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PREPRINT

Unstructured 3-D Electromagnetic Calculations Using the Discrete Surface Integration Method

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J. Brian Grant, David Steich, Dale E. Nielsen, Jr.

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September 7, 1994

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Lawrence Livermore National Laboratory

DISCLAIMER

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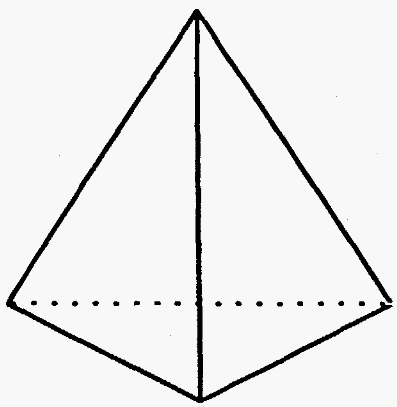
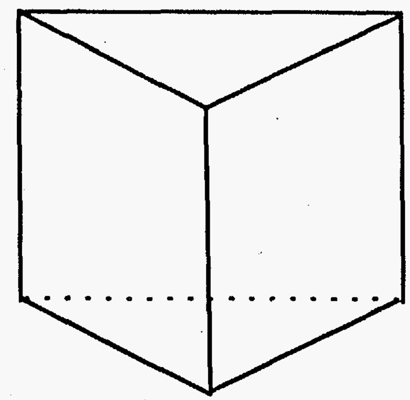
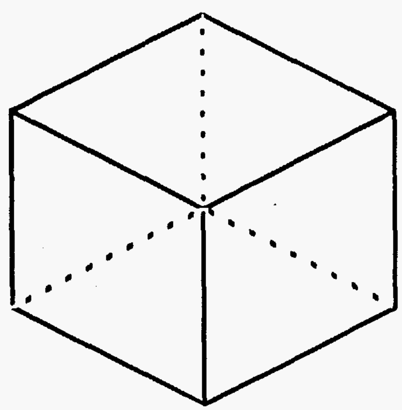
Supported Elements



