-D. This is most easily visualized as a sewing-together of Cartesian and polar coordinates, but in principle allowing a continuously-variable curvature in one plane of the beam line [4]. The usual longitudinal position is replaced by another coordinate, s , denoting path length along a centerline, often (but not necessarily) the center of the beam pipe (Fig. 4a). In a bend, particles each have, at any step, their own associated Cartesian coordinate system, aligned with the local tangent to the curve along which s is defined. It is possible to handle bends “without approximation” by advancing each particle as if in a straight beam line, then re-labeling the position and velocity at the end of the step to those associated with the local coordinate system at that value of s [11]. Warp uses a somewhat faster but approximate algorithm that carries out the particle advance with additional pseudo-forces associated with the coordinate system rotating underneath the particle as it moves. [12]. As an example, Warp was recently used to study beam stripping by a foil, followed by charge selection in a chicane (Fig. 4b-d) [13].

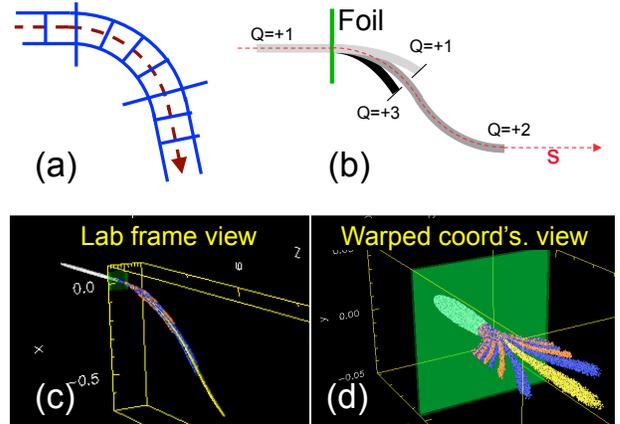


Fig. 4. Treatment of bent beam lines: (a) sketch of typical bent beam line; dashed arrow shows line along which s is measured; (b) overall geometry of foil and chicane, showing charge separation; (c) lab frame view (reconstructed); (d) view in Warp’s native “warped” coordinates.

A “cut cell” boundary representation on the field grid offers a subgrid-scale conductor-edge description, and thus removes the common limitation that conducting surfaces be built up like “Lego bricks.” This is especially important for problems involving electrostatic elements, *e.g.*, electrostatic quadrupole lenses for beam focusing, where the focusing strength depends upon the boundary’s location. In a cut-cell treatment, the finite-difference stencil at nodes within one cell of a conductor is

modified so that the specified potential on the conductor is enforced at the conductor edge, rather than at the nearest node. Warp made early use of 3-D cut-cell boundaries in a PIC code; the technique itself was invented many years earlier [14]. Building on this technique, Warp also offers time-dependent Child-Langmuir space-charge limited injection from specified curved surfaces.

For field solvers (such as the FFT solvers also available in Warp) which cannot accommodate non-uniform stencils, a capacity-matrix capability is included; the technique is efficient for simple extruded pipe shapes, which are well defined by a modest number of boundary points.

Warp was used extensively to model the Electrostatic Quadrupole (ESQ) Injector [15] and the High Current Experiment (HCX) [16] at LBNL, wherein a beam was generated on a curved emitting surface, accelerated across a gap, then both accelerated and focused (confined) by a sequence of alternating-gradient quadrupole elements with an overall longitudinal voltage gradient superposed (Fig. 5).

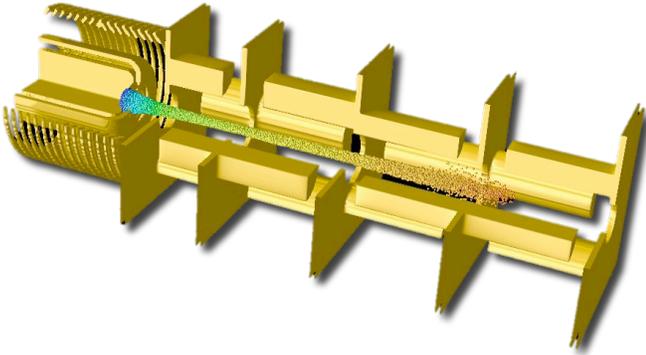


Fig. 5. Snapshot of Warp simulation of HCX electrostatic-quadrupole injector showing curved electrode surfaces. One quadrant has been cut away in this projected view.

