ELECTROMAGNETIC PLASMA SIMULATION IN REALISTIC GEOMETRIES

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INTRODUCTION

Particle-in-Cell (PIC) calculations have become an indispensable tool to model the nonlinear collective behavior of charged particle species in electromagnetic fields. Traditional finite difference codes, such as CONDOR[1](2-D) and ARGUS[2](3-D), are used extensively[3,4,5,6,7,8] to design experiments and develop new concepts. A wide variety of physical processes can be modeled simply and efficiently by these codes. However, experiments have become more complex. Geometrical shapes and length scales are becoming increasingly more difficult to model. Spatial resolution requirements for the electromagnetic calculation force large grids (50-100 thousand mesh points) and small time steps. Many hours of CRAY YMP time may be required to complete 2-D calculations - many more for 3-D calculations. In principle, the number of mesh points and particles need only to be increased until all relevant physical processes are resolved. In practice, the size of a calculation is limited by the computer budget. As a result, experimental design is being limited by the ability to calculate, not by the experimenters ingenuity or understanding of the physical processes involved.

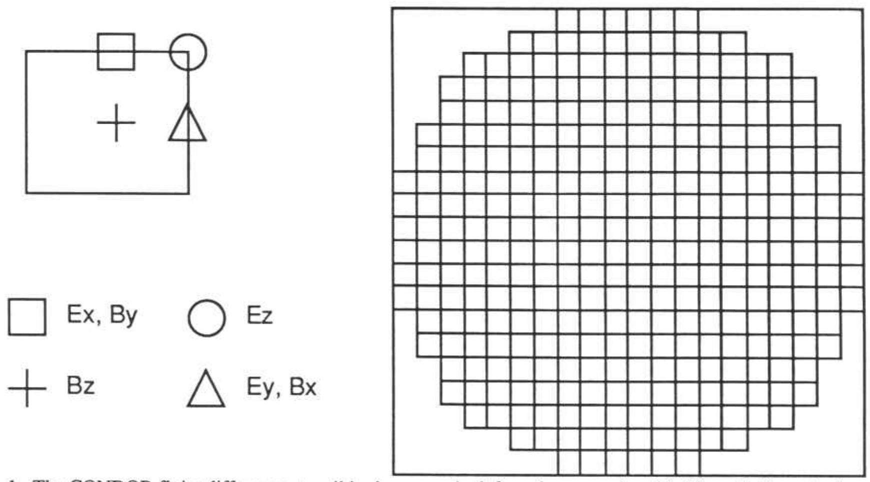

Fig. 1. The CONDOR finite difference stencil is shown on the left, active zones in a 20x20 mesh discretization of a circle are shown on the right.

Several approaches to meet these computational demands are being pursued. Traditional PIC codes continue to be the major design tools. These codes are being actively maintained, optimized, and extended to handle larger and more complex problems. Two new formulations are being explored to relax the geometrical constraints of the finite difference codes. A modified finite volume[9] test code, TALUS, uses a data structure compatible with that of standard finite difference meshes. This allows a basic conformal boundary/variable grid capability to be retrofitted to CONDOR (Mesh generation is accomplished via a point & click interface using the SMaRT[10] code running on a Macintosh). We are also pursuing an unstructured grid finite element code,[11] MadMax (mesh generation begins with a simple description of the boundaries and is "advanced" into the interior as fronts[12]). The unstructured mesh approach provides maximum flexibility in the geometrical model while also allowing local mesh refinement. Both innovative approaches to electromagnetic PIC calculations are generalizable to 3-D.

FINITE VOLUME FORMULATION

Finite volume formulations of electromagnetic PIC codes are being pursued in order to relax the geometrical meshing constraints of the traditional finite difference mesh. The field propagator we are investigating in the TALUS test code uses a distorted rectangular mesh with a staggered centering of the field components which reduces to the standard leap-frog algorithm on a uniform mesh. Thus, CONDOR (ARGUS) can be easily retrofitted to the new finite volume propagator. Physicists would then have access to conformal boundaries and distorted grids with a minimum of change in the computer codes - however problem setup and diagnostic visualizations may be substantially more difficult.

