Advances in Self-Consistent Accelerator modeling: status report

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Presented at ANL

13 March 06

and the VORPAL TEAM

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NSF, the DOE/HEP SBIR program

(and we hope to SciDAC)

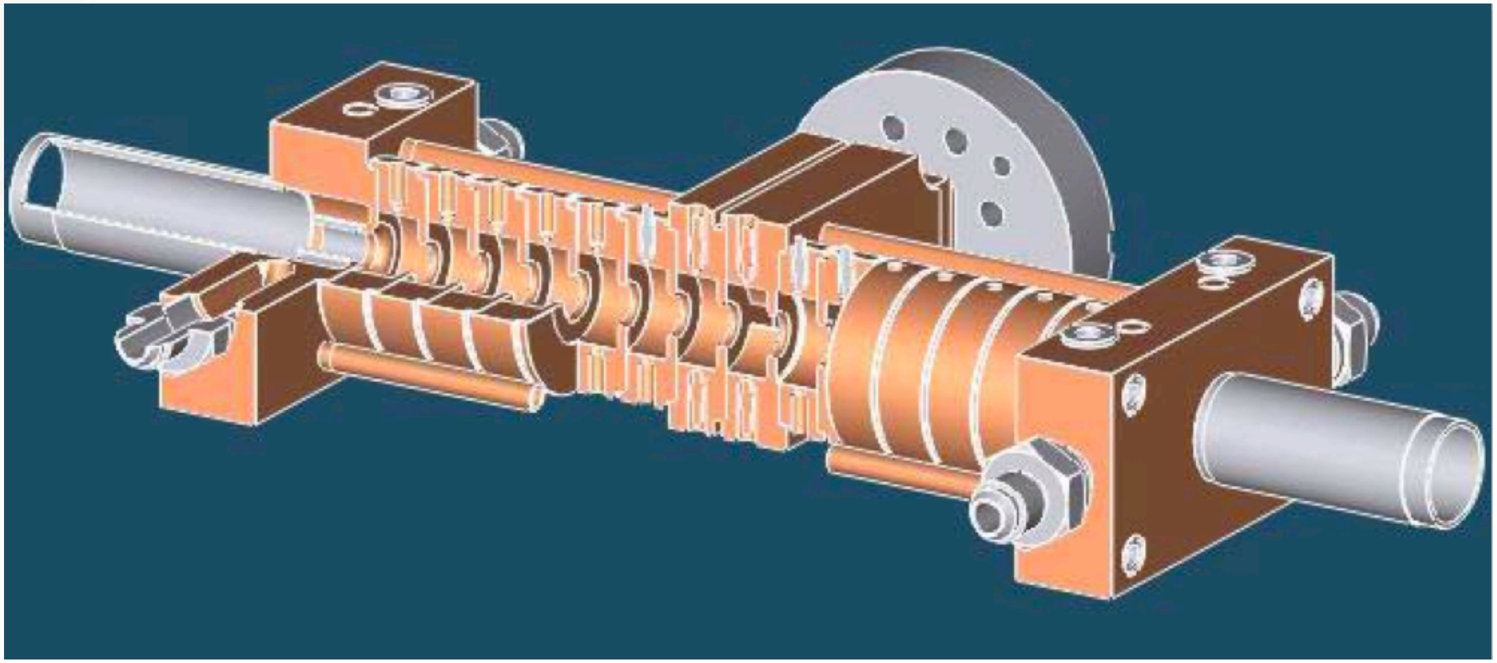
Advances in Self-Consistent Electromagnetic Modeling

- Complex cavity computations with particles have been improved through algorithms, including parallelization, making possiblle computations of wakefields in complex structures, intrabunch effects, injectors, …
- Summary of some of what has made this possible
  - Local charge and current deposition methods
  - Parallelization
  - Improved stability
  - Boundary representations
- Comparison with
  - Finite element approaches
  - Unitary separation approaches

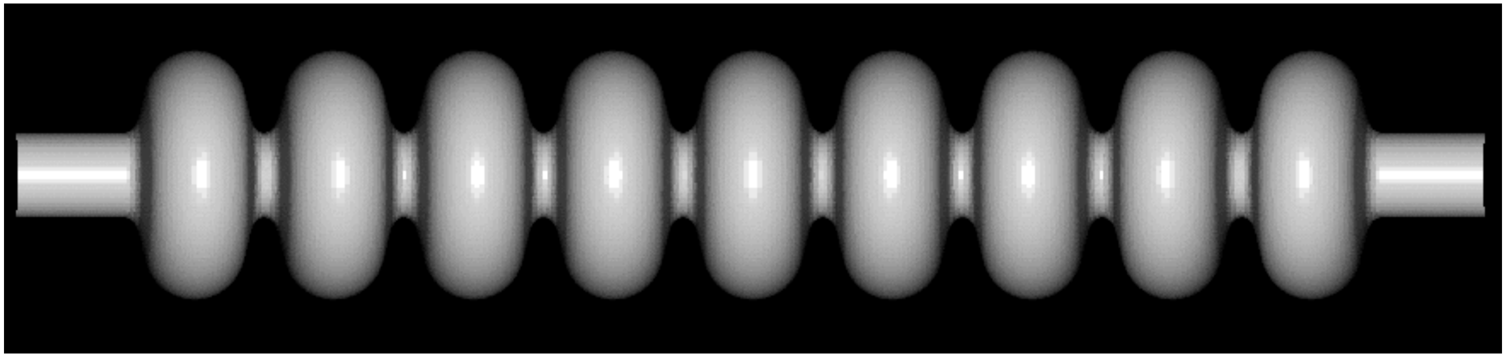
The goals of modeling?

- Part of the design process
  - Create
  - Simulate
  - Build
  - Test
- Simulation for prediction of
  - Cavity losses
  - Instability
- In general for
  - Exploration
  - Confirmation
  - Elucidation

Modeling allows one to answer questions without construction cost



NLC



ILC (Tesla)

Basic problem in charge particles moving in EM fields

Auxiliary equations

- Maxwell

$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E}$$

$$\nabla \bullet \mathbf{B} = 0$$

$$\frac{\partial \mathbf{E}}{\partial t} = c^2[\nabla \times \mathbf{B} - \mu_0 \mathbf{j}]$$

$$\nabla \bullet \mathbf{E} = \rho / \varepsilon_0$$

- Particle sources

$$\mathbf{j} = \sum q_i \mathbf{v}_i \delta(\mathbf{x} - \mathbf{x}_i)$$

$$\rho = \sum q_i \delta(\mathbf{x} - \mathbf{x}_i)$$

- Particle dynamics

$$\frac{d(\gamma \mathbf{v})}{dt} = \frac{q_i}{m_i}[\mathbf{E}(\mathbf{x}_i, t) + \mathbf{v}_i \times \mathbf{B}(\mathbf{x}_i, t)]$$

$$\frac{d\mathbf{x}_i}{dt} = \mathbf{v}_i$$

With much other physics added for a complete model

- Particle injection
- Dark currents
- Multipactoring
- Photon (short wavelength) production
- Surface resistance
- Secondary emission