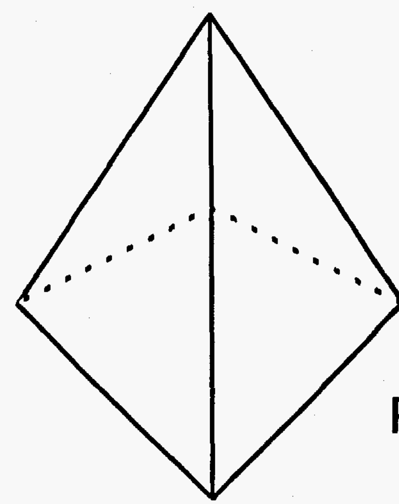
Tetrahedron



Triangular Prism

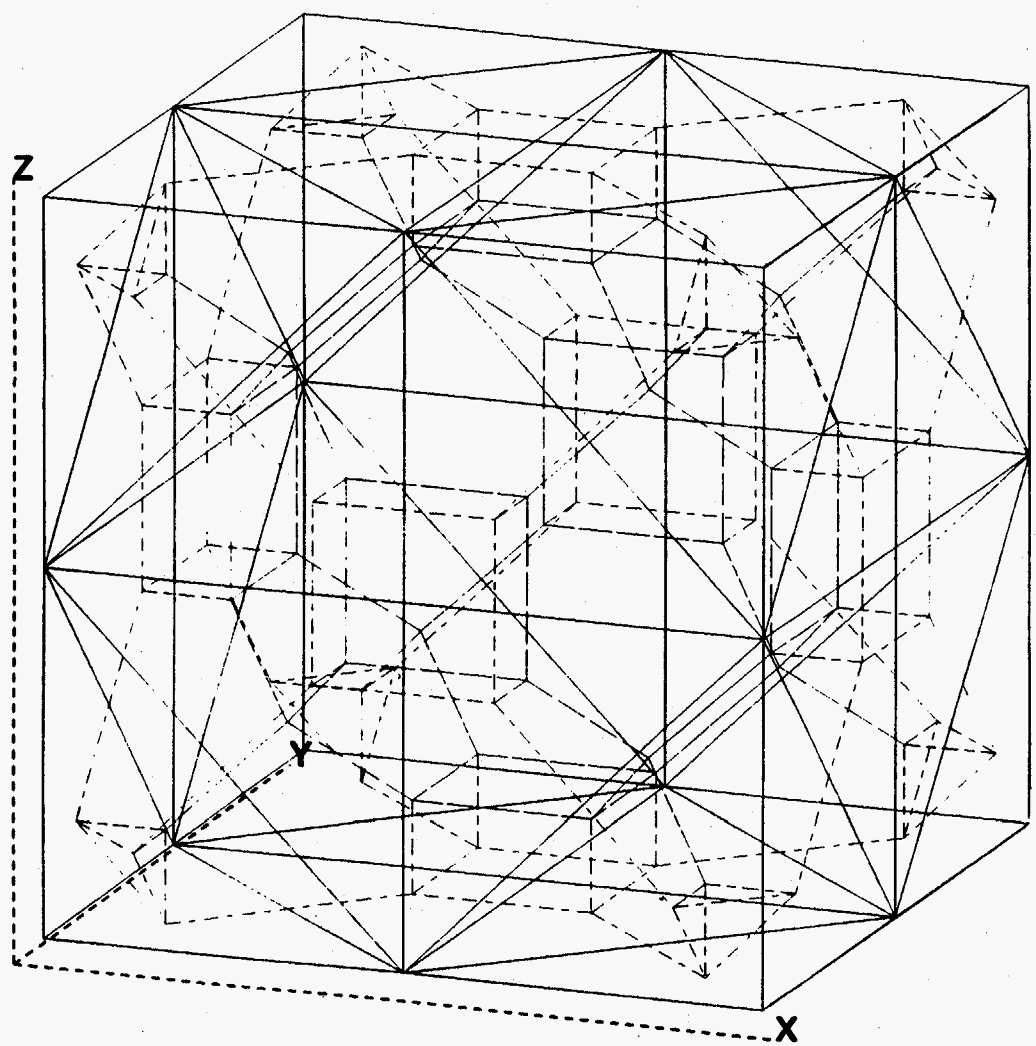


Hexahedron



Pyramid

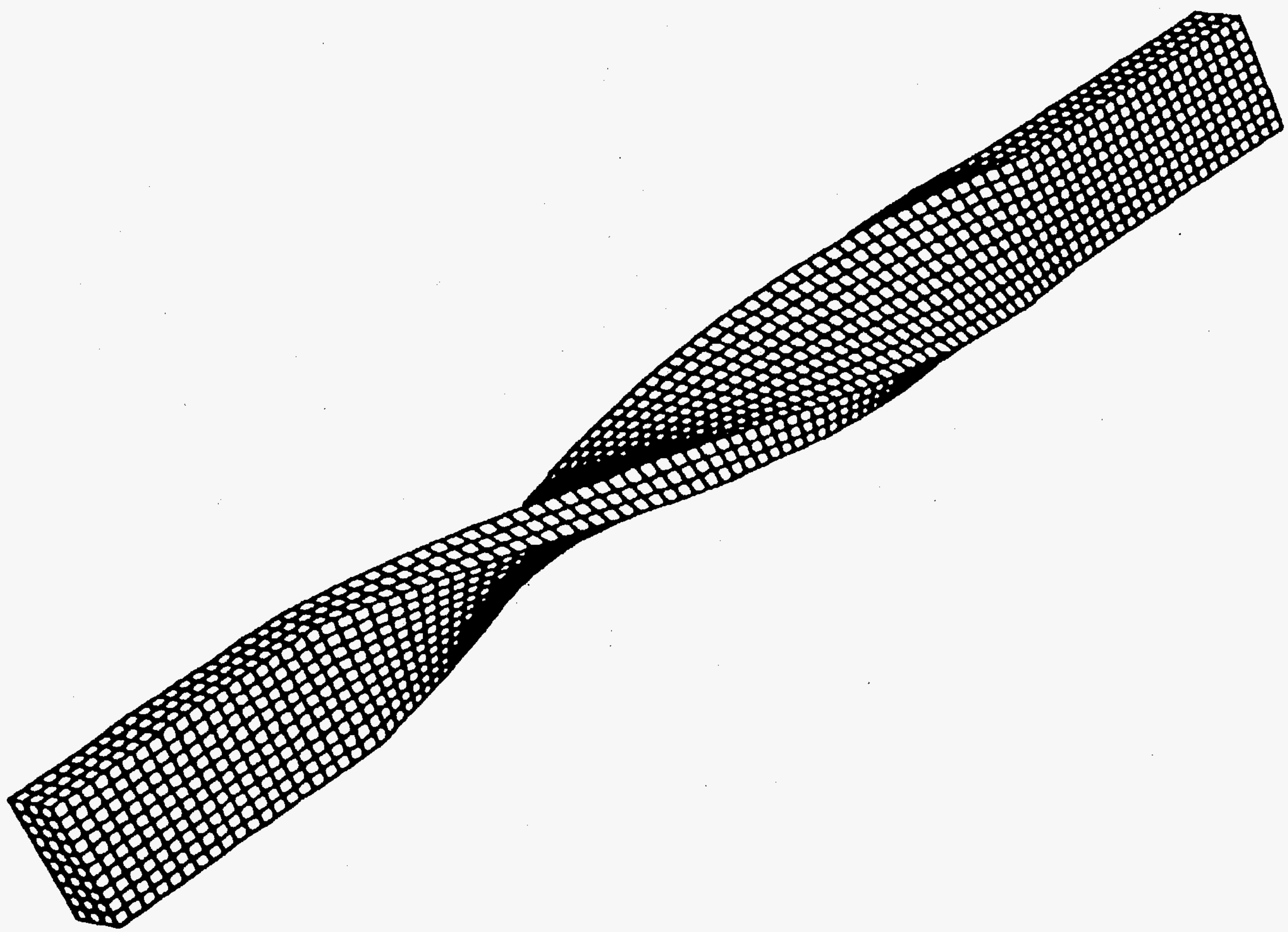
Primary and Dual Grids



View Angle (75.00, 20.00)

Distorted Regular Grid

Twisted waveguide discretized into hexahedral cells.