The Talus Field Solve

As shown in Fig. 2, the field propagator uses a staggered centering of the electric field projections along the four sides of each 2-D mesh cell (zone) to represent the transverse electric triad solutions to Maxwell's equations. The electric fields are updated in a three step process. First, the dEn/dt along the dual side *normal* is calculated from a simple difference of the two neighboring Bz values as in a normal leap-frog propagator. Then the total dEx/dt and dEy/dt is calculated by a finite volume integral around the six nearest zones. Finally, the value of dEt/dt (along the zone boundary) is solved using the value of the total dE/dt and the dEn/dt calculated in the previous step. The Bz values are updated from a line integral around the zone boundary using the side directed electric field values.

The exact form of the finite volume path integral determines the stability and accuracy of the resulting field propagator. The present field propagator uses a volume weighted average to center Bz to the zone vertices. A simple difference provides the dEn/dt values. Again the dEt/dt value is found from a projection of the known electric fields to the zone edge. This field propagator is stable and preserves local divergence constraints.

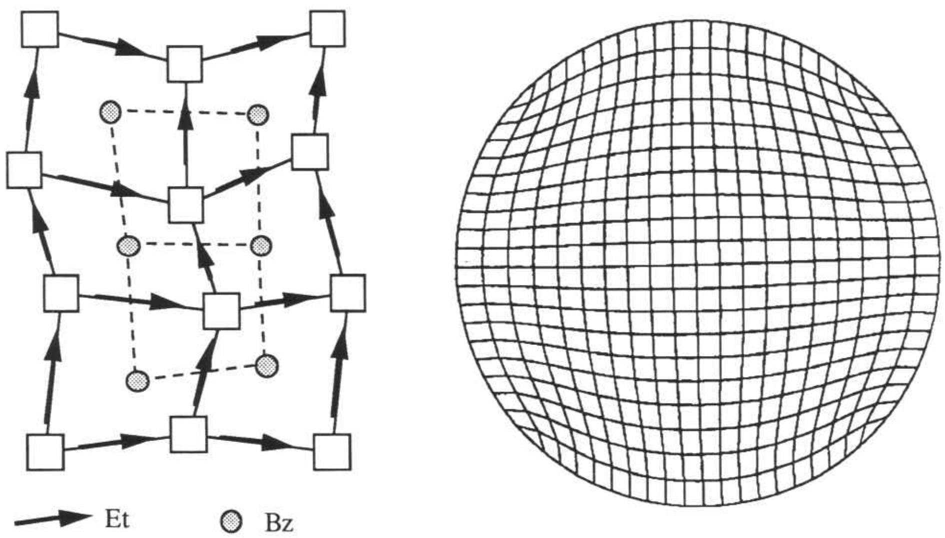

Fig. 2. The finite volume staggered grid is shown on the left, a 20x20 mesh of quadrilaterals "stretched" into a circle is shown on the right.

The Talus Particle Push

Logical space (uniform rectangular) coordinates are used in a standard bilinear area weighting scheme for both field interpolations and current depositions. For simplicity, the particle's field interpolation and current deposition is all done using quantities centered on the vertices of the primary grid. These quantities are averaged as necessary to obtain values at other locations. This process introduces some smoothing of the particle source terms and of the field actually seen by the particles. If the problem is well resolved, this may be an advantage compared to the normally noisy finite difference codes. However, in most practical problems, this introduces an inaccuracy in the TALUS result which is not present in CONDOR or ARGUS.

Tracking particles efficiently through an irregular mesh of quadrilaterals can be challenging. We have chosen to combine the problem of particle tracking and calculating the particle weights by using a bilinear mapping suggested by Westermann[13] which maps an arbitrary (but convex) quadrilateral onto a unit square. After the particle advance, the weights are calculated relative to each particle's previous zone. If the new logical weights are all between zero and one, the particle is still in the same zone and we are done. However, if the particle has crossed a zone boundary, the values of the resulting logical weight functions will suggest the direction to continue the search. The weights are then calculated for the new zone. This process is iterated until the particle is located. However, the bilinear mapping of the quadrilaterals to the unit square is only guaranteed to exist inside the quad. For highly distorted quads, the mapping may not exist. In this case a more robust "area" method is used to determine the direction to continue the search.