Here we remark upon another of Ned Birdsall’s teachings: that it is important to simulate realistic systems, not just ideal ones. The early use of cut-cells enabled Warp to treat complex geometries accurately and efficiently.

IV. DRIFT-LORENTZ MOVER, E-CLOUD MODELS

In ion accelerators, stray electrons can be liberated from structures by the impacts of “halo” ions or generated by the ionization of background gas. We sought to efficiently compute the motion of such electrons, and to answer such questions as whether they can be accelerated (upstream) to high energies by the accelerating fields of a series of induction cells. Direct integration of the Lorentz force law in regions where electrons are strongly magnetized requires a very small timestep due to the gyroperiod being much shorter than other timescales of interest; but in such regions, the gyro phase is unimportant and a drift approximation suffices. In regions of weaker magnetic field (such as between electrostatic quadrupoles of opposite polarity), accurate direct integration is possible with relatively modest timestep sizes. Thus, we developed a hybrid “Drift-Lorentz” mover [17] to address the challenge of short electron timescales in typical magnetic fields. This mover

interpolates between full-particle dynamics (“Boris mover”) and drift kinetics (motion along the magnetic field \mathbf{B} plus drifts) using:

$$\mathbf{v}_{eff} = \mathbf{b}(\mathbf{b} \cdot \mathbf{v}_L) + \alpha \mathbf{v}_{L,\perp} + (1 - \alpha) \mathbf{v}_d \quad (1)$$

where \mathbf{b} is a unit vector aligned with \mathbf{B} , \mathbf{v}_d is the drift velocity, and \mathbf{v}_L is the velocity updated using the full Lorentz force (via the Boris mover) plus $(1 - \alpha)$ times the field-aligned magnetic-mirror (“ $\mu\nabla B$ ”) force from drift kinetics. The correct gyroradius is obtained when the interpolating fraction $\alpha = 1/[1+(\omega_c \Delta t/2)^2]^{1/2}$, with ω_c the gyrofrequency, is used. See Fig. 6.

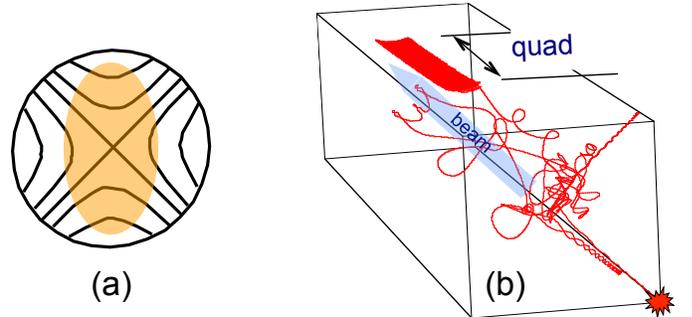


Fig. 6. Illustration of use of Drift-Lorentz mover: (a) schematic cross-section of ion beam in field of a magnetic quadrupole; (b) typical electron orbit showing drift motion where strongly magnetized, chaotic motion near field null between quadrupoles.

Warp contains Monte-Carlo models for ionization, capture, charge exchange, and secondary electron emission (with energy and angular dependence). Particle emission can be space charge limited, thermionic, a hybrid of the two, or specified arbitrarily by the user. Ion impact- or photo-induced electron emission, and ion impact-induced gas emission (with the gas tracked as neutral particles) are also simulated. The TXPhysics package from Tech-X is also available [18].

The Posinst code [19] has been integrated into the Warp framework, and its routines can be employed in Warp runs. As a well-benchmarked model for secondary electron emission, this feature, together with the Drift-Lorentz mover, has made Warp a capable tool for studies of “electron cloud” buildup and its effects on a positively-charged beam.

The integration of Posinst with Warp exemplifies the utility of our Python-based code framework. Posinst can still be run as a stand-alone code, but its functionality is fully available in Warp. For Fortran-based codes, such integrations are enabled by the Forthion system; it is also possible to couple in C and C++ coding.