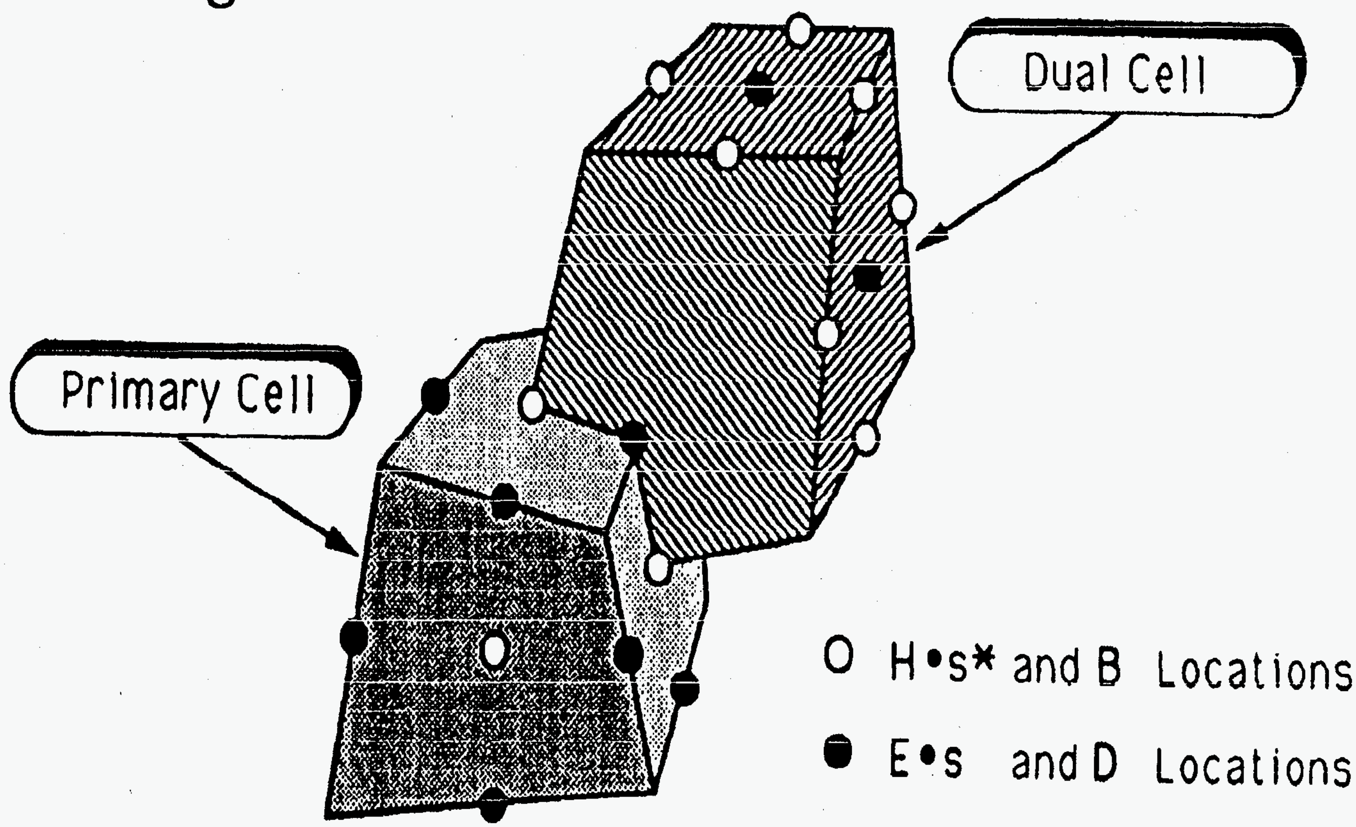


Criteria for a reliable/robust 3-D electromagnetic field solve

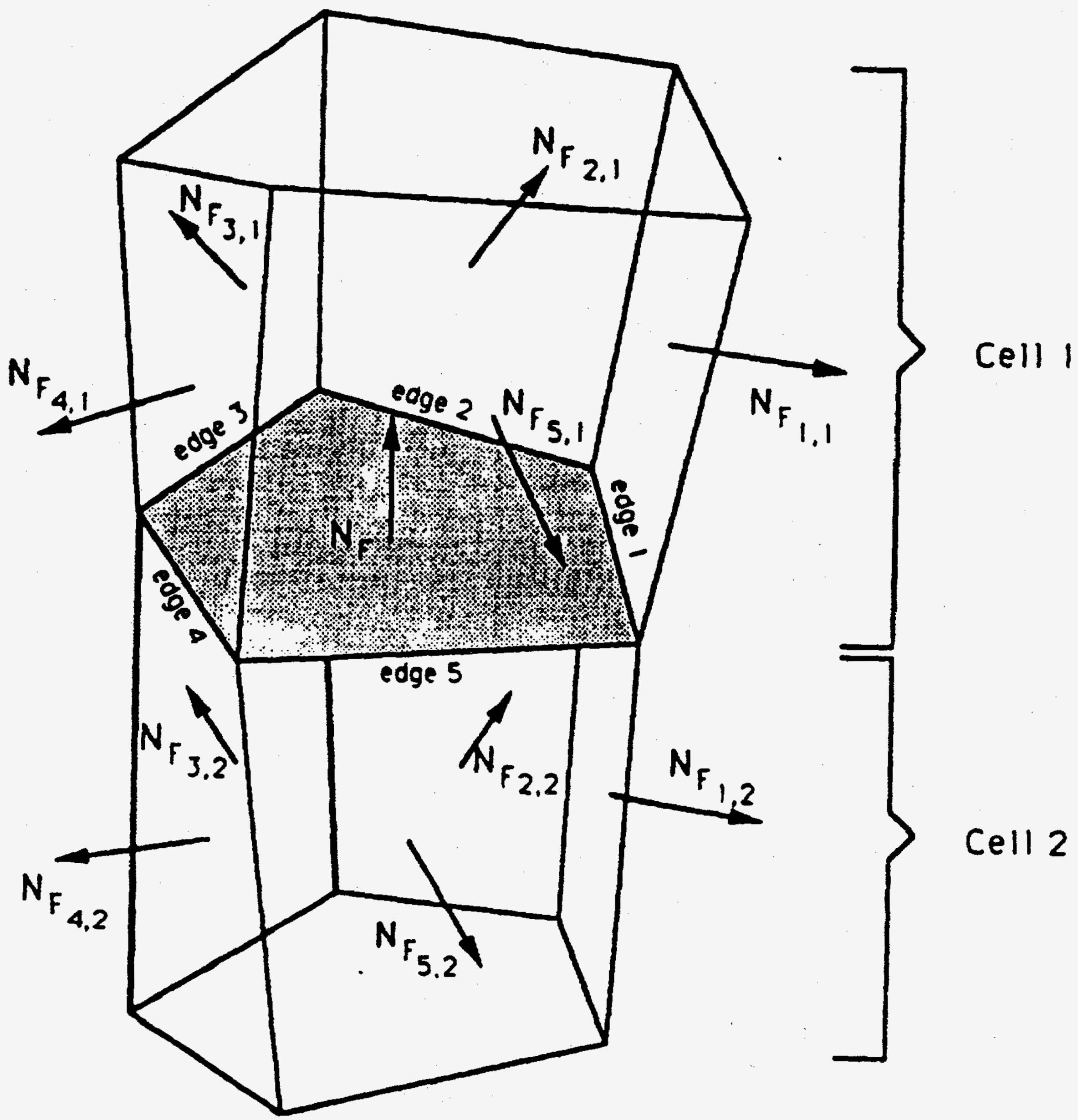
- allow use of unstructured non-orthogonal grids while retaining accuracy
- allow a variety of cell or element types
- reduce to standard FDTD method when orthogonal grids are used
- preserve charge/divergence locally (and globally)
- conditionally stable
- non-dissipative

Spatial Discretization

Electric and magnetic field locations relative to the primary and dual grid cells

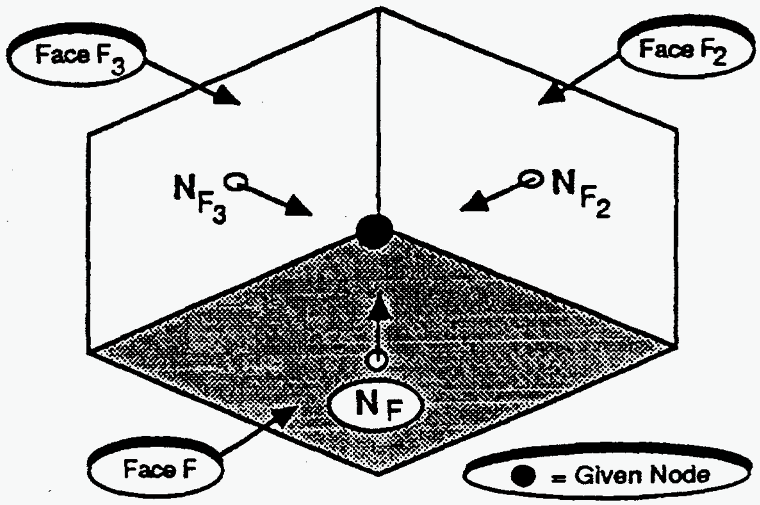


Face values for B advance



APS-11-93-7-DL&SB

Node values of B dot



$$\frac{dB_{ij}^{k}}{dt} \bullet N_F = -\oint_F E^k \bullet dl$$

$$\frac{dB_{ij}^{k}}{dt} \bullet N_{F_{i,j}} = -\oint_{F_{i,j}} E^k \bullet dl$$

$$\frac{dB_{ij}^{k}}{dt} \bullet N_{F_{m,j}} = -\oint_{F_{m,j}} E^k \bullet dl$$

APS-11-93-8-DL&SB

Face values of B dot

The node B dot values are averaged to obtain a single B dot value for the face

The fully volume weighted scheme

$$\frac{dB_F^k}{dt} = \frac{\sum_{j=1}^{N_c} \sum_{i=1}^{P} \left|\omega_{ij}\right| \frac{dB_{ij}^k}{dt}}{\sum_{j=1}^{N_c} \sum_{i=1}^{P} \left|\omega_{ij}\right|}$$

where the weight

$$\omega_{ij} = N_F \bullet \left(N_{F_{i,j}} \times N_{F_{i+1,j}}\right)$$

represents the volume of the jth coordinate system at node i of face F

works out well in our implementation.