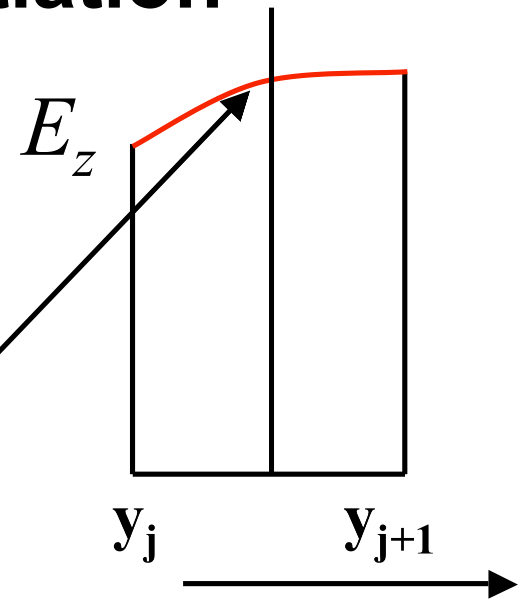
ELECTROMAGNETICS

Yee: 2nd order accurate spatial differentiation

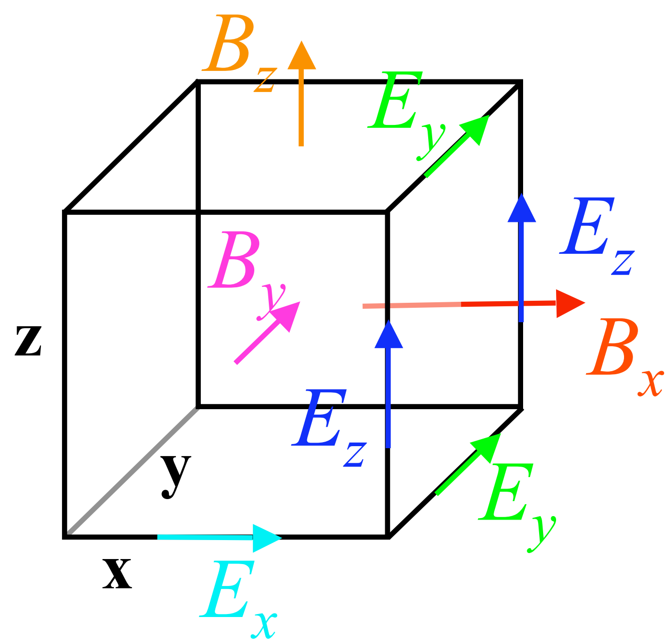
$$\frac{\partial B_x}{\partial t} = -\frac{\partial E_z}{\partial y} + \frac{\partial E_y}{\partial z}$$

- At the midpoint

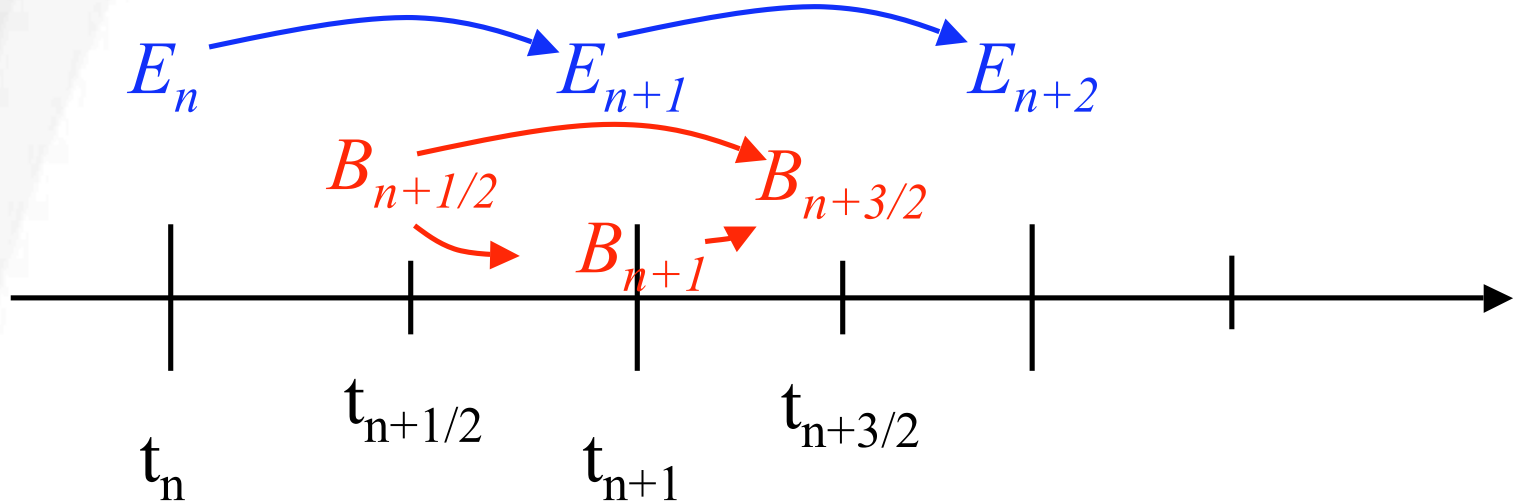
$$\frac{\partial E_z}{\partial y} = \frac{E_{z,j+1} - E_{z,j}}{\Delta y} + O(\Delta y^2)$$



- Leads to special layout of values in a cell
- *Yee mesh* gives 2nd order accuracy of spatial derivatives



Second-order in time by leap frog



$$\frac{\partial B_x}{\partial t} = -\frac{\partial E_z}{\partial y} + \frac{\partial E_y}{\partial z}$$

$$B^{n+1/2}_{x,i,j,k} - B^{n-1/2}_{x,i,j,k} = \Delta t \left(\frac{E^n_{z,i,j,k} - E^n_{z,i,j+1,k}}{\Delta y} + \frac{E^n_{y,i,j,k+1} - E^n_{y,i,j,k}}{\Delta z} \right)$$

- Time centered differences give second order accuracy in Δt
- Can get time-collocated values by half-stepping in B
- Similar for E update, except c^2 factor

Matrix representation useful for stability

$$\frac{dB_{x,i,j,k}}{dt} = \left(\frac{E_{z,i,j,k} - E_{z,i,j+1,k}}{\Delta y} + \frac{E_{y,i,j,k+1} - E_{y,i,j,k}}{\Delta z} \right)$$

$$\frac{d\mathbf{b}}{dt} = -\mathbf{C} \bullet \mathbf{e} \qquad \frac{d\mathbf{e}}{dt} = c^2 \mathbf{C}' \bullet \mathbf{b} \qquad \frac{d^2\mathbf{b}}{dt^2} = -c^2 \mathbf{C} \bullet \mathbf{C}' \bullet \mathbf{b} = -\mathbf{D} \bullet \mathbf{b}$$

- Magnetic and electric spaces are different
- **C**, **C'** are adjoints, so **D** is self-adjoint (symmetric)
- Diagonalize into separate harmonic oscillators
- Leap frog for harmonic oscillator, stability limit at

$$\omega_{\max} \Delta t_{CFL} = 2 \qquad \Delta t_{CFL} = \frac{1}{c\sqrt{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2}}}$$

Gershgorin Circle Theorem gives stability bound

- Frequencies are eigenmodes of $D = c^2 C'C$
- Eigenvalues in range

$$0 < \omega^2 < \max\left(\sum_j \left|D_{ij}\right|\right) \textit{ over } i$$

- Gives precise range for infinite grid
- Points to relation between coefficients and frequencies for other cases

Many other methods available

- Finite element - later
- Hamiltonian splitting (de Raedt): into exactly solvable parts $$\frac{d(\mathbf{b},\mathbf{e})}{dt} = \mathbf{A}\bullet(\mathbf{b},\mathbf{e}) = \mathbf{M}\bullet\mathbf{N}\bullet(\mathbf{b},\mathbf{e})$$
  - known: $\frac{d\mathbf{U}_M}{dt} = \mathbf{M}\bullet\mathbf{U}_M \quad \frac{d\mathbf{U}_N}{dt} = \mathbf{N}\bullet\mathbf{U}_N$
  - stable approximate solution (since unitary): $$\mathbf{U}(\Delta t) = \mathbf{U}_N(\Delta t/2)\bullet\mathbf{U}_M(\Delta t)\bullet\mathbf{U}_N(\Delta t/2)$$
  - Similar to drift-kick of symplectic integration
  - Lee and Fornberg (2005) have improved method based on Zheng et al (1999)
- *None of these has yet proven as effective for self-consistent particle simulation as FDTD, explicit or implicit*