As a test of electron-cloud physics and the Warp models, the ion beam in HCX was deliberately directed onto a metal end-plate, leading to copious back-streaming of electrons [20], [21]. Warp predicted an electron oscillation which was concurrently observed in the experiment and found to be in excellent agreement with the simulation (Fig 7). This calculation also used Warp’s Mesh Refinement (MR) capability, described below in Section V. The run time was ~ 3 cpu-days; without the Drift-Lorentz electron mover and MR, it would have been ~ 1 -2 months.

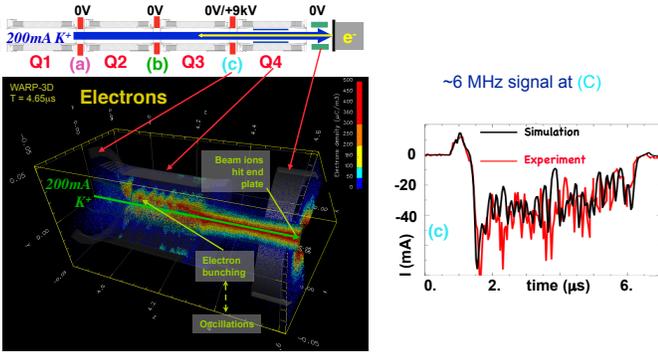


Fig. 7. Electron oscillations in HCX, as simulated in Warp, and as observed.

V. MESH REFINEMENT

Mesh refinement (MR) is a family of techniques used to concentrate grid resolution where it is needed, while avoiding fine gridding where it is unnecessary. Adaptive mesh Refinement (AMR) is a variation, wherein refinement patches are automatically moved or generated as needed, guided by the evolving flow; various refinement criteria are available. Warp offers both electrostatic and electromagnetic AMR capabilities. Either may be combined with a capability for independent timestep sizes, so that particle motion over a step can be constrained by the local cell size as necessary.

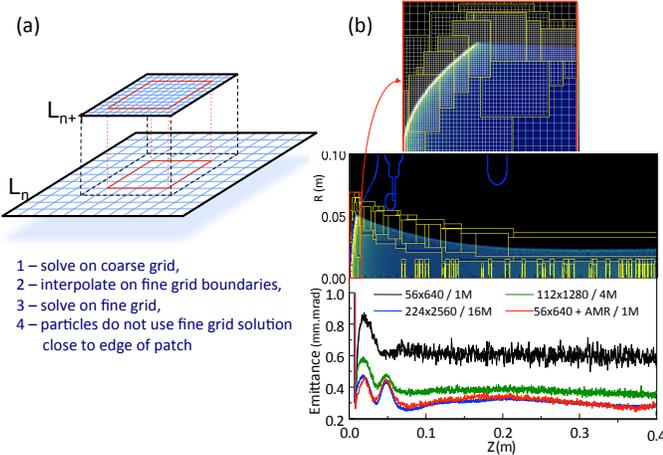


Fig. 8. Electrostatic Adaptive Mesh Refinement: (a) depiction of MR scheme; (b) application to an ion injector, showing (from top to bottom) overlapped refinement patches near the injection surface and at beam edge; snapshot of generated refinement patches; comparison of runs at various resolutions and particle numbers, and an AMR run (which was ten times faster than the high-resolution run).

Electrostatic MR (Fig. 8a) uses a straightforward algorithm whereby the field is first solved on a coarse level and then interpolated to the boundaries of the finer patches; a solution for the field on the patches is then carried out. Particles in the central regions of the patches (but not those close to the edges) use the refined field [22], [23]. This procedure minimizes artifacts due to the asymmetry of the prescription near the patch boundary. Electrostatic (and magnetostatic) field solvers in Warp include FFT's (with optional capacity matrix for boundaries) and a multigrid solver; the latter is used for

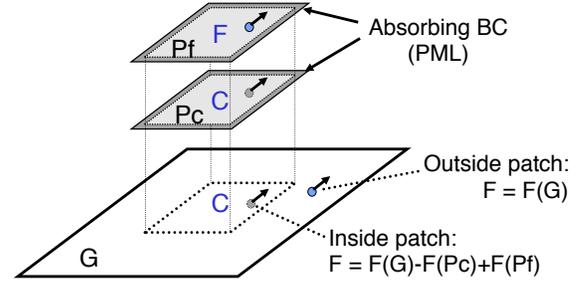


Fig. 9. Electromagnetic AMR. Fields F in a refinement patch are obtained as a linear combination of those on the main coarse grid G , the coarse patch P_c , and the fine patch P_f , with coarse data interpolated to finer resolution as necessary. The patches are terminated using PML absorbing boundary conditions.