DSI* algorithm for B

Face aligned B dot

$$\frac{\partial B^k}{\partial t} \bullet N_F \equiv \int_F \left(\frac{\partial B^k}{\partial t} \bullet n \right) dS = -\int_F \left(\nabla \times E^k \right) \bullet n \, dS$$

$$= -\oint_F E^k \bullet dl$$

Node centered B dot

$$\frac{dB^k_{ij}}{dt} \bullet N_F = -\oint_F E^k \bullet dl$$

$$\frac{dB^k_{ij}}{dt} \bullet N_{F_{i,j}} = -\oint_{F_{i,j}} E^k \bullet dl$$

$$\frac{dB^k_{ij}}{dt} \bullet N_{F_{m,j}} = -\oint_{F_{m,j}} E^k \bullet dl$$

Interpolate to face centers

$$\frac{dB^k_F}{dt} = \frac{\sum_{j=1}^{N_c} \sum_{i=1}^{P} \left| \omega_{ij} \right| \frac{dB^k_{ij}}{dt}}{\sum_{j=1}^{N_c} \sum_{i=1}^{P} \left| \omega_{ij} \right|} \qquad \omega_{ij} = N_F \bullet \left(N_{F_{i,j}} \times N_{F_{i+1,j}} \right)$$

Leapfrog advance

$$B^{k+\frac{1}{2}} = B^{k-\frac{1}{2}} + \Delta t \frac{dB^k}{dt}$$

Project to dual edge

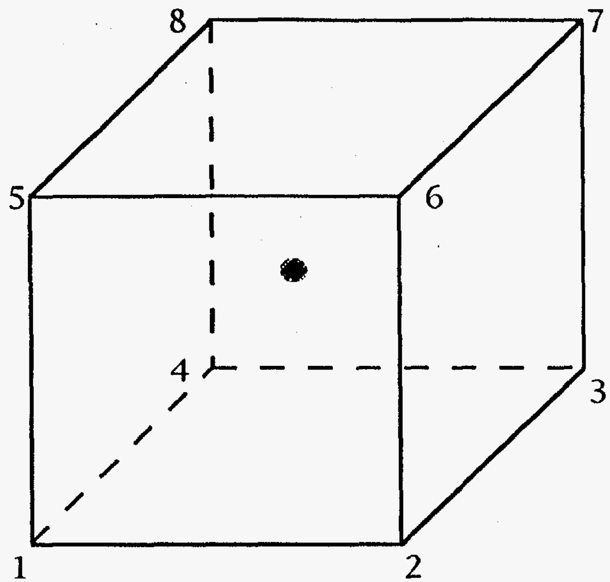
$$\left(H \bullet s^* \right)^{k+\frac{1}{2}} = \frac{B^{k+\frac{1}{2}} \bullet s^*}{\mu}$$

* Niel Madsen, February, 1992, UCRL-JC-109787

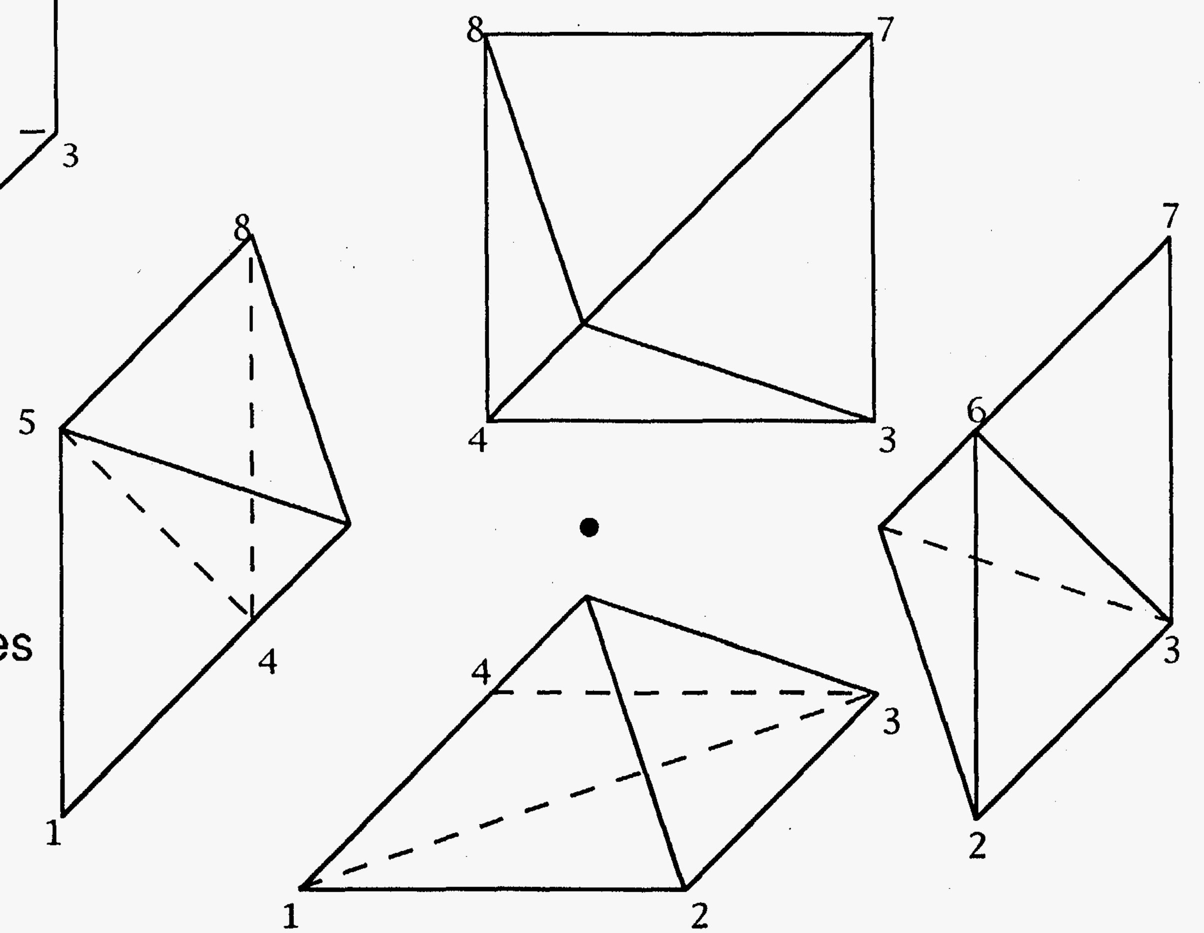
Particle Tracking

- Locate the element in which the particle resides. The first guess is the element associated with the particle's previous position.
- Calculate the interpolation weights required to deposit the particle current and to interpolate the E and B fields to the particle position.
- Mesh elements are decomposed into tetrahedral volumes defined by the particle location and the element faces.
- A negative weight indicates that the particle has left the current element and provides some clue as to where to look next.

Hexahedral Element



A simulation particle within a hexahedral mesh element.

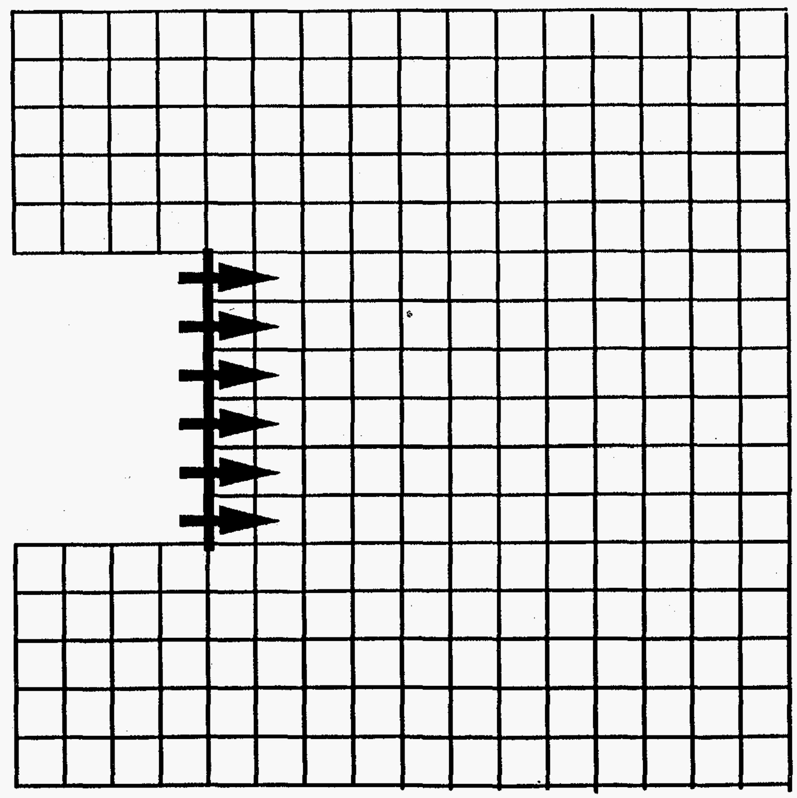


Eight of the twelve volumes required to calculate the interpolation weights.