PARTICLES

Computing particle-particle interactions is prohibitive

- Coulomb interaction leads to N_p^2 force computations

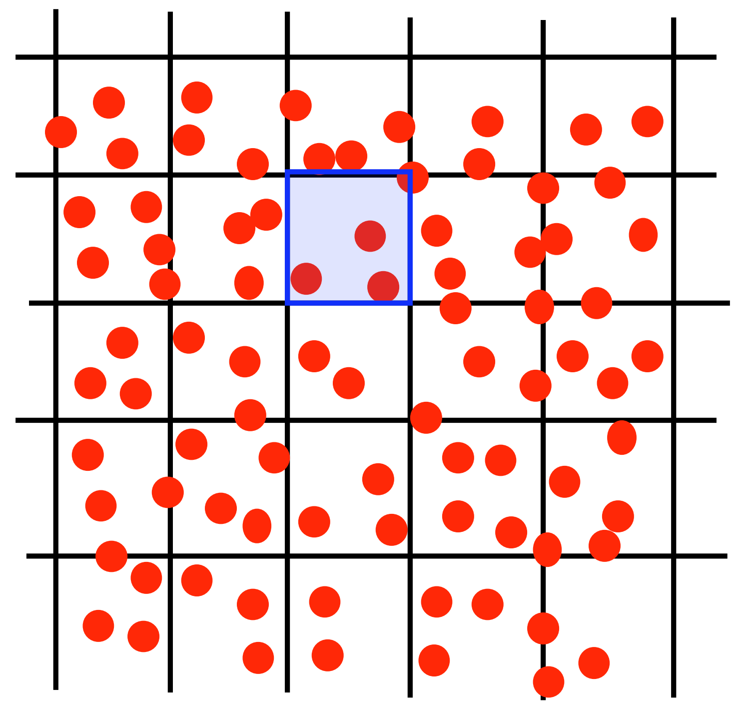
$$\frac{d\gamma_i \mathbf{v}_i}{dt} = \frac{q_i}{\varepsilon_0 m_i} \sum_j q_j \frac{\mathbf{x}_i - \mathbf{x}_j}{\left|\mathbf{x}_i - \mathbf{x}_j\right|^3}$$

- Lenard-Weichert (retarded potentials) - worse due to need to keep history

$$\frac{d\gamma_i \mathbf{v}_i}{dt} = \frac{q_i}{\varepsilon_0 m_i} \sum_j q_j \mathbf{F}_{ij}(\mathbf{x}_i, \mathbf{x}_j(t - \tau))$$

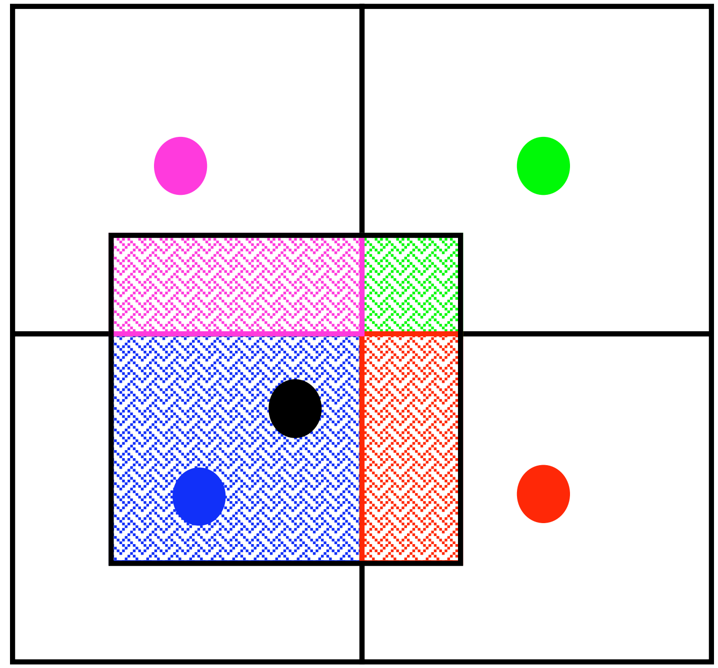
Particle In Cell (PIC) reduces to N_p scaling

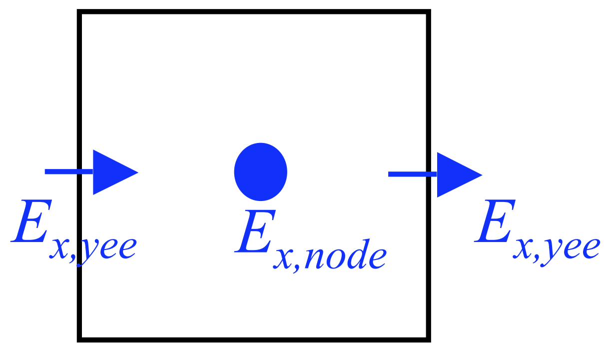
- Particle contributions to charges and currents are added to each cell: $O(N_p)$ operations
- Forces on a particle are found from interpolation of the cell values: $O(N_p)$ operations



Finding the force: interpolation (gather)

- Linear weighting for each dimension
  - 1D: linear
  - 2D: bilinear = area weighting
  - 3D: trilinear = volume weighting
- Force obtained through 1st order, error is 2nd order
- For simplicity, no loss of accuracy, weight first to nodal points





Only certain EM algorithms ensure Poisson satisfied

$$\nabla \bullet \mathbf{E} = \rho / \varepsilon_0$$

satisfied always if

$$\frac{\Delta E_x}{\Delta x} + \frac{\Delta E_y}{\Delta y} + \frac{\Delta E_z}{\Delta z} = \rho / \varepsilon_0$$

$$\frac{\partial \mathbf{E}}{\partial t} = c^2[\nabla \times \mathbf{B} - \mu_0 \mathbf{j}]$$

finite difference version

and

$$\nabla \bullet \mathbf{E} = \rho / \varepsilon_0$$

initially

$$\frac{\Delta E_x}{\Delta x} + \frac{\Delta E_y}{\Delta y} + \frac{\Delta E_z}{\Delta z} = \rho / \varepsilon_0$$

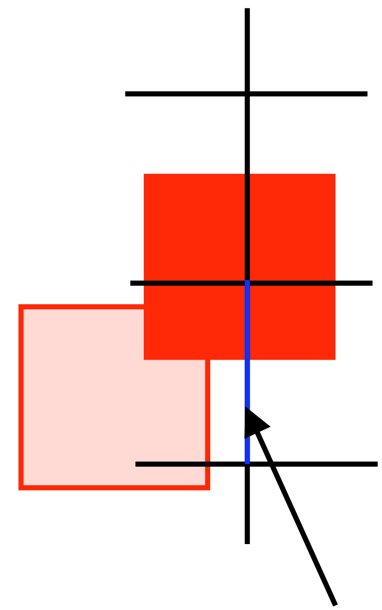
and

$$\frac{\partial \rho}{\partial t} = -\nabla \bullet \mathbf{j}$$

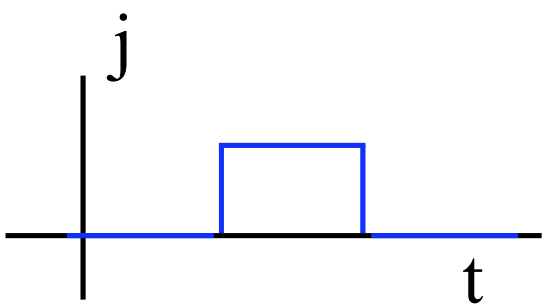
$$\frac{\Delta \rho}{\Delta t} = -\frac{\Delta j_x}{\Delta x} + \frac{\Delta j_y}{\Delta y} + \frac{\Delta j_z}{\Delta z}$$

