Petascale self-consistent electromagnetic computations using scalable and accurate algorithms for complex structures

John R. Cary,1,2 D. Abell,1 J. Amundson,3 D. L. Bruhwiler,1 R. Busby,1 J. A. Carlsson,1 D. A. Dimitrov,1 E. Kashdan,2 P. Messmer,1 C. Nieter,1 D. N. Smithe,1 P. Spentzouris,3 P. Stoltz,1 R. M. Trines,4 H. Wang,5 G. R. Werner2

1 Tech-X Corporation, Boulder, CO 80303, USA
2 University of Colorado, Boulder, CO 80309, USA
3 Fermi National Accelerator Laboratory, Batavia, IL 60510, USA
4 Rutherford Appleton Laboratory, Chilton, DIDCOT, OX11 0QX, UK
5 Thomas Jefferson National Accelerator Facility, Newport News, VA 23606, USA

Email: cary@txcorp.com

Abstract. As the size and cost of particle accelerators escalate, high-performance computing plays an increasingly important role; optimization through accurate, detailed computer-modeling increases performance and reduces costs. But consequently, computer simulations face enormous challenges. Early approximation methods, such as expansions in distance from the design orbit, were unable to supply detailed accurate results, such as in the computation of wake fields in complex cavities. Since the advent of message-passing supercomputers with thousands of processors, earlier approximations are no longer necessary, and it is now possible to compute wake fields, the effects of dampers, and self-consistent dynamics in cavities accurately. In this environment, the focus has shifted towards the development and implementation of algorithms that scale to large numbers of processors. So-called charge-conserving algorithms evolve the electromagnetic fields without the need for any global solves (which are difficult to scale up to many processors). Using cut-cell (or embedded) boundaries, these algorithms can simulate the fields in complex accelerator cavities with curved walls. New implicit algorithms, which are stable for any time-step, conserve charge as well, allowing faster simulation of structures with details small compared to the characteristic wavelength. These algorithmic and computational advances have been implemented in the VORPAL[1] Framework, a flexible, object-oriented, massively parallel computational application that allows run-time assembly of algorithms and objects, thus composing an application on the fly.

1. Introduction

Charged particle accelerators are critical to the advance of science (high-energy physics, light sources, electron microscopes), manufacturing (semiconductor processing), the health industry (cancer therapy), and many other areas. Such accelerators are particularly important to the Department of Energy, which maintains many accelerator facilities for advancing the knowledge frontier. Improvements to particle accelerators therefore have wide impact on society and the DOE mission.
Improvements that arise from computational modeling have the advantage of low cost. With computational modeling much of the build-test-repeat cycle is eliminated, as physical prototypes are not built until many of the problems have been found through simulation and removed from the designs. This can potentially save multiple millions of dollars in the building of the next large accelerator systems. However, there is an increasing difficulty with computational modeling because particle accelerators have become increasingly complex. The original accelerators of vacuum tubes and cyclotrons had little more than a filament, a simple structure, and a power supply, and they could fit in a human hand. By contrast, the proposed ILC \[2\], a TeV electron-positron collider identified to be the highest priority concept for the next high-energy physics facility \[3\], will consist of two 20 km long superconducting linear accelerators, cooling rings, complex RF galleries, etc. Modeling difficulty is further increasing because of the large-scale separations of these problems. For example, the beam for ILC at the final focus will be tens of nanometers high, while the system is, as noted, 20 km long, for a scale ratio of \(2 \times 10^{12}\)!

These challenges can be met by moving to petascale computing, but this will require the development of accurate and fast algorithms that scale well to thousands of processors; to be efficient, such algorithms must minimize global communication. Electromagnetic algorithms must accurately simulate the intricate boundaries of accelerator structures, especially with the recent move to superconducting RF (SRF) cavities, which have curved surfaces. These fast, detailed, and accurate electromagnetic algorithms must treat charged particles self-consistently, with particles reacting to the fields created by the particles. Because these particles are relativistic, their dynamics can depend critically on the difference between the velocity of the particles (close to the speed of light) and the phase velocity of the electromagnetic waves; therefore, the electromagnetic algorithms need to simulate the phase velocity accurately. Furthermore, one would like to be able to model intra-beam effects, which requires resolving lengths smaller than the beam size while simulation the macroscopic electromagnetics of the much larger cavity.

The results presented here indicate that the combination of these requirements can be met by particle-in-cell (PIC) methods with fields defined on logically cartesian meshes and field-updates based on cut-cell (aka embedded boundary) methods. Logically cartesian meshes greatly simplify the incorporation of particles, since the locations and the weighting of the particles relative to the mesh is straightforward. This contrasts with finite-element methods, where complex connections must be followed to determine the elements with which a particle interacts. To this end, we have begun by implementing the Dey-Mittra \[4\] cut-cell method within VORPAL.