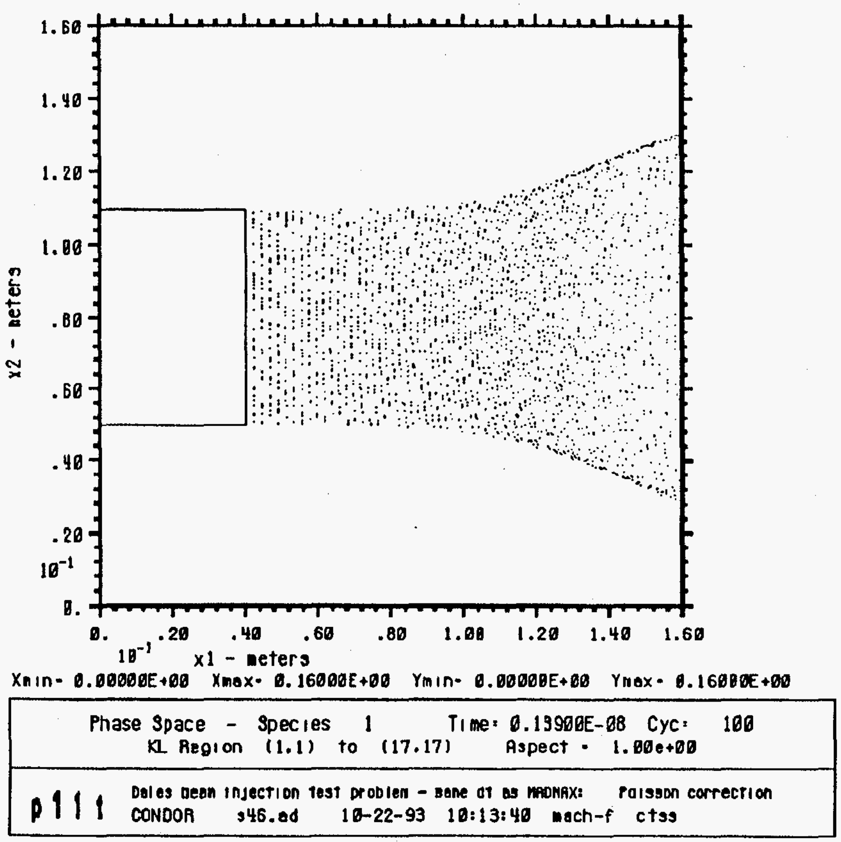
Test Problem

Test Problem: Space Charge "Almost" Limited Injection

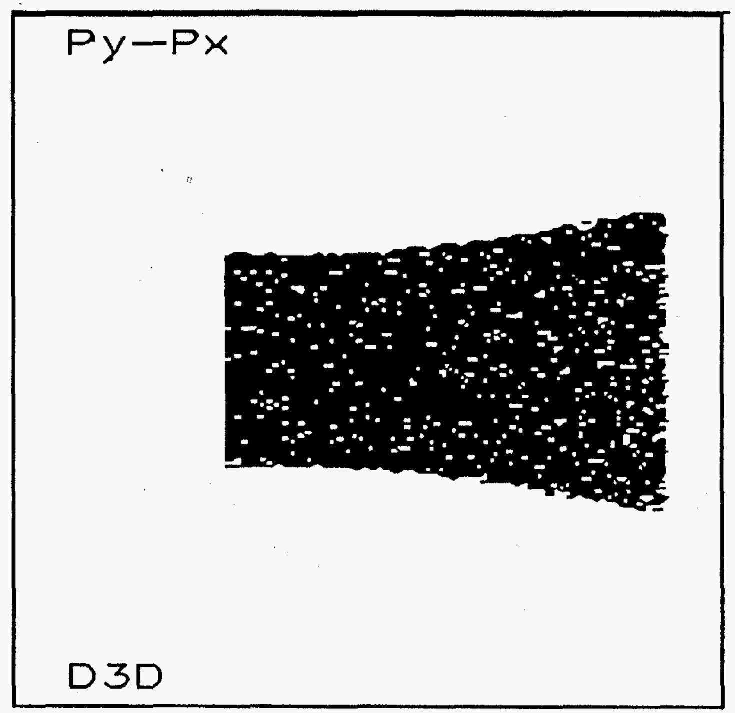
We inject 80 kA/m^2 of 100 keV electrons from all 36 zones on the face of the "pedastal" shown in the grid below. There are 16 zones in all three dimensions with $\Delta x = \Delta y = \Delta z = 0.01$ meters. A square mesh is chosen to allow comparison with the results from other well tested EM PIC codes. The "coarse" resolution accentuates the effects of interpolation.