FINITE ELEMENT FORMULATIONS on UNSTRUCTURED GRIDS

One of the most promising approaches to performing simulations in realistic geometries makes use of unstructured grids. A single point may be connected to any number of neighbors to form a grid of triangles and quadrilaterals. Even when the grid is restricted to triangles, the arbitrary point connectivity of unstructured grids provides tremendous geometric flexibility. An example of a geometrically complex grid is shown in Fig. 3. Another feature made possible by the unstructured grid is the capability to perform local adaptive refinement during the calculation. This becomes advantageous in plasma simulations by allowing various plasma sheaths or density perturbations to be resolved and tracked without greatly increasing the number of grid points which must be calculated. We are using the MadMax finite element PIC code to explore unstructured-grid formulations.

The MadMax Field Solve

The unstructured grid field propagator uses both conforming and non-conforming elements. The conforming elements have sample points located on the vertices, while the non-conforming elements have sample points located on the element sides. The resulting staggering of field quantities, as shown in Fig. 4, is more like the standard staggered finite difference schemes. Analysis of this new formulation indicates that the local divergence constraints are preserved (within round-off).

Particle Tracking

One apparent difficulty with using particle techniques on unstructured grids is that the particles must be located on the mesh before their charge or current can be assigned to the appropriate nodes. However, for a mesh of triangles, the linear function which interpolates the charge of a particle inside an element onto a particular node is easily evaluated. The weight functions have a value of unity at the node and fall to zero on the line joining the remaining two nodes. If, a particle is outside the element, at least one of the weights will be negative. This simple property can be used to define an efficient particle search procedure. After the particle advance, the particle weights are calculated with respect to the element it was in on the last time step. If all of the weights are positive, the particle is still in the old element. If not, we guess the new particle's element to be the one adjacent to the side opposite the node whose weight is most negative. The particle weights are then calculated for the new element. This process is iterated until the particle is located. Given the normal Courant limit for the time step size, most particles will be located in under three iterations. This search technique can be made more efficient on vector machines. The addition of a small amount of sorting[14] can produce vector-to-scalar speedups of up to 14:1.

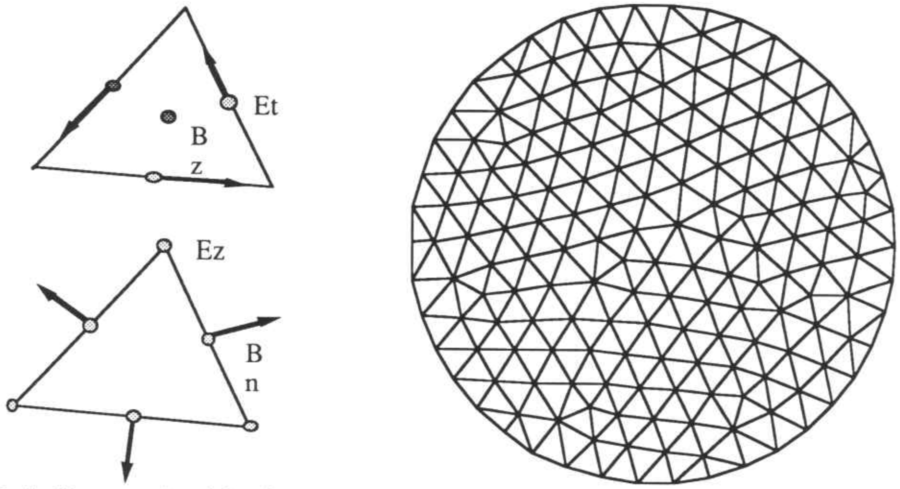

Fig. 4. The staggered mesh locations of the field quantities are shown on the left for the non-conforming finite element formulation. The TE and TM representations of one element are shown separately. Et is the electric field tangent to the element side. Bn is the component of the B field normal to the element side. A finite element triangular discretization of a circle using 314 elements is shown on the right.

SUMMARY

Design and analysis of experiments requires a rich variety of physical models. Traditional finite difference codes provide detailed physical models, but allow only simple geometries. This leads to stair-stepped boundaries and large grids. Innovative conformal boundary techniques promise to relax this restriction. The finite volume structured grid approach offers conformal boundaries and variable grids with a minimum of change in the standard finite difference codes. Unstructured grids provide the maximum geometric flexibility but represent a radical departure (e.g. data structures) from the current generation of production codes. Future development work must provide both detailed physical models and flexible geometries.

ACKNOWLEDGEMENTS

We wish to thank our many colleagues for their insightful comments and suggestions. In particular we thank Niel Madsen, Scott Ray, Rainald Löhner, Alex Friedman, Bruce Langdon, and Peter Rambo for their contributions to this research.

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