A special scatter ensures finite difference charge conservation

- Principle: apportion via some weighting
- Computing the charge density
  - Compute the current density and find the charge density from finite difference
  - Directly weight particles to the grid
- If these two methods do not agree, then one can have false charge buildup from the Ampere-Maxwell equation. Requires Poisson solve to remove.
- Villasenor/Buneman explicitly conserves charge, but is noisier



Current contrib. to this interface must match charge difference change across separated cells



EM algorithm must take *numerically* divergenceless to *numerically* divergenceless

$$\frac{\Delta E_x^n}{\Delta x} + \frac{\Delta E_y^n}{\Delta y} + \frac{\Delta E_z^n}{\Delta z} = 0$$

and

$$\mathbf{E}^{n+1} = \mathbf{M} \bullet \mathbf{E}^n$$

implies

$$\frac{\Delta E_x^{n+1}}{\Delta x} + \frac{\Delta E_y^{n+1}}{\Delta y} + \frac{\Delta E_z^{n+1}}{\Delta z} = 0$$

Mardahl and Verboncoeur show importance of getting this right

ELSEVIER

Computer Physics Communications 106 (1997) 219–229

Charge conservation in electromagnetic PIC codes; spectral comparison of Boris/DADI and Langdon–Marder methods

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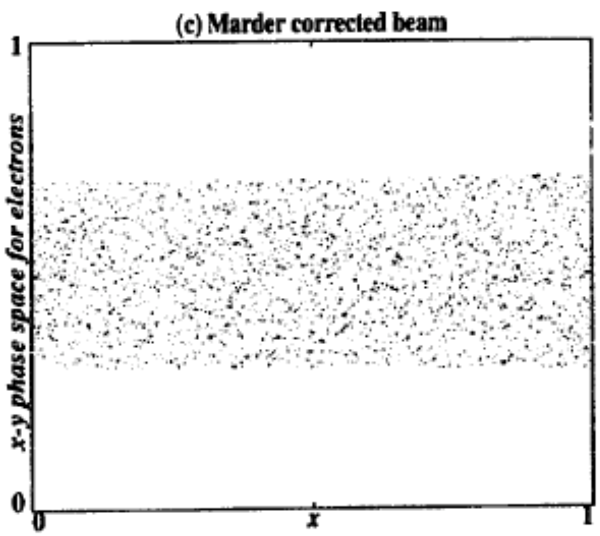
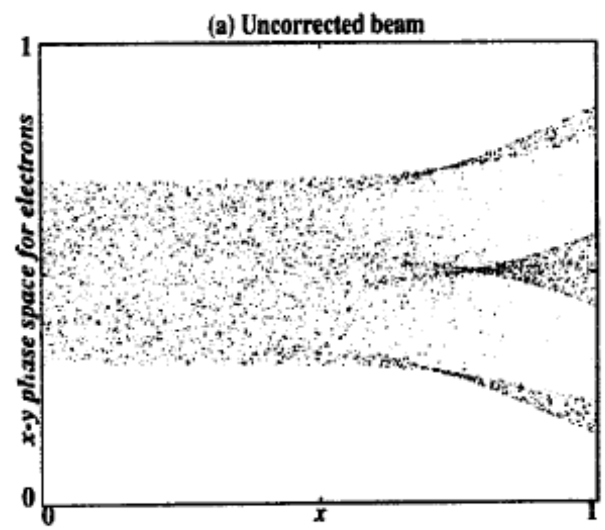
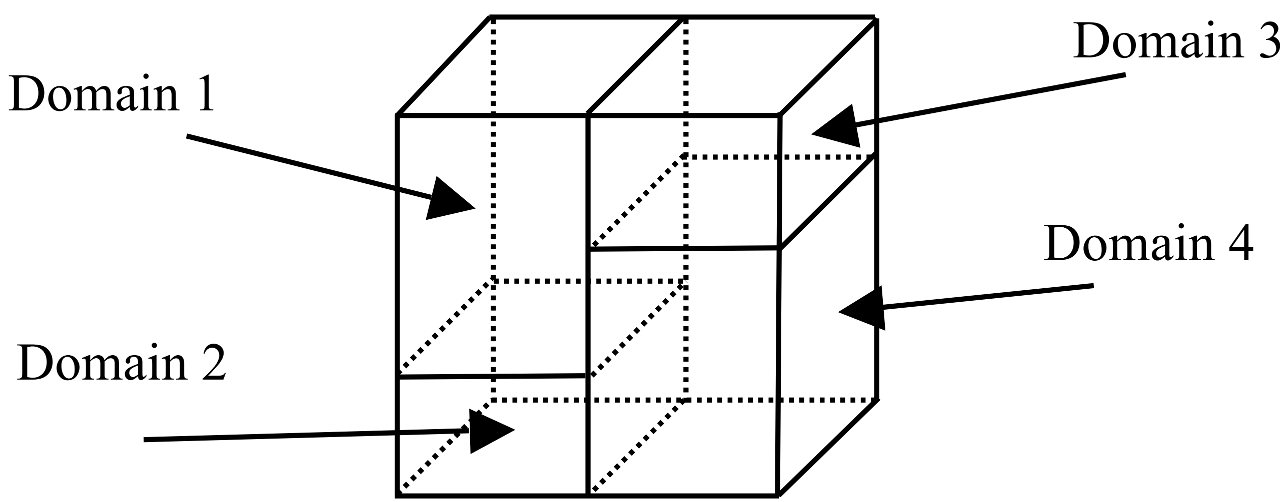
Received 1 April 1997; revised 11 August 1997