Particle Postion

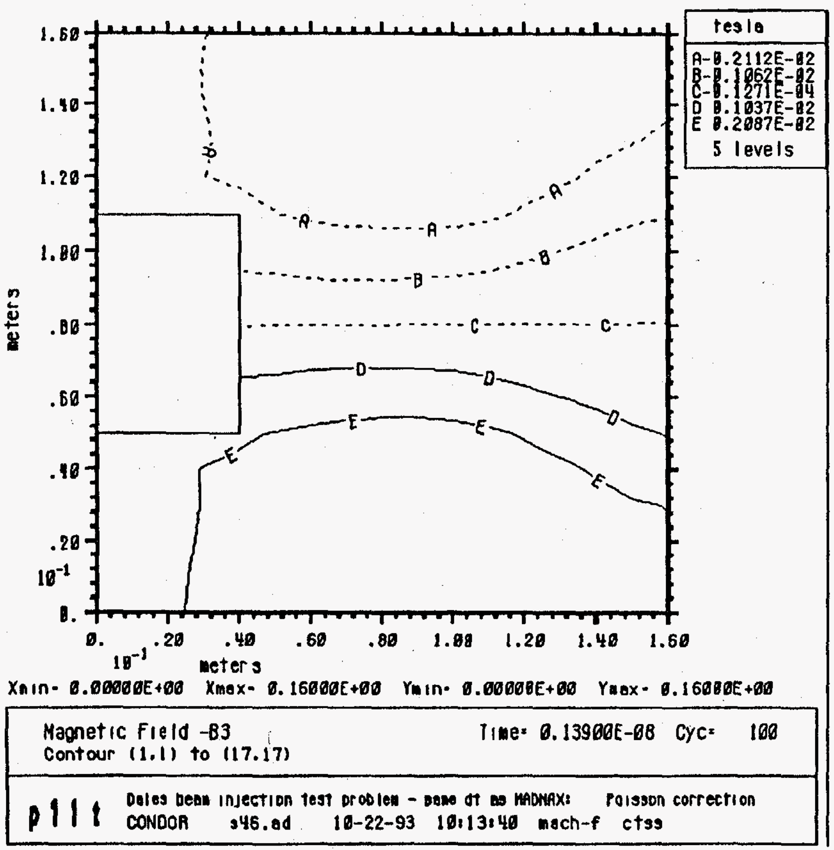


2-D Calculation

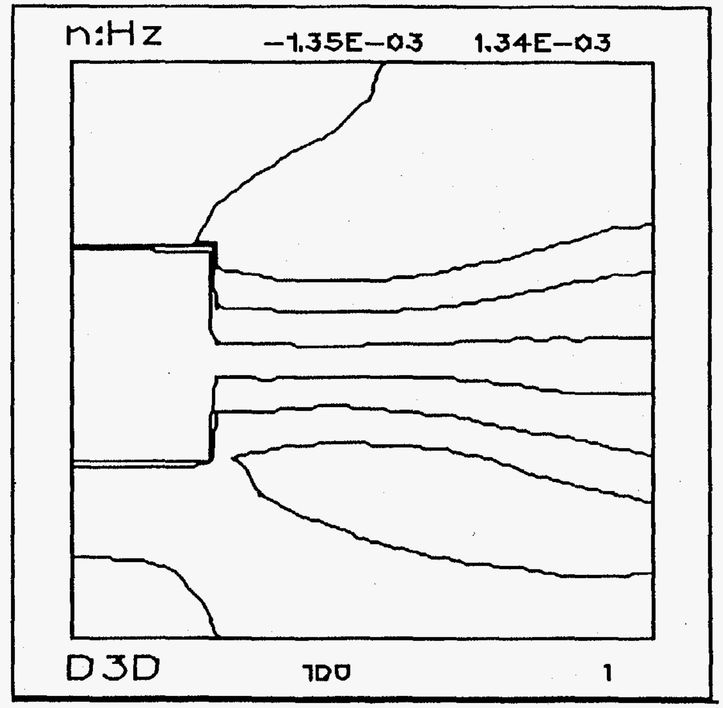


3-D Calculation

Bz Contour Plot

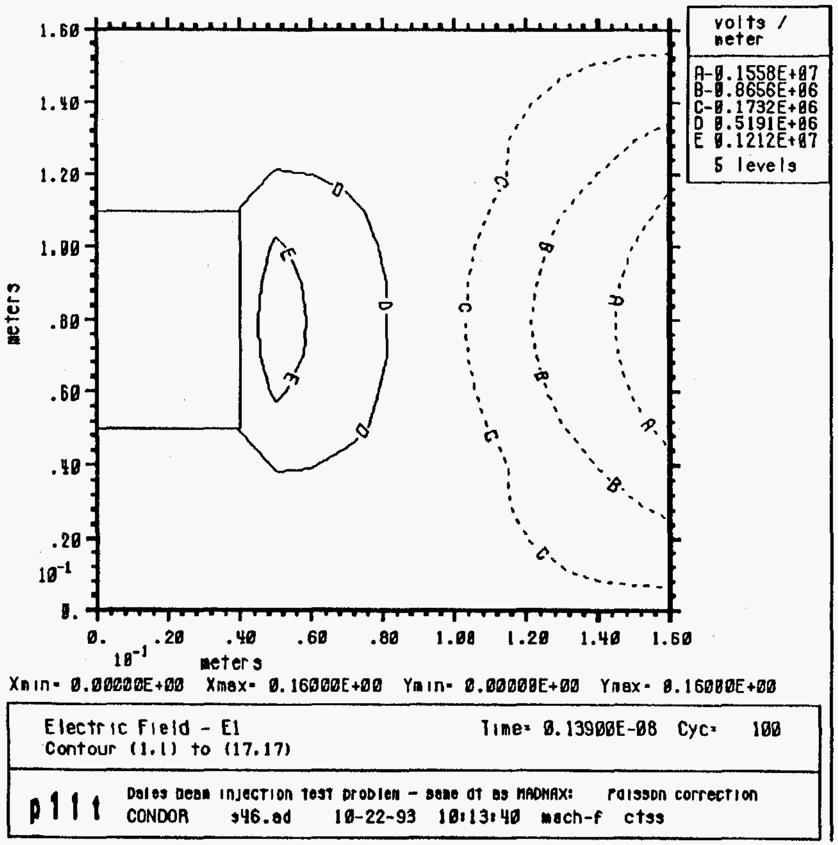


2-D Calculation

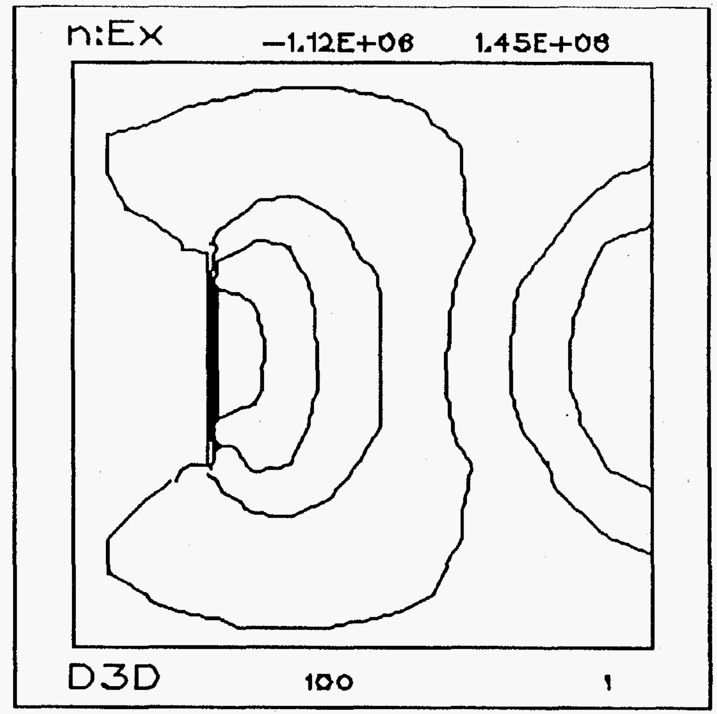


3-D Calculation

Ex Contour Plot



2-D Calculation



3-D Calculation

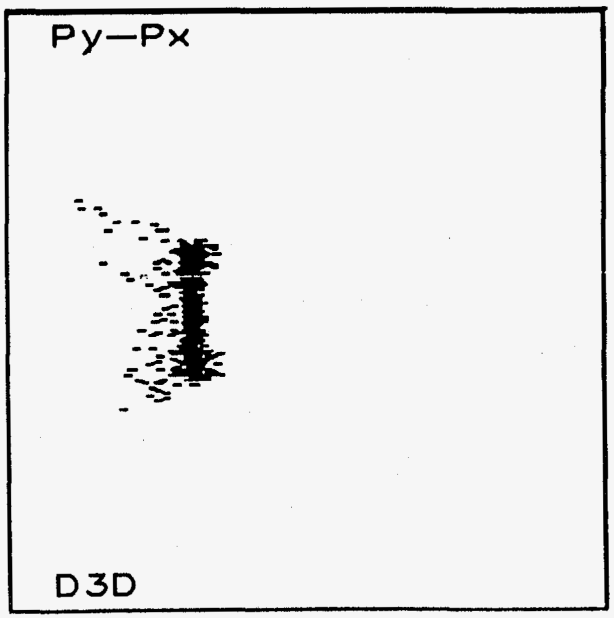
Marder current correction

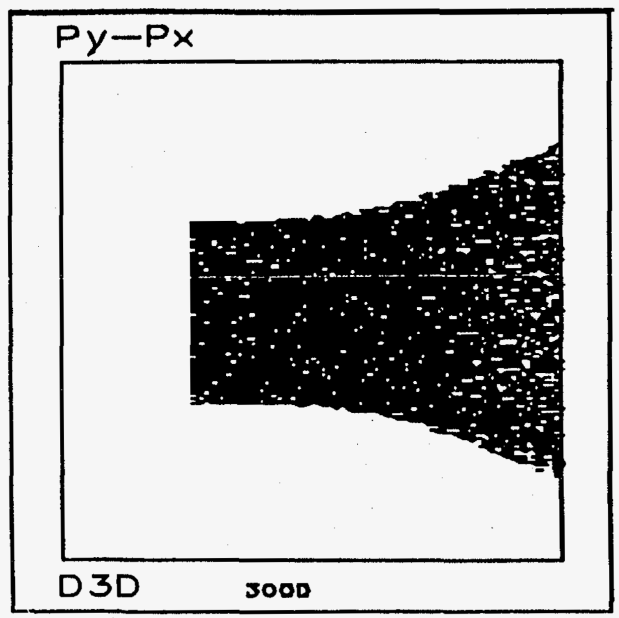
PROBLEM: Gauss' law $\nabla \bullet \mathbf{D} = \rho$ is not preserved due to numerical inaccuracies.

The Marder pseudo-current algorithm adds diffusion to Ampere's Law in order to bound the error in Gauss' Law.

Define: $F = \varepsilon_0 \nabla \bullet \mathbf{E} - \rho$ then $\varepsilon_0\, \partial \mathbf{E}/\partial t = \nabla \times \mathbf{B}/\mu_0 - \mathbf{J} + c_m \nabla F$

<u>3000 Δt without the Marder correction</u> <u>with the Marder correction</u>





Divergence Calculation

The conventional finite-difference method of calculating divergence on an orthogonal grid

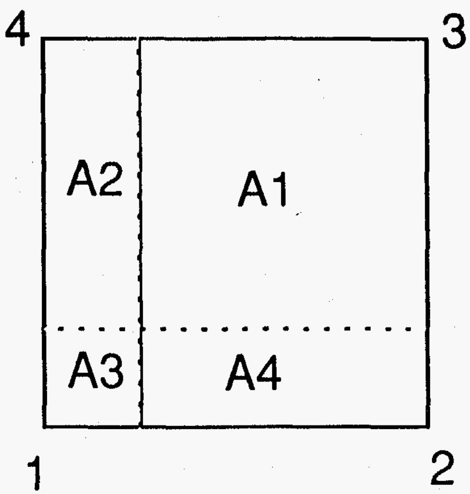
$$\nabla \bullet \mathbf{E} = (E_x^{i+1} - E_x^{i-1})/2\Delta x + \ldots$$

does not generalize to an unstructured grid. Instead we use the definition of divergence:

divergence = the outgoing flux per unit volume.

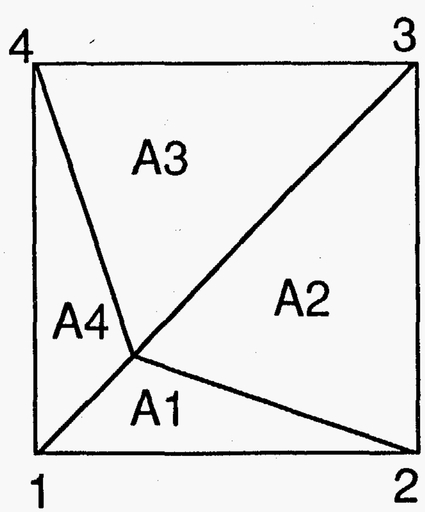
We obtain the divergence of **E** by taking the dot product of the primary edge **E** values with the associated dual-face area normals for all the primary edges connected to a primary node. This sum is then divided by the volume of the dual cell, yielding the divergence at the primary node.

Weighting Algorithms



Area weighting using conventional PIC technique on a 1 X 1 square:

W(n1) = Area 1 = 9/16
W(n2) = Area 2 = 3/16
W(n3) = Area 3 = 1/16
W(n4) = Area 4 = 3/16

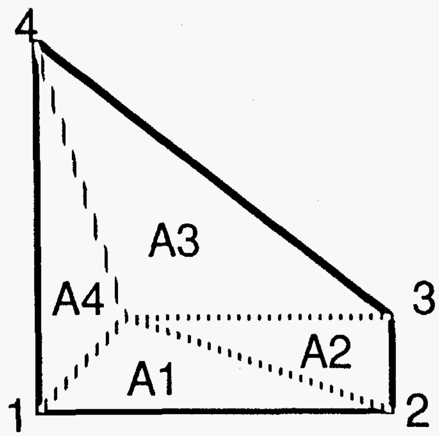


Weighting using our present side-based scheme on an "unstructured grid":

W(n1) = w2*w3 = 9/16
W(n2) = w3*w4 = 3/16
W(n3) = w1*w4 = 1/16
W(n4) = w1*w2 = 3/16

where A1 = 1/8 A2 = 3/8   A3 = 3/8   A4 = 1/8
and
w1 = A1/(A1+ A3) = 1/4   w2 = A2/(A2 + A4) = 3/4
w3 = A3/(A1+ A3) = 3/4   w4 = A4/(A2 + A4) = 1/4

Distorted Element

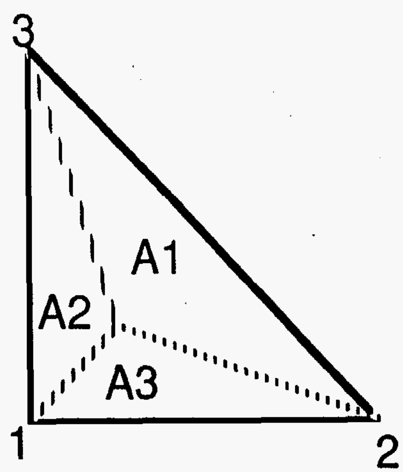


Our present hexahedral weighting algorithm produces erroneous results:

W(n1) = 27/91 W(n2) = 36/91
W(n3) = 16/91 W(n4) = 12/91

In addition we would like to have consistent weights calculated by our triangular and quadrilateral element algorithms. If side 2-3 of the above quad vanishes (the element becomes a triangle) the weights become

