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QUICKSILVER — A General Tool for Electromagnetic PIC Simulation

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Abstract. The dramatic increase in computational capability that has occurred over the last ten years has allowed fully electromagnetic simulations of large, complex, three-dimensional systems to move progressively from impractical, to expensive, and recently, to routine and widespread. This is particularly true for systems that require the motion of free charge to be self-consistently treated. The QUICKSILVER electromagnetic Particle-In-Cell (EM-PIC) code has been developed at Sandia National Laboratories to provide a general tool to simulate a wide variety of such systems. This tool has found widespread use for many diverse applications, including high-current electron and ion diodes, magnetically insulated power transmission systems, high-power microwave oscillators, high-frequency digital and analog integrated circuit packages, microwave integrated circuit components, antenna systems, radar cross-section applications, and electromagnetic interaction with biological material. This paper will give a brief overview of QUICKSILVER and provide some thoughts on its future development.

OVERVIEW OF QUICKSILVER

Charged-particle simulations in three dimensions are performed routinely in the Pulsed Power Sciences Center at Sandia with the QUICKSILVER (1) suite of codes. QUICKSILVER is a three-dimensional, relativistic, finite-difference, electromagnetic, particle-in-cell (PIC) code developed at Sandia. It was originally targeted for vector supercomputers, such as the Cray Y-MP, which are characterized by large, shared memory and multiple processors. It now runs on a wide variety of platforms, including most UNIX workstations, and is presently being ported to the Intel Paragon, a massively-parallel distributed memory supercomputer.

QUICKSILVER is actually a suite of codes; in addition to the main simulation code there are several support codes. The problem geometry is generated using various preprocessors and the simulation results are examined with one or more postprocessors. The original MERCURY command-driven preprocessor assists the user in defining the mesh, boundary conditions, and other input parameters. Recently, a

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set of widget-based tools have been developed to further simplify the process of mesh generation. These widget-based tools, built upon the IDL data analysis and visualization tool[1] have been incorporated in PFIDL (2), QUICKSILVER's primary simulation data postprocessor. In its role as postprocessor, PFIDL provides the capability to manipulate and examine 3D scalar and vector field data as well as 6D particle phasespace data. Additionally, PFIDL can be used to examine and manipulate time histories of various simulation quantities. AVS[2] is used for the visualization and/or animation of field and particle distributions as well as the 3D model geometry. These pre- and postprocessing tools are available on a wide variety of platforms. The potentially vast amount of simulation data is shared between the simulation code and the postprocessors via the Portable File Format (PFF) (3), a portable, compact, machine-independent binary file format developed expressly for the QUICKSILVER suite but widely used for many other applications.

QUICKSILVER's Preprocessors

Generating input data for three-dimensional simulations can be difficult, time-consuming, and error-prone. MERCURY is a command-driven preprocessor that is used in defining the finite-difference grid, the problem geometry, the boundary conditions, and other input parameters. MERCURY allows free-format input and provides menus for guiding simulation setup and on-line help. It processes all input for a QUICKSILVER simulation and checks for errors and inconsistencies. QUICKSILVER uses a nonuniform, multiple-block, rectilinear grid with staggered grids. The MERCURY grid generator provides straightforward tools to facilitate the generation of these multi-block, nonuniform grids, automatically ensuring that the grid is both continuous and smoothly varying.

A nonuniform grid defined by the relationship between the grid index i and the physical grid location x,

$$x(i) = x_0 + ai + bi^2 + ci^3 ,$$

is supported by QUICKSILVER. Different regions of the grid can have different descriptions of the relationship between i and x. Across any interface between such grid regions, $x(i)$ and $dx(i)/di$ must be continuous in order to retain accuracy in the field solution. The MERCURY grid generator ensures that this condition is met as the mesh is produced. Cartesian, cylindrical, and spherical coordinate system multiple-block grids can be generated. By multiple block, we mean that the grid is composed of logically connected blocks, each of which is a coordinate-system-conformal region of space with its own local grid.