### 2. Self-consistent electromagnetic algorithms

The workhorse algorithm of the simulations discussed here is the electromagnetic PIC algorithm \[5\], in which the electromagnetic field lives on a grid, while particles move through space. The forces on the particles are computed by interpolation of the fields from the grid nodes to the particle positions. The particles are then accelerated and moved. The motion of the particles implies a flux of charge crossing the faces of the cells. This gives the grid-based current density, which acts as a source for the electromagnetic fields. The full system is
advanced with second order accuracy in space and time.

In more detail, the EM fields live on the so-called Yee [6] mesh. With this layout, each of the spatial derivatives in the curls of Maxwell’s equations is computed through first-order accuracy (second-order error) with respect to the cell size. Temporally, the leap-frog algorithm is used to obtain second order accuracy with respect to the time step.

Parallelization is achieved through domain decomposition, illustrated in Fig. 1. In this methodology, a domain is responsible for the red and lavender cells of Fig. 1, but it has copies of the data from neighboring cells in the green cells of Fig. 1. This allows a finite difference throughout the red and lavender cells in one step. However, to begin the next step, the green cells must be filled with the data from the neighboring cells again. If done at the end of the update, all computations must stop while messages are passed, and this creates a performance bottleneck.

To obtain good parallelization, one overlaps computation with communication. This is accomplished by first updating only the lavender cells, which comprise the skin. The guard cells of one processor are the skin cells of another, so after the skin update, this information can be sent. Then the interior, or body, can be computed. By the end of the body update, the messages have been sent and can be received and loaded into the guard cells. With such overlap of computation and communication, one can obtain very good speedup of computations on multi-processor machines, as shown in Fig. 2.

However, a requirement for such type of parallelization is that the updates on the grids remain local. This is true for electromagnetics even in the presence of particles, through use of the Villasenor-Buneman [7] current deposition algorithm. However, it can be problematic for certain finite-element calculations, as there can be a requirement for a global solve to remove “null-space modes” and impose the divergence equations of the Maxwell set.

For electromagnetic simulations, well-posed boundaries are found by specifying the tangential electric field at a boundary. A metallic boundary is specified by setting the tangential electric field to vanish at its surface. A simple way to do this in the present scheme is to use the boundary to either keep cells in the simulation or disregard them. The electric field is then set to zero on all cell edges that separate interior cells from exterior cells. Such works very well when the metallic surfaces are aligned with the grid, but it works poorly when one has misaligned surfaces, such as curved surfaces. Of course, such surfaces are critical in accelerator modeling, as modern, superconducting accelerating cavities, such as those to be used in the ILC, are curved to maximize acceleration gradient given the limitations of breakdown and quench. Figure 3 shows the resulting stair-step boundary for the Tesla cavities.

The problem with such boundary approximations is that they reduce accuracy dramatically. The original algorithm was second order in space. Stair-stepping leads to the elimination of cells, each giving a relative volume error that is $O(\Delta x^3/L^3)$, where $L$ is a typical scale length. The number of such errors is proportional to the number $O(N_{1d})$ of cells on the surface, where $N_{1d} = O(L/\Delta x)$ is the number of cells in one direction. Thus, the overall error is $O(\Delta x/L)$, a reduction of accuracy by one order compared with that of the algorithm used to update the bulk.

Such error would preclude high-accuracy computations of accelerator cavities. Figure 4 shows, as the red points, the results of using VORPAL with stair-step boundaries to compute cavity mode frequencies. This figure indicates that for accuracy of one part in $10^4$, one must have of the order of 5000 cells per direction, or $10^{11}$ cells in the volume. Another order of magnitude is needed for more complex structures such as shown in Fig. 4. Hence, algorithmic improvement is needed if one is to proceed with the FDTD algorithm on a regular mesh.

![Fig. 4. Comparison of cut-cell(blue), stair-step (red) error, and Richardson extrapolation (green).](image)
3. Improved boundary conditions

An important algorithmic advance was the development of the Dey-Mittra [4] cut-cell boundaries. One can derive standard FDTD electromagnetics through the integral formulation of Maxwell’s equations, with the integrations being around cells, and those integrals giving the changes of the fluxes. This provides a picture for how to implement the update for a cell that is cut by a metallic boundary. The integral is simply the sums of the oriented electric fields on edges multiplied by the lengths of those edges. That gives the change of the magnetic flux in the face. Dividing by the area gives the change of the magnetic field for that face. That magnetic field is then used in the usual discretization of Ampere’s law to give the update of the electric fields.