Parallelism: domain decomposition

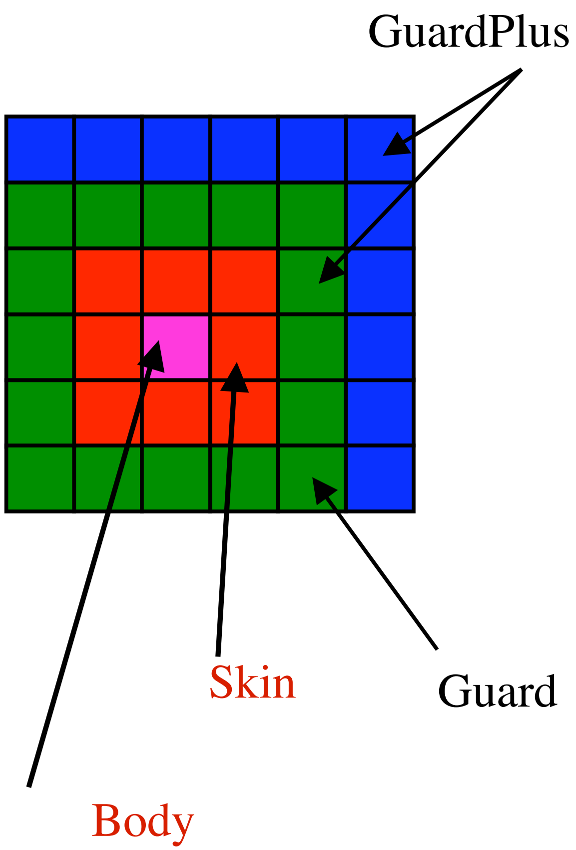


Parallelism rules of thumb

- Communication is expensive
- Global solves are really expensive

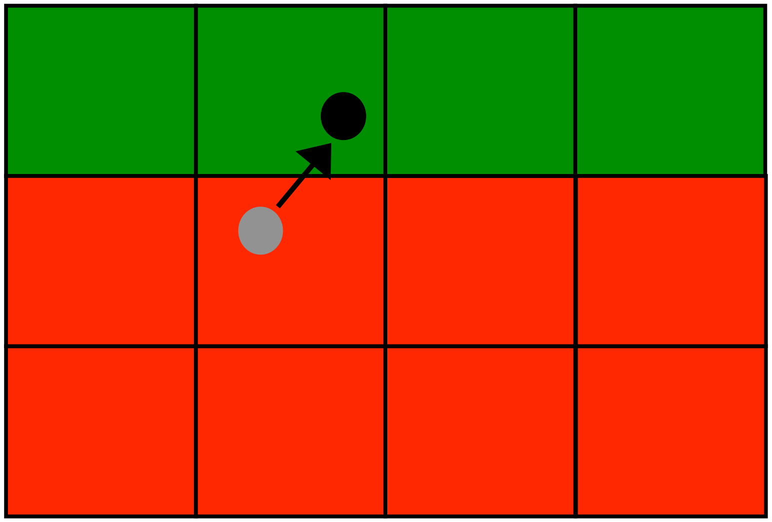
Overlap of communication and computation needed for speed

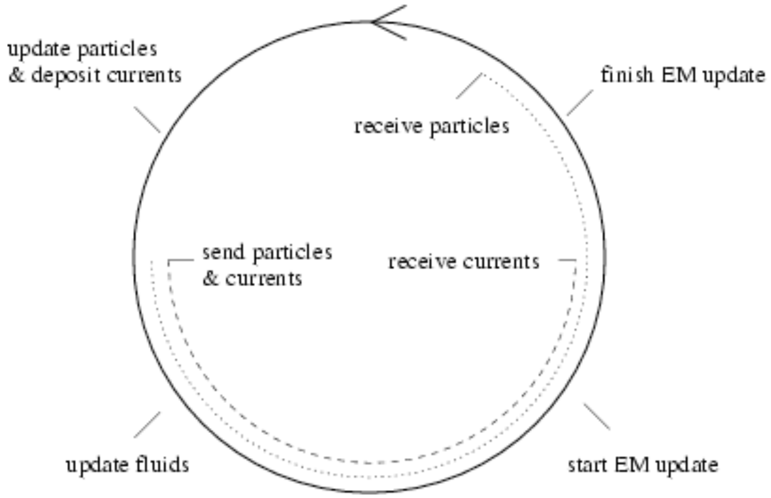
- Non overlap algorithms:
  - Compute domain
  - Send skin (outer edge)
  - Receive guard
  - Repeat
- Overlap algorithms
  - Compute skin
  - Send skin
  - Compute interior
  - Receive guard
  - Repeat



Similar overlap possible for particles

- Move particles and weight currents to grid
- Send currents needed by neighboring processors
- Send particles to neighboring processors
- Update B for half step
- Receive currents and add in
- Update E, B
- Receive particles





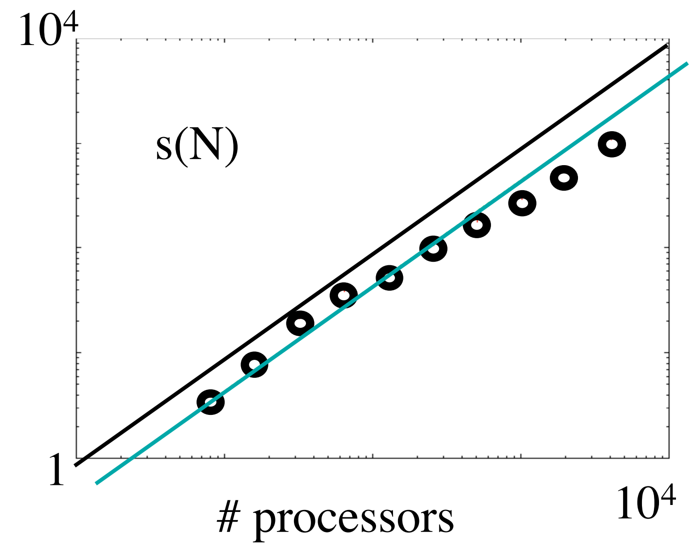
Without charge conserving current deposition, further costly global solve

VORPAL implements basic algorithms in highly scalable manner

<u>Object-oriented and flexible</u>

(Arbitrary dimensional)

- Self-consistent EM modeling
  - Full EM or electrostatic + cavity mode
  - Particle in cell with relativistic or nonrelativistic dynamics
- But has other capabilities
  - Impact and field ionization
  - Fluid methods for plasma or neutral gases
  - Implicit EM
  - Secondary emission
- And is modern
  - Serial or Parallel (general domain decomposition)
  - Cross-platform (Linux, AIX, OS X, Windows)
  - Cross-platform binary data (HDF5)