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1) IDL is a product of Research Systems, Inc., 2995 Wilderness Place, Suite 203, Boulder, Colorado 80301.

2) AVS is a product of Advanced Visual Systems, 300 Fifth Ave., Waltham, MA 02154.

Conducting and dielectric volumes are easily generated with MERCURY by combining (sequentially adding or removing) objects selected from a provided set of simple solid-object primitives. MERCURY then fits the resulting compound volume description to the simulation's underlying finite-difference grid. MERCURY also computes the memory requirements for arrays in QUICKSILVER so that only the minimum memory required for a simulation is used.

In addition to MERCURY's capabilities, widget-based tools have been added to PFIDL to ease some of the more difficult facets of simulation setup. For example, since often a description of the problem geometry is available from solid modeling or CAD tools, PFIDL currently has a tool for editing DXF[1] files and converting them to MERCURY format, and we are working on extending that capability to allow the use of ACIS[2] files. Also, one of the difficulties of constructing grids for complex system simulations is that often the locations of structure surfaces are critical to the fidelity of the simulation, and since material interfaces must coincide with grid locations it is thus difficult and time consuming to design a grid conforming to these constraints. To address this problem we have added an interactive "point-and-click" graphical tool to PFIDL that allows the user to tie grid locations to various surfaces of the model structure while providing continuous visual feedback on the size and quality of the resulting mesh.

The QUICKSILVER 3D Physics Simulation Code

QUICKSILVER, the member of the suite for performing 3D physics simulations, can be divided into two distinct parts, the field solver and the particle handler. In the following sections, the features of each will be described.

The QUICKSILVER field solver utilizes explicit (4) and implicit (5) finite-difference, leap-frog algorithms. Multiple lossy, non-dispersive dielectrics are allowed for regions without particles. Available boundary conditions include conductors, inlet and outlet boundaries, mirror symmetry, and periodic symmetry. Simulations can be performed in Cartesian, cylindrical or spherical coordinate systems. Currently, inlet wave boundaries can be driven either with multiple, independent TEM modes or a 1D, multi-line Telegraphers' model. In both cases, outgoing waves are treated with a 1st-order Mur (6) radiation-absorbing boundary condition. The code also supports a variety of outlet boundary conditions, including 1st-order Mur, 2nd-order dispersive (7), and the Perfectly Matched Layer (PML) (8). QUICKSILVER also has models for embedded current source excitation and surface impedance.

Recently, the capabilities of the QUICKSILVER's field solver have been extended to use unstructured grid methods. Although unstructured grids provide consider-

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1) DXF is a registered trademark of Autodesk, Inc., 111 McInnis Parkway, San Rafael, California 94903.

2) ACIS is a registered trademark of Spatial Technology, Inc., 2425 55th St., Bldg. A, Boulder, Colorado 80301.

able modeling flexibility for complex geometries, they can require an extremely large number of cells; in addition, their cost of computation (and memory) per cell is significantly higher than that of QUICKSILVER's structured-grid finite-difference algorithm. The finite-volume hybrid-grid (FVHG) field algorithm (9) enables unstructured grids to be combined with rectangular-cell structured grids, thus combining the modeling flexibility of unstructured grids with the efficiency of standard finite-difference methods. This approach was first incorporated in the VOLMAX solver (10) and, with its inclusion in QUICKSILVER's field solver, allows its modeling flexibility to be combined with QUICKSILVER's extensive boundary condition and diagnostic features. Currently, we use I-DEAS[1] to build the solid models and to subsequently generate the grid for the unstructured region of the simulation space.