W(n1) = 0 W(n2) = 2/3
W(n3) = 1/3 W(n4) = 0



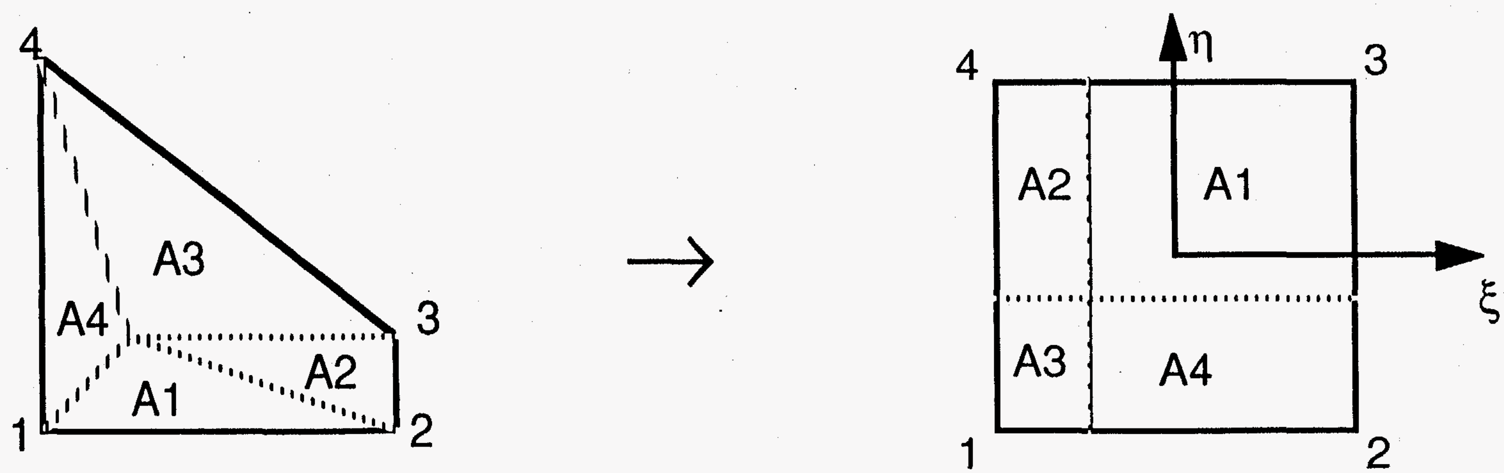
while our current triangular element weighting scheme yields

W(n1) = A1/(A1+A2+A3) = 1/2
W(n2) = A2/(A1+A2+A3) = 1/4
W(n3) = A3/(A1+A2+A3) = 1/4

Isoparametric Maps

We are considering the use of isoparametric maps in order to circumvent these difficulties. Mapping distorted elements to regular elements allows the use of standard bi or tri-linear weighting.

Consider a quadrilateral element → triangular element as side 2-3→ 0. The quadrilateral element maps to a 2x2 square in (ξ,η) space.



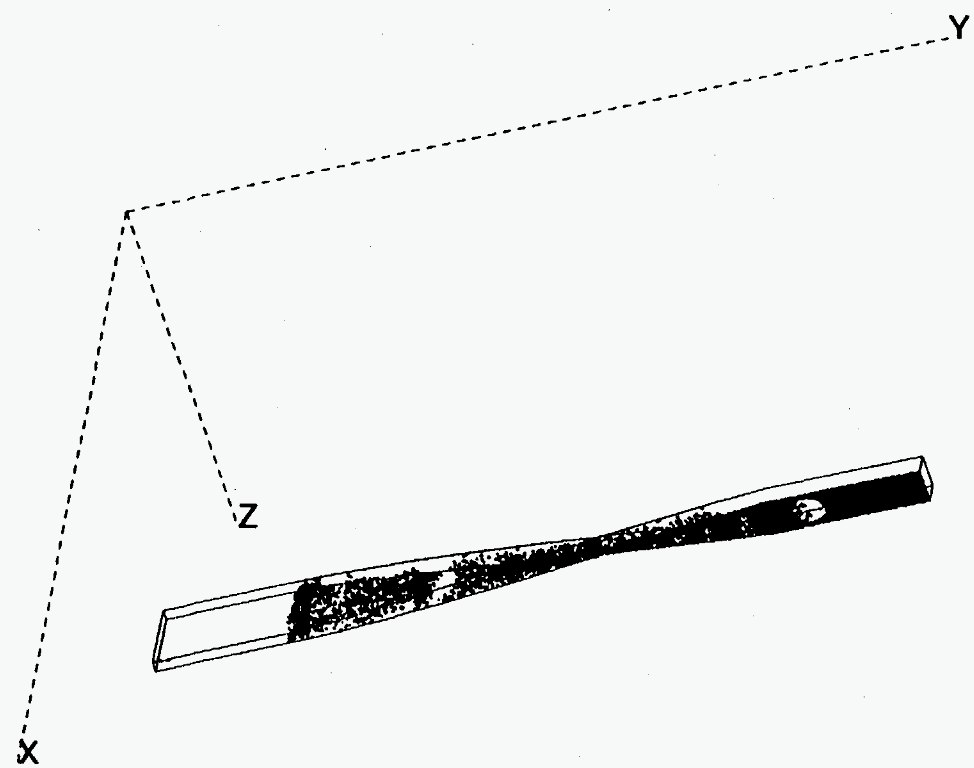
In the mapped coordinate space we use bilinear weighting

$W(n1) = (24+3\varepsilon)/(48+4\varepsilon) = 1/2$ $W(n2) = (8+\varepsilon)/(48+4\varepsilon) = 1/6$

$W(n3) = 1/(12+\varepsilon) = 1/12$ $W(n4) = 3/(12+\varepsilon) = 1/4$

As $\varepsilon \to 0$ the weights at nodes 2 and 3 combine to give a weight of 1/4. These results are consistent with the triangular element weighting scheme.

Field Emission in a Twisted Waveguide



Post Processing

- During a run the code dumps data that can be read by several different LLNL-developed graphics packages: GRIZ, PDBview, and Mesh-TV.
- GRIZ produced the twisted waveguide field plot.
- PDBview produced the primary and dual grid plots and the plot of particles in the twisted waveguide.

Parallel Particles

- The particle push will coexist nicely with the domain decomposed field blocks
- particles will be sorted in spatially distinct domains
- each particle domain will be completely contained in a single field domain
- every field block will keep at least 1 particle domain (may have zero particles)
- particle domains can be split or combined arbitrarily
- load balancing is accomplished by moving daughter particle blocks to idle processors (with a rather large communications penalty) or returning particle blocks to the original field processor

Computer Science

- Standard Fortran77 coding
- all variables explicitly declared
- COMMON blocks avoided
- no POINTER statements
- static memory management (for now)
- GRAPHICS based on GL or GKS
- source code control via CVS
- Parallel processing via domain decomposition
- Field regions split automatically via the Recursive Spectral Bisection algorithm (H. D. Simon - NASA Ames)
- About 4000 elements are required per node on the Intel iPSC/860 to amoritize communication time

Summary

- Self-consistent plasma simulation on grids composed of tetrahedrons, hexahedrons, triangular prisms, and pyramids.
- Successful simulation of beam injection and field emission in a twisted waveguide.
- Divergence errors controlled by the Marder pseudo-current algorithm.
- Simple particle and field boundary conditions.
- Future plans include more boundary condition options (periodic, etc.)
- Parallel implementation on the Meiko CS-2 is underway, with general procedures for handling parallel particles currently undergoing tests.