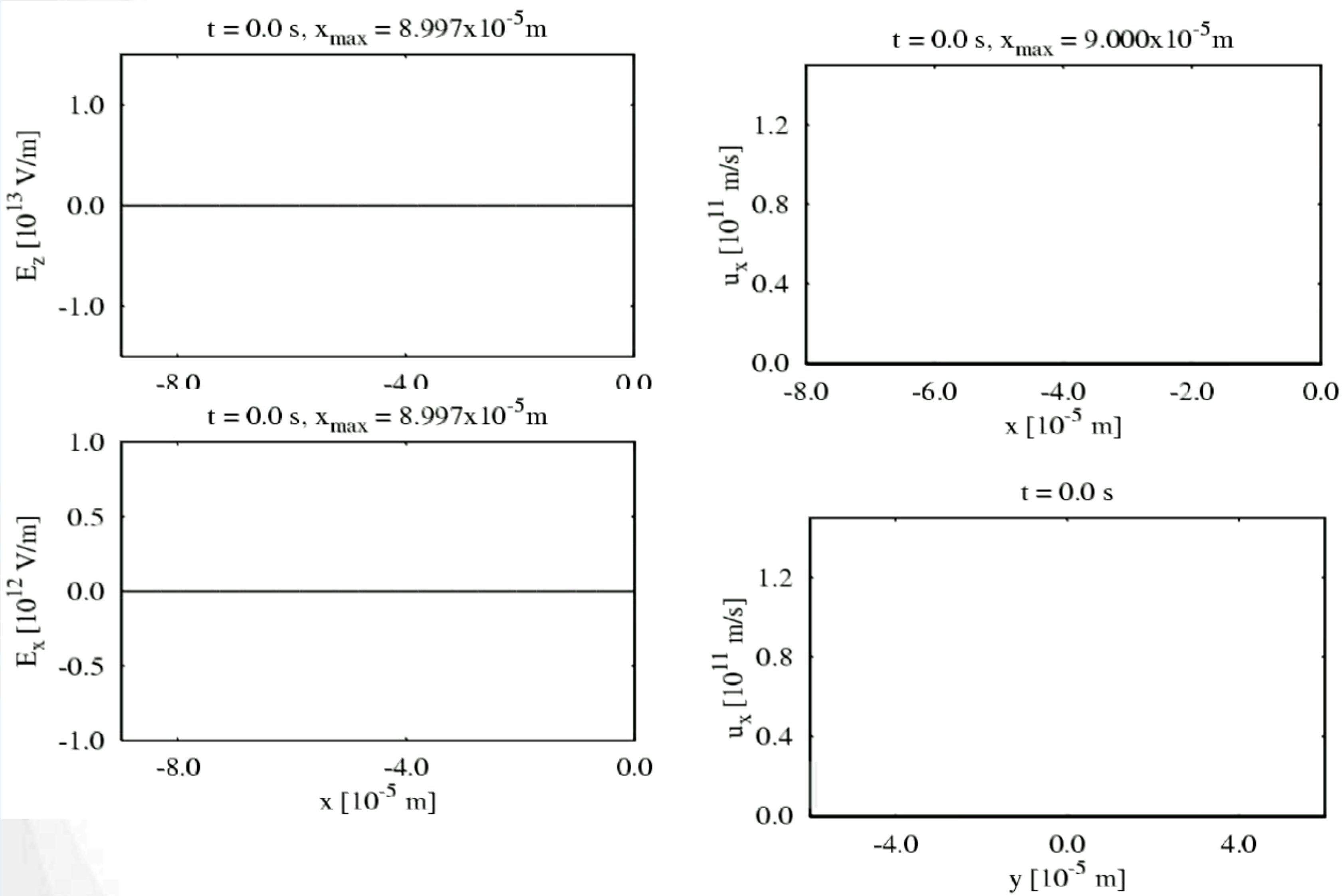


VORPAL scales well to 1,000's of processors (strong scaling)

Simplest algorithm allows complex computations

- Example: formation of beams in laser-plasma interaction

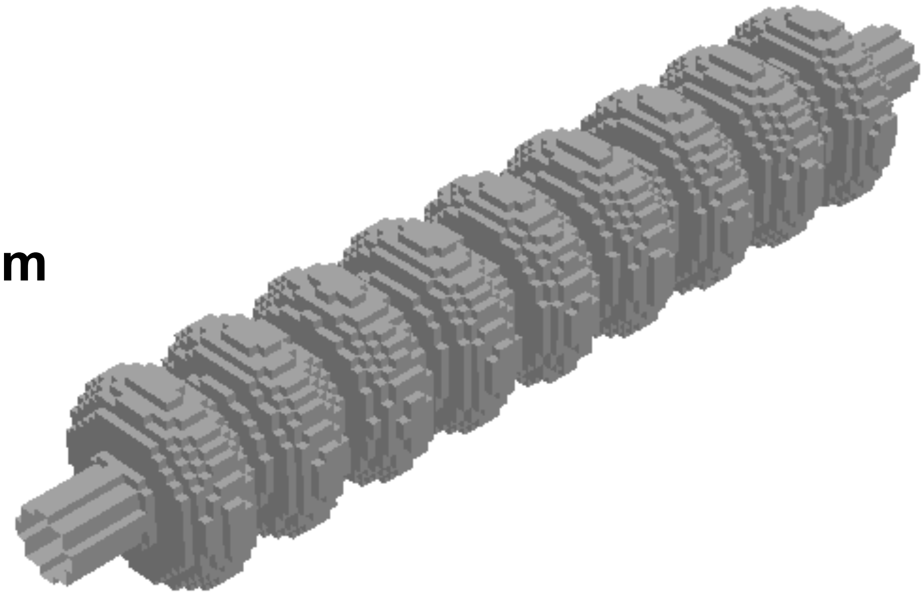
Elucidation: long pulses shorten to resonance, capture, loading, acceleration



Complications: boundaries

Early work on structured meshes had *stair-step* boundary conditions

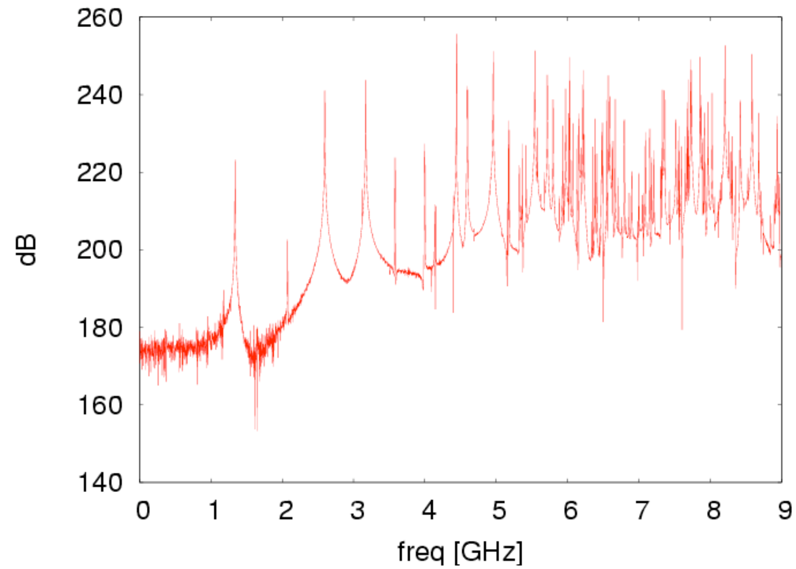
120x24x24 = 71,424 cells
= 215,000 degrees of freedom



- N ($L/\Delta x$) cells in each direction
- Error of $(\Delta x/L)^3$ at each surface cell
- $O(N^2)$ cells on surface
- Error $= N^2(\Delta x/L)^3 = O(1/N)$

Modes computed with combination of FFT and fitting

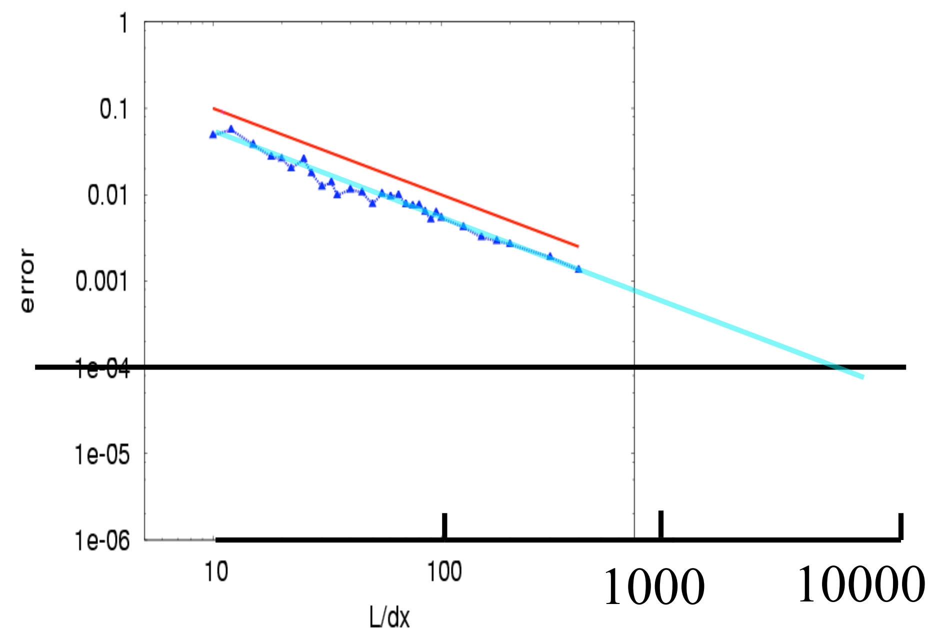
- 3 cell SRF
- High density of higher-order modes
- FFT allows extraction of field shape
- Excite that field, measure frequency by fitting



Excite with delta-function initial condition
Run 25000 steps
FFT

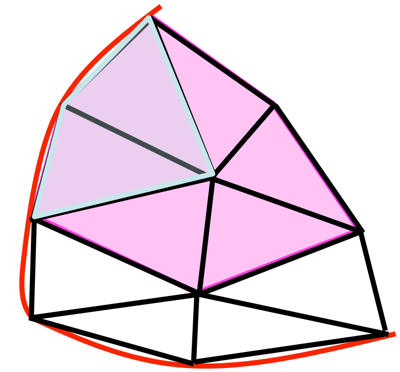
Convergence studies confirm result, indicate modeling problem

- Stair-step error is 10^{-3} at 1000 cells per dimension, error linear with cell size
- Requires 10,000 cells per dimension to get 10^{-4} accuracy
- 10^{12} cells for 3D problem



This approach will not give answer even on large, parallel hardware

Finite elements give one approach to improved boundary modeling



- Tau3P, HFSS, …

$$\mathbf{B} = \sum b_k(t)\mathbf{u}_k^B(x) \qquad \mathbf{E} = \sum e_\ell(t)\mathbf{u}_\ell^E(x)$$

$$\frac{\partial \mathbf{B}}{\partial t} = \sum \frac{db_k}{dt}(t)\mathbf{u}_k^B(x) \qquad \nabla \times \mathbf{E} = \sum e_\ell(t)\nabla \times \mathbf{u}_\ell^E(x)$$

$$\sum \frac{db_k}{dt}(t)\mathbf{u}_k^B(x) = -\sum e_\ell(t)\nabla \times \mathbf{u}_\ell^E(x)$$

$$\int d^3x \sum_k \frac{db_k}{dt}(t)\mathbf{u}_{k'}^B(\mathbf{x})\mathbf{u}_k^B(\mathbf{x}) = -\int d^3x \sum_\ell e_\ell(t)\mathbf{u}_{k'}^B(\mathbf{x}) \bullet \nabla \times \mathbf{u}_\ell^E(\mathbf{x})$$

$$\mathbf{M}_b \bullet \frac{d\mathbf{b}}{dt} = -\mathbf{C} \bullet \mathbf{e}$$

$$\mathbf{M}_e \bullet \frac{d\mathbf{e}}{dt} = c^2\mathbf{C}' \bullet \mathbf{b}$$

Finite elements require global solves, more intense particle calculations

- Global mass matrix inversion required at each step

$$\mathbf{M}_b \bullet \frac{d\mathbf{b}}{dt} = -\mathbf{C} \bullet \mathbf{e}$$

- Self consistency difficult and charge conservation not guaranteed

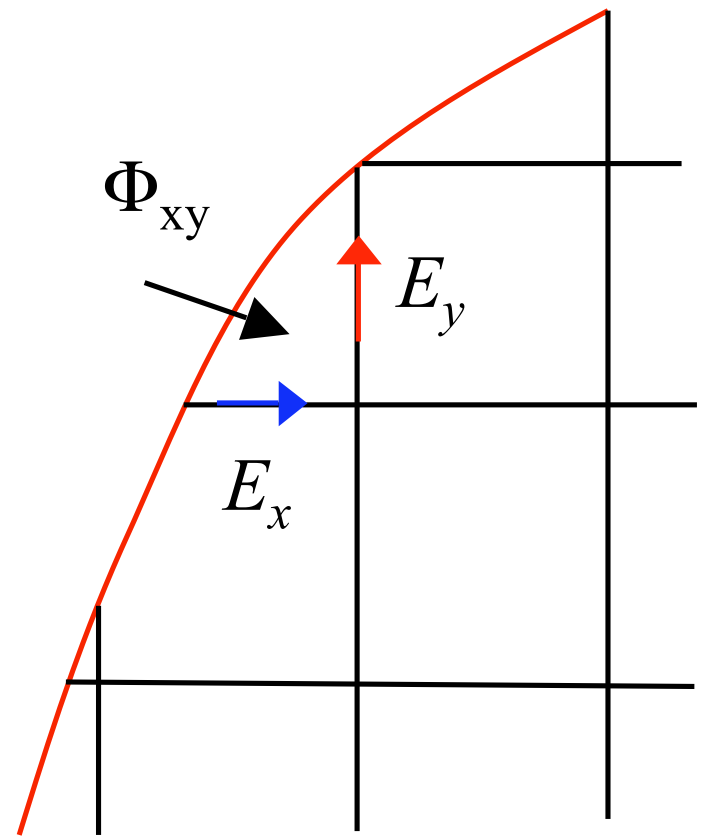
$$\mathbf{M}_e \bullet \frac{d\mathbf{e}}{dt} = c^2\left(\mathbf{C}' \bullet \mathbf{b} - \mu_0 \mathbf{j}\right)$$

$$j_\ell = \sum_{ptcls\ i} q_i \mathbf{v}_i \mathbf{u}_\ell^E\left(\mathbf{x}_i((n+1/2)\Delta t)\right)$$

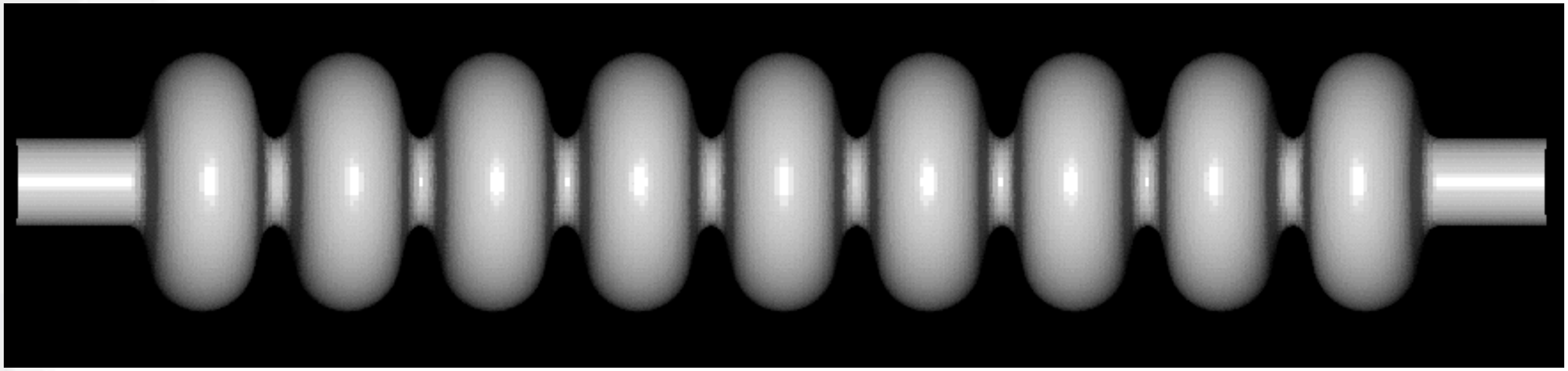
- Difficult to follow particles
  - List of regions
  - List of FE's with support in that region
  - Complex FE element evaluation at each time step for each particle

Resurgence of regular grids: cut cells give same accuracy as finite elements

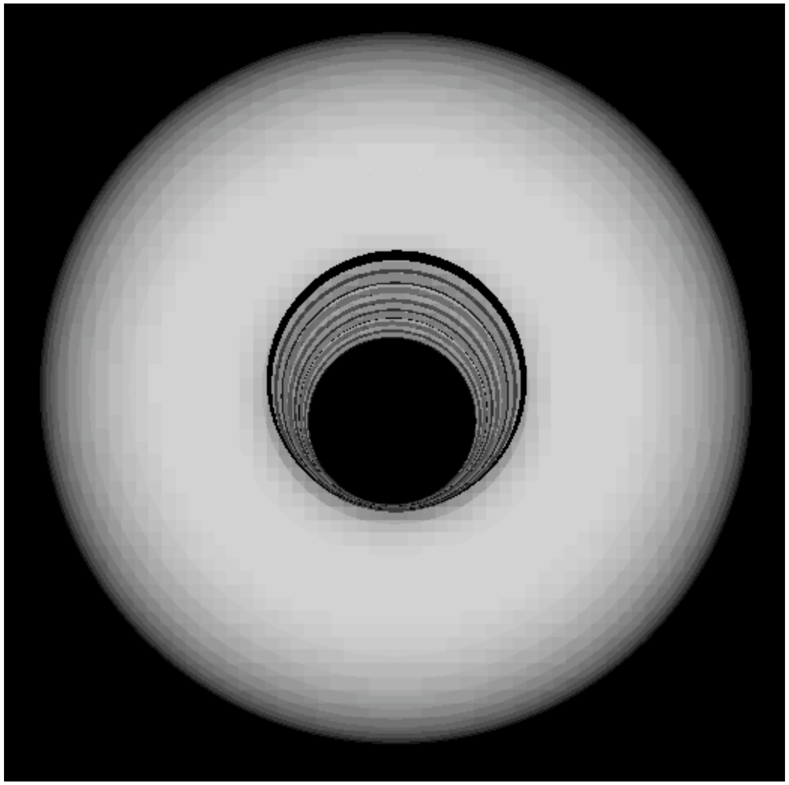
- For cells fully interior, us regular update
- For boundary cells:
  - Store areas and lengths
  - Update fluxes via
    $$\dot{\Phi}_{xy} = -E_x \ell_x - E_y \ell_y$$
  - Update fields via
    $$B_z = \Phi_{xy} / A_{xy}$$



Cut-cell boundary conditions accurately represent geometry

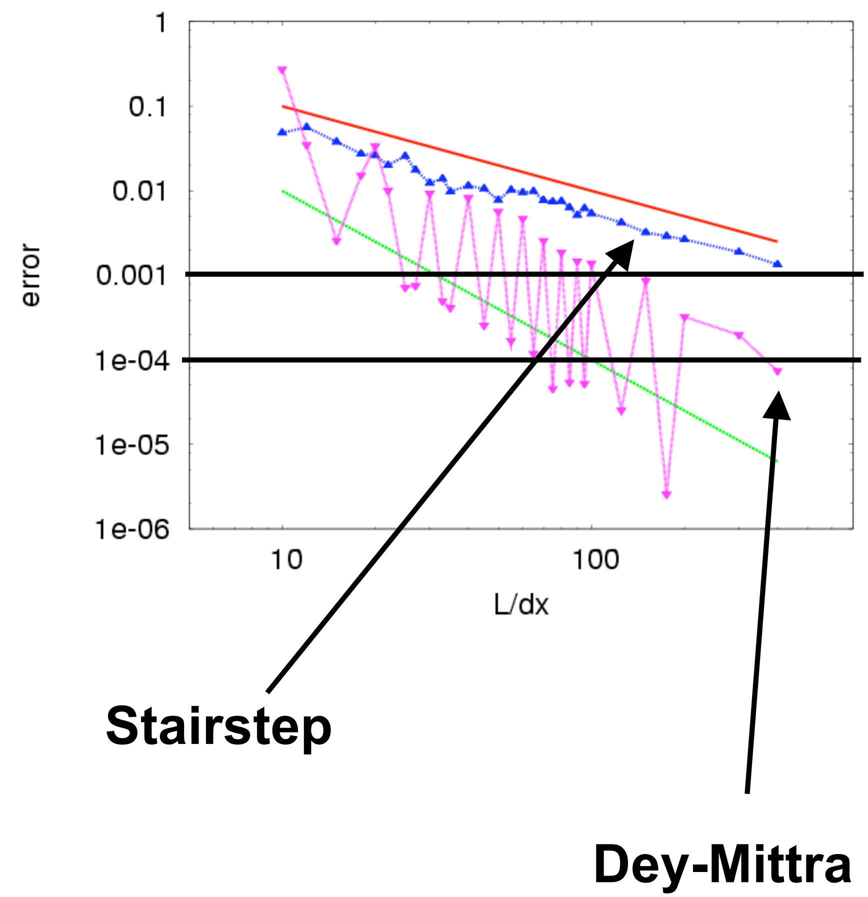


- Tesla 2000 cavities
- 312x56x56 (10^6) cells



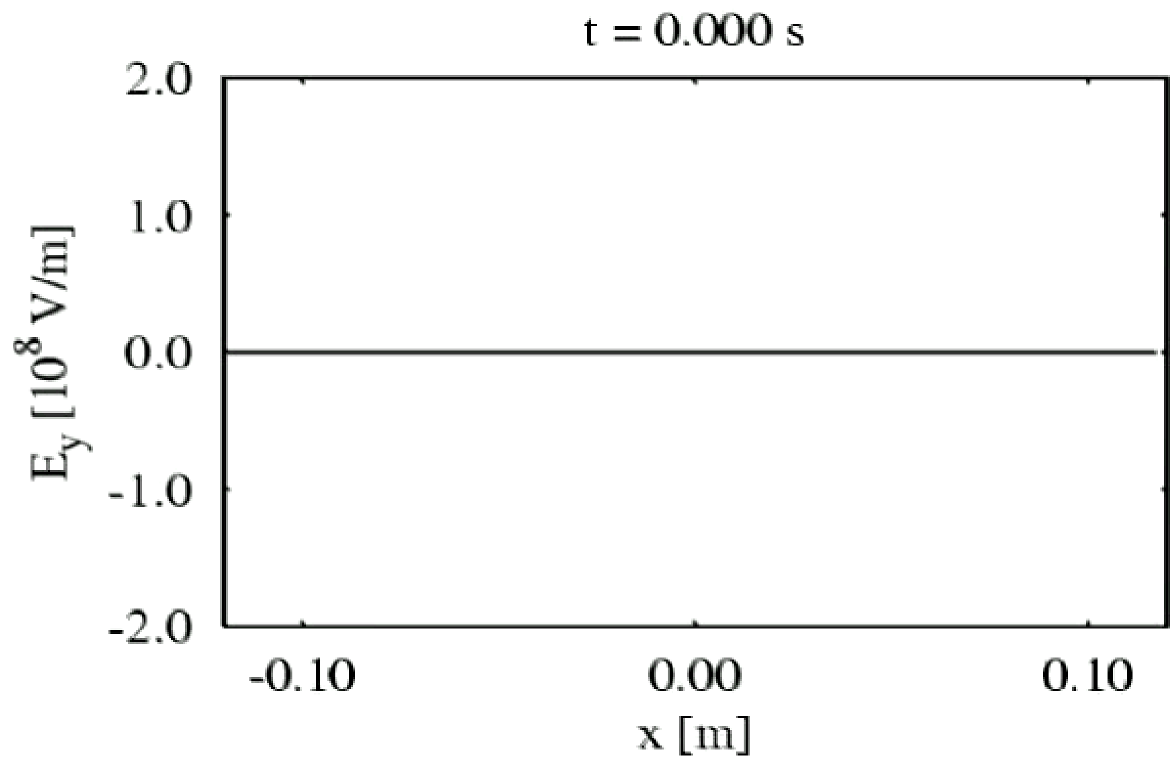
Dey-Mittra (1997) cut-cells allow 10^{-4} accuracy

- Fewer than 10^8 cells for cavity modeling at one part in 10^4
- Implementation exists now in VORPAL



Dey-Mittra problem: small triangles give high frequencies, small time steps

- B update matrix coefs ~ length/area
- Length/area becomes infinite as area vanishes
- Get localized, high-frequency modes
- Must throw out small cell fragments