The second major portion of the QUICKSILVER code is its particle handler, whose job is to advance particle positions with 3D, fully-relativistic kinematics and to subsequently allocate each particle's contribution to the current back to the finite-difference grid for use by the field solver. QUICKSILVER's particle handler allows multiple particle species with particle creation via preloading, beam injection and space-charge-limited field emission. It supports the same boundary conditions and coordinate systems as the field solver. Currently the code uses a current/charge density allocation algorithm that locally conserves charge exactly. A pseudo-current algorithm (11) which diffuses errors in the charge to the simulation boundaries has recently been added to PML regions to allow that boundary condition to function properly with a low density particle flux at the boundary. It will also be used to ensure charge conservation on both the structured and unstructured grid regions of the hybrid QUICKSILVER/VOLMAX code when it is extended to treat particles.

Diagnostics

The QUICKSILVER code has a wide variety of diagnostics available to the user which can be divided into two basic types: snapshots and time histories. Snapshot diagnostics provide detailed spatial information about some simulation quantity at specified instants of time (or averaged over specified intervals of time). On the other hand, time histories provide, as a function of time, a simulation quantity at a fixed spatial location or integrated over some spatial region of the simulation.

QUICKSILVER can provide snapshots of both vector and scalar field quantities: electric (**E**) and magnetic (**B**) fields, current density (**J**), and charge density (ρ). Snapshots of simulation particles in 6D phasespace (x, y, z, p_x, p_y, p_z), or a subset of that phasespace, can also be obtained.

Time histories can be requested for ρ or any component of **E**, **B**, or **J** at any spatial location in the simulation. In addition, line integrals $\int E \cdot dl$ and $\int B \cdot dl$ are available, each along a complex path composed of one or more coordinate-confor-

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[1] I-DEAS is a product of Structural Dynamics Research Corporation, Milford, Ohio.

mal subpaths. Similarly, the area and volume integrals $\int \boldsymbol{E} \cdot dA$, $\int \boldsymbol{B} \cdot dA$, $\int \boldsymbol{J} \cdot dA$, $\int \boldsymbol{S} \cdot dA$, $\int \rho dV$, $\int W_E dV$, $\int W_M dV$, and $\int W dV$ can be obtained, each over one or more coordinate-conformal subareas or subvolumes, respectively. Here, $\boldsymbol{S}$ is the Poynting vector ($\boldsymbol{E} \times \boldsymbol{H}$), and W_E, W_M, and W are the electric ($\varepsilon E^2/2$), magnetic ($B^2/2\mu$), and total ($W_E + W_M$) field energy densities, respectively. Time histories are also available for several particle-related items, including count, energy, or charge of surviving, created, or killed particles, by species. Also, time-history data for the current, energy, and momentum of particles killed on specified conductor surfaces is available. Furthermore, selected subsets of such killed particles can be saved, either for postprocessing in IDL, or as input to other codes, e.g., beam transport codes. To examine simulation charge conservation, maximum and RMS values of the error in charge density ($\nabla \cdot D - \rho$) are also available as time histories.

A LOOK TO QUICKSILVER'S FUTURE

As the demands on the modeling capabilities of QUICKSILVER expand, it has become increasingly difficult, and consequently more expensive, to enhance the code to meet these new demands. A substantial portion of this difficulty is connected with the limitations inherent in current versions of FORTRAN-77, in which almost all of the QUICKSILVER suite is written. However, the modern object-oriented design software methods and their embodiment in programming languages such as C++ offer the prospect of developing an integrated capability that will be portable, extendable, reusable, and will be well suited to next-generation high performance computing platforms. It is our goal to develop an EM-PIC toolset based upon these methods that will both integrate our present capabilities as well as provide for a cost-effective route for extensions in those capabilities that will be needed to meet our simulation requirements for at least the next decade.

New physics modeling capability will be needed to provide the high degree of confidence that will be required as our ability to perform key experiments decreases and consequently our reliance upon simulation increases. This includes adding multi-scale physics (e.g., wires, slots, thin films, etc.) on hybrid mesh structures, non-linear devices (e.g., coupled solid-state components), fluid descriptions of high density plasmas, the desorption and ionization of contaminants from electrodes, secondary electron emission models, and beam transport and scattering through low density gas. These physics packages will require greatly increased computational capacity as well as a highly-modular object-based code framework.