Use of Dey-Mittra cut cells gives much improved accuracy, as shown by the blue points in Fig. 4, which compares the error of Dey-Mittra and stair-step as one increases the number of cells. This figure shows that for Dey-Mittra, the error falls off as $1/N^2$, as it should, up to a point, at which it then falls off more like $1/N$. This occurs because with Dey-Mittra, the very tiny faces lead to large coefficients in the update matrix for the magnetic field, and this causes the maximum stable time step to be reduced relative to that of the infinite grid. To avoid the tiny time steps that would be required to integrate a system with tiny faces, we discard the faces depending on a computed “size” that ensures stability according to Gershgoren’s theorem. This algorithm works very well. However, it implies that at some point the first-order error associated with discarding small faces can dominate the second-order error otherwise.

Recently we have shown that one can obtain very accurate results using Richardson extrapolation, which assumes that the error is second-order, and then fits two or more results at modest resolution ultimately to eliminate the error to one higher order. This is indicated by the green line shown in Fig. 4. With Richardson extrapolation we have been able to reduce the error by another order of magnitude, so that with two simulations having of order 60 cells across, one can obtain the frequency to one part in $10^5$.

We note that recently there has been an improved algorithm published by Zagorodnov, et al [8]. This algorithm uses area borrowing methods to eliminate the reduction in the maximum stable time step. We will be implementing this algorithm within VORPAL in the coming year.

With these implementations we are immediately able to simulate particles and fields self-consistently, at least when they are in the center of the cavities. A visualization of one such simulation is shown in Fig. 5. These simulations are stable and automatically give the wake fields and particle-particle interactions occurring in the acceleration cavities. In addition, we are able to simulate such self-consistent dynamics in complex cavities, such as the crab cavity shown in Fig. 6. We can now define such cavities through some flavors of CAD descriptions, and we can also define such shapes through imported python scripts, which allow great flexibility, generality, and are easily used in parameter scans and within exterior loops for solving for cavities with improved properties.

To complete this stage of modeling, we are now implementing conformal particle boundaries. This can be an extensive task, depending on requirements. Absorbers are relatively straightforward, but we are also working towards emitters as are needed for multipactoring computations.

4. Moving towards the Petascale

It has long been known that EM solves on regular meshes with appropriate charge deposition algorithms scale very well and so would be able to take advantage of petascale
computing. However, use of such algorithms for complex structures has been problematic until recently, due to their lack of accurate boundary representations. This situation has now changed with the development of the new embedded boundary (or cut-cell) algorithms discussed here. We have shown that these new algorithms can give very accurate answers for a modest number of cells while retaining the good parallelization properties of FDTD electromagnetic solves. In fact, the algorithms are so accurate that computing the propagation of moderately sized beams through cavities requires much less computational power. These savings in computational cost then allow an entire new area of simulation to be attacked through petascale computing. One can now imagine, with appropriate algorithmic improvements, resolving the tiny beams expected in the ILC while computing multi-cavity and multi-bunch wakefield interactions, ultimately in an end-to-end simulation.

5. Conclusions
High-accuracy computations of charged particles interacting with cavities are now possible due to the emergence of cut-cell algorithms that provide accurate boundary representations for computations on regular meshes. Because these algorithms have excellent parallelization properties, they are the lead candidates for moving towards the petascale in computational accelerator science. However, there remains significant work in implementing advanced solvers and particle boundary conditions.

6. Acknowledgments
This work is primarily supported by the U.S. Department of Energy (DOE) Office of Science, Office of High Energy Physics through the SciDAC project “Advanced Computing for 21st Century Accelerator Science and Technology” under various grant and contract No.’s, including DE-FC02-01ER41178. Additional support was provided by the same office, under multiple grant No.’s, including DE-FG03-95ER40926. This work used resources of the National Energy Research Scientific Computing Center, which is supported by the DOE Office of Science under Contract No. DE-AC02-05CH11231. Partial support was also provided by Tech-X Corp.

References
[1] Nieter C and Cary J R 2004 J. Comp. Phys. 196 538. The VORPAL web site; http://www.txcorp.com/products/VORPAL
[2] The International Linear Collider (ILC); http://www.linearcollider.org/cms/
[3] "Facilities for the Future of Science: A Twenty-Year Outlook" Department of Energy, Office of Science Report (Dec. 2003). Available at http://www.er.doe.gov/sub/Facilities_for_future/20-Year-Outlook-screen.pdf
[4] Dey S and Mittra R 1997, IEEE Microwave and Guided Wave Lett. 7 273.
[5] Birdsall C K and Langdon A B 1985 Plasma Physics via Computer Simulation (McGraw-Hill, New York); Hockney R W and Eastwood J W 1981 Computer Simulation Using Particles (McGraw-Hill, New York);
[6] Yee K S 1966 IEEE Trans. Ant. Prop. 14 302
[7] Villasenor J and Buneman O 1992 Comp. Phys. Comm. 69 306
[8] Zagorodnov I A, Schuhmann R, and Weiland T 2003 J. Num. Modeling 16 127.