MR field solutions. The approach has been highly successful, offering savings of an order of magnitude or more on problems of interest, such as injectors (Fig. 8b).

Electromagnetic AMR is more challenging, in large part because some waves that can be resolved on a refined patch cannot be resolved on the coarser parent patch. When they reach the edge of the fine patch, they can nonphysically reflect back into it, often with amplification, and disrupt the solution. To minimize such ill effects, Warp employs absorbing “Perfectly-Matched Layer” (PML) boundary conditions at the patch edges [24], [25]. In the method developed for use in Warp [7], [25], each fine patch is overlaid by a coarse patch spanning the same subdomain, and a subtractive correction yields the field on the fine patch (Fig. 9). No interpolation at the boundaries is used. As in the electrostatic case, the fields on coarser levels are unaffected by those on finer levels, and the refined field is not used within a guard region near the patch boundary.

VI. EM AND PARTICLE ADVANCE, BOOSTED FRAME

Warp offers several options for the time-advance of the electromagnetic field via Maxwell's equations. Most of these use a staggered “Yee” discretization of the field components [26], with either a traditional leapfrog stencil or a Non-Standard Finite-Difference (NSFD) stencil. The latter was adapted from the Cole-Karkkainen free-space prescription [27]–[29] so that source currents using “exact” charge-preserving prescriptions are usable [30].

Most recently, a pseudo-spectral Maxwell solver was implemented in Warp. It builds on Haber's earlier method [31], which is accurate to machine precision for modes resolved by the grid, has no Courant or accuracy-based limit on the timestep size (in a uniform medium with time-invariant source terms), and no numerical dispersion or anisotropy. In contrast with most commonly employed methods that use a staggered grid (*e.g.* Yee solver), it represents all field values at a common set of nodes, thus avoiding interpolation errors associated with staggering. Though the original method required global FFT's, good performance on modern multi-processor systems was made possible by a recent realization: the finite speed of light enables rapid pseudo-spectral solution of the Maxwell

equations on a set of overlapping subdomains. As described in [32], [33], the method requires only local FFT's and the exchange of guard cell data between neighboring subdomains, and introduces only very small errors in the resulting field values.

A “tunable damping” algorithm is available to control noise in EM simulations induced by particle fluctuations [30], [34]–[37]. Its purpose is to rapidly damp those modes which are poorly resolved by the grid and most susceptible to excitation by random motions, while preserving the dispersion properties of the underlying scheme for lower-frequency modes which are well resolved in space and time (the scheme preserves those modes more faithfully than would the common damping approach of simply de-centering the system of equations). The degree of damping is adjustable by the user, and can be “tuned” to match the needs of the problem being simulated. An implementation used in Warp, employing the lag-averaged electric field $\bar{\mathbf{E}}$, is shown in eqns. (2):

$$\begin{aligned} \mathbf{E}^{n+1} &= \mathbf{E}^n + \Delta t \nabla \times \mathbf{B}^{n+1/2} - \Delta t \mathbf{J}^{n+1/2} \\ \mathbf{B}^{n+3/2} &= \mathbf{B}^{n+1/2} \\ -\Delta t \nabla \times &\left[\left(1 + \frac{\theta}{4}\right) \mathbf{E}^{n+1} - \frac{1}{2} \mathbf{E}^n + \left(\frac{1}{2} - \frac{\theta}{4}\right) \bar{\mathbf{E}}^{n-1} \right] \\ \bar{\mathbf{E}}^{n-1} &= \left(1 - \frac{\theta}{2}\right) \mathbf{E}^n + \frac{\theta}{2} \bar{\mathbf{E}}^{n-2} \end{aligned} \quad (2)$$

where θ is the damping parameter; when $\theta = 0$, the system of equations is time-reversible and undamped.

The tunable NSFD EM solver (but not the Yee FDTD solver) allows use of $c\Delta t = \Delta z/\sqrt{2}$ for (near) cubic cells. At this step size there is a sharp decrease in the numerical Cherenkov instability. The existence of such “special” time step sizes was discovered with Warp [30] and is explained in [38]. Numerical filtering is also helpful in suppressing the instability, and to this end a new and efficient “strided” filtering algorithm was developed and implemented in Warp [30].

For highly relativistic particle beams, the standard “Boris” implementation of the particle advance introduces significant errors associated with summing imperfectly-computed, nearly-opposite electric and magnetic contributions to the acceleration. To address this, a modification of the Boris advance was developed and implemented in Warp [39]. It strictly preserves Lorentz invariance, and can readily be implemented in codes that use the traditional advance. It has proven useful in simulations of relativistic beam interactions with background electrons, and elsewhere [7].

Many systems of emerging interest are characterized by a wide spread in space and/or time scales, posing challenges for numerical simulations. A few years ago, it was recognized [40] that, by carrying out the calculation in a Lorentz-transformed frame, dramatic reductions in the required computational effort could be achieved for such systems. That is, even though in any frame the relevant interactions need to be captured, the required computational effort is not invariant. When disparate scales are involved, computation in a suitable frame effectively

Lorentz-contracts some of the larger features of importance to the physics while Lorentz-expanding some of the smaller features, conveniently bringing them closer in scale. Furthermore, The Lorentz transformation to an optimal boosted frame may be cast as a hyperbolic rotation in space-time. For a laser-wakefield acceleration simulation, such a transformation can effectively convert laser spatial oscillations (requiring fine gridding) to time-beating.

For computations in a boosted frame, no changes to the underlying simulation algorithms are needed (since the laws of physics are the same in that frame). However, because simultaneity is not frame-invariant, Warp must properly set up initial conditions at a fixed time in the boosted frame, must handle particle and laser injection from fixed planes in that frame (see [41]), and must generate diagnostic “snapshots” in the lab frame using data accumulated over multiple time steps at multiple planes in the boosted frame (Fig. 10).

The method can yield extremely large speedup factors [42], and has already enjoyed broad applicability [43], [44].

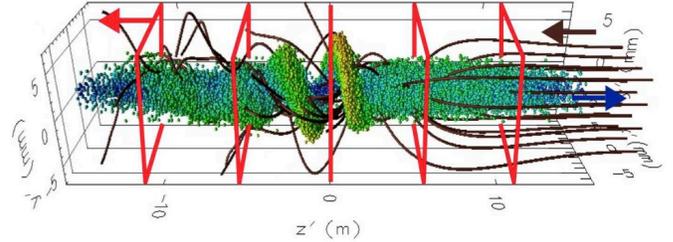


Fig. 10. Illustration of data gathering for production of a laboratory-frame diagnostic in a calculation being carried out in a Lorentz-boosted frame. Red boxes denote moving planes in the simulation frame, on which data is gathered over multiple timesteps. The image is from a study of e-cloud induced instability in a proton bunch [40].

VII. NDCX-II, UMER, AND OTHER APPLICATIONS

As noted above, Warp has long been the work-horse code for beam dynamics studies in the Heavy Ion Fusion research program, and its applications in support of that program are too numerous to mention here. The reader is referred to References [2], [4]–[7], [45] for information on these applications. Here we limit our summary to recent uses of Warp in support of two prominent accelerator facilities, NDCX-II and UMER, and briefly list selected other applications of the code.

The Neutralized Drift Compression Experiment-II (NDCX-II) [46], [47] at Berkeley Lab is a novel, pulse compressing ion induction accelerator designed to generate intense, ns-duration pulses of Li^+ ions and focus them into mm-scale spots on thin-foil targets. It was developed specifically for studies of ion-heated matter in the Warm Dense Matter regime; key aspects of heavy-ion beam-driven inertial fusion energy targets (including techniques such as ramping the beam kinetic energy to achieve more efficient coupling of beam energy); and the dynamics of space-charge-dominated beams. Extensive simulations were required to develop the “physics design,” along with much iteration between the simulators and the engineering team (especially in regard to the acceleration voltage waveforms). See Refs. [46], [48].

Because of the very large multi-dimensional space of possible waveform sets, a simpler 1-D particle-in-cell code, ASP (for “acceleration schedule program”) [49], was constructed using Fortran and drawing on elements of Warp. ASP was used for rapid scoping and development of the longitudinal dynamics in NDCX-II. The process was reminiscent of that used in designing pulse shapes for the implosion of inertial-fusion target capsules. We believe that Ned Birdsall would have appreciated this highly interactive use of a relatively simple PIC model coupled with sophisticated optimizers and a large portion of intuition.

Because the field model in ASP is approximate (and because transverse and longitudinal dynamics are coupled), final optimizations of the longitudinal dynamics were carried out in both 2-D and 3-D using Warp itself. Warp was also important to the development of the final neutralized drift compression and final focusing sections of NDCX-II; it led to the adoption of a design with minimal gaps in the plasma density, and to new physical insights, *e.g.*, regarding non-paraxial effects in the focusing of a finite-radius particle beam [50].

In NDCX-II, the beam emerges from the injector as a long pulse (of order 600 ns) and is compressed in an initial (plasma-free) “bunching” section using waveforms that accelerate its “tail” portions much more than its “head” portions. Drift space is included so that this “non-neutral drift compression” can reduce the beam’s duration to roughly 70 ns, at which point space-charge forces halt the compression. The high-voltage Blumlein power supplies (from the decommissioned ATA facility at LLNL) can then apply rapid acceleration at 250 kV/m. The final Blumlein-powered cells apply a head-to-tail velocity “tilt” to the beam, which then enters into a plasma filled line wherein neutralized drift compression can take place. The beam evolution is illustrated in Fig. 11.

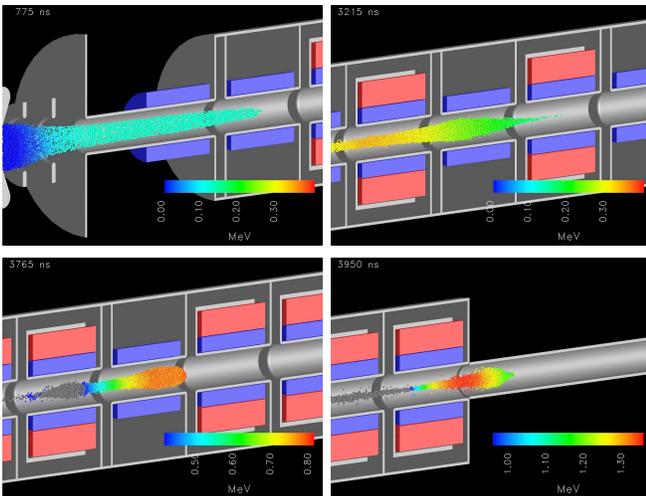


Fig. 11. Snapshots of Warp simulation of beam in NDCX-II accelerator. At upper left the beam is being injected; at upper right it is undergoing initial unneutralized bunching; at lower left bunching is nearly complete, and at lower right the beam is exiting the linac with a velocity “tilt” and entering the plasma-filled line for final neutralized drift compression. Colors denote local kinetic energy.

Iterative design was employed to develop the nominal accelerating waveforms, and especially to establish their timing and

the required tolerance for “jitter” in the firing of the voltage pulsers for acceleration and compression. To this end Warp was run (using the NERSC computer facility) in “ensemble” mode, wherein a large number of independent simulations ran at once, each with unique parameters that varied slightly among the cases. The process is illustrated in Fig. 12.

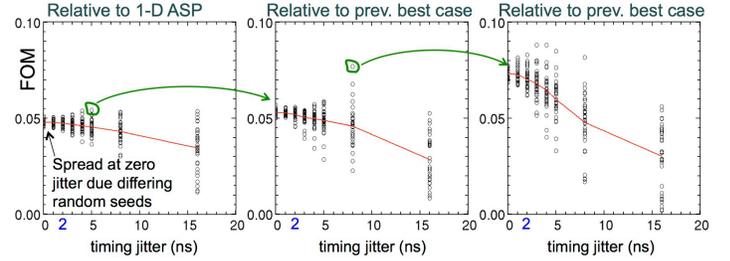


Fig. 12. Use of “ensemble” runs to iteratively improve the NDCX-II nominal operating point. Starting from a set of 256 runs shown in the left-most panel, the run with the highest figure-of-merit (labeled FOM; a quantity roughly proportional to the pressure induced in a nominal target) was selected as the baseline for the second set of runs, and the process repeated. Quasi-Newton optimization methods have been ineffective due to discrete-particle-induced fluctuations.

The University of Maryland (in particular the University of Maryland Electron Ring – UMER – group) has made extensive use of Warp for both research and teaching. For example, Warp simulations of multipactoring predicted the existence of new “ping-pong” modes which subsequently were observed experimentally [51]. As another example, virtual cathode oscillations in UMER gun, predicted by Warp simulations, were measured near the predicted frequency [52]. The many simulations of transverse and longitudinal collective beam dynamics in UMER’s various operating modes have yielded much insight [53], [54].

Beyond the above applications, Warp has been used to simulate a wide variety of devices and physical processes, among them: the temperature evolution during the acceleration of intense beam pulses [55]; plasma traps for the production of anti-Hydrogen [56], [57]; Paul traps for experimental modeling of accelerator beams [58], [59]; a non-conventional Penning-Malmberg micro-trap [60]; electron-cyclotron resonance (ECR) ion sources [61]; coherent synchrotron radiation (CSR) [62]; Free-Electron Lasers [63]; and the capture and control of laser-accelerated proton beams [64].

VIII. DISCUSSION

The name “Warp” is not an acronym; it originally was motivated by our desire for a relatively narrowly scoped but fast PIC code tuned specifically to the needs of the Heavy Ion Fusion research program. (Fans of the “Star Trek” movies and television series will recognize the term as referring to a starship’s most rapid mode of operation). Subsequently, the need to accurately and efficiently treat bent beam lines led to the invention of a new method; it was natural to call the resulting coordinate system “warped coordinates.” The original notion was that of a wooden chair, with its back made up of laminated strips glued together and then “warped” in the presence of heat and moisture. To this day the code

developers wonder whether the code's name subliminally led to the development of the method. Such serendipity was no stranger to Ned Birdsall, and it may be that in this case it visited us as well.

We are gratified that, despite our intention to develop a simple code with a programmatic focus, the growth of that program and of the code, coupled with an architecture that has proven robust, has led to the beneficial use of Warp for a broad range of applications. Indeed, the variety of the code's uses has far exceeded our expectations.

With the recent adoption of an open-source license for Warp, we are hopeful that the code and its associated framework will find additional uses and will attract an even broader community of developers and users. Since adding functionality (such as diagnostics) via Python scripts offers that language's rapid-prototyping benefits, the barrier to contributing is low. Development of major new functionality will, of course, continue to require an understanding of the code's internal structure. The Warp web site [8] contains documentation, the code source, and examples.

This summary has necessarily been abbreviated. It has omitted discussion of significant code features and methods, and of important applications. The interested reader may consult the references for further information.

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Fig. 13. Ned Birdsall and Alex Friedman, November 2005.

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The major emphasis of Dr. Haber's recent work has been continuing demonstration of the capability of numerical simulation to reproduce, in detail, experimental measurements in particle beam systems, and the development of the appropriate numerical tools for this purpose. He has authored in excess of 200 papers and reports.



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effects, computation, and multipactor, where he made groundbreaking contributions to its theoretical modeling.

He has published over 170 scientific papers, delivered 45 invited talks, and has over 1000 citations to his work. Dr. Kishek is a scientific consultant for multiple companies and has chaired several workshops, most recently the 4th Workshop on the Microbunching Instability in FELs, held at UMD in April 2012. He has advised or co-advised 11 graduate students and guided the research of dozens more graduate, undergraduate, and high school students, and regularly teaches both at UMD and at the US Particle Accelerator School.