To meet our modeling needs in the next decade, even with the expected advances in computing hardware, we will need the capability to partition a problem into coupled regions, each of which could treat a potentially different subset of available physics models, using different algorithms, on different types of meshes.

The QUICKSILVER/VOLMAX integration is only a first small step toward this capability; more generalized modeling/meshing of this sort can only be achieved using modern object-oriented design techniques.

The need for higher resolution for increasingly complex systems, coupled with more realistic physics modeling, clearly drives us to take full advantage of the new generation of massively-parallel supercomputers. QUICKSILVER is now running (fields only) on Sandia's 1800+-processor Intel Paragon; in one year it will be running in full PIC mode on that machine as well as on the Sandia/Intel Teraflop machine that is scheduled for availability in early 1997. To take full advantage of the capacity afforded by these machines, it is also clear that we will need to significantly alter the way in which we set up and mesh our simulations as well as the way in which we retrieve, store, and analyze their complex and voluminous data. We anticipate that our pre- and postprocessing tools will require significant, if not radical, new development in order to meet this challenge.

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REFERENCES

1. D. B. Seidel, M. L. Kiefer, R. S. Coats, T. D. Pointon, J. P. Quintenz, and W. A. Johnson, "The 3-D, Electromagnetic Particle-In-Cell Code, QUICKSILVER." in *The CP90 Europhysics Conference on Computational Physics*, Armin Tenner, Ed., World Scientific, Amsterdam, 1991, pp. 475–482; J. P. Quintenz, D. B. Seidel, M. L. Kiefer, T. D. Pointon, R. S. Coats, S. E. Rosenthal, T. A. Mehlhorn, M. P. Desjarlais, and N. A. Krall, *Laser and Particle Beams* **12**, 283-324 (1994).
2. L. P. Mix, R. S. Coats, and D. B. Seidel, "PFIDL: Procedures for the Analysis and Visualization of Data Arrays," presented at the 1st Biennial Tri-Laboratory Engineering Conference on Computational Modeling, Pleasanton, California, Oct. 31–Nov. 2, 1995.
3. D. B. Seidel, R. S. Coats, M. L. Kiefer, T. D. Pointon, and L. P. Mix, "PFF — A Compact, Machine-Independent File Format for Simulation Data," presented at the 9th Biennial CUBE Symposium, Santa Fe, New Mexico, Nov. 27–30, 1990.
4. K. S. Yee, *IEEE Trans. Antennas Propagat.* **14**, 2155–2163 (1966); O. Buneman, "Fast Numerical Procedures for Computer Experiments on Relativistic Plasmas," in *Relativistic Plasmas*, O. Buneman and W. Pardo, Eds., New York: Benjamin, 1968, pp. 205–219.
5. B. B. Godfrey, presented at the 9th Conference on Numerical Simulation of Plasmas, Evanston, Illinois, June 30–July 2, 1980.
6. G. Mur, *IEEE Trans. Electromagnetic Compatibility* **23**, 1191–1196 (1982).
7. Z. Bi, K. Wu, C. Wu, and J. Litva, *IEEE Trans. Microwave Theory Tech.* **40**, 774–777 (1992).
8. J.-P. Berenger, *J. Comp. Physics* **114**, 185–200 (1994).
9. D. J. Riley and C. D. Turner, *IEEE Microwave and Guided Wave Letters* **5**, 284–286 (1995).
10. D. J. Riley and C. D. Turner, "VOLMAX: A Solid-Model Based, Transient *Vol*umetric *Max*well Solver Using Hybrid Grids," to appear in *IEEE Antennas & Propagation Magazine*.
11. B. Marder, *J. Comp. Phys.* **68**, 48–55 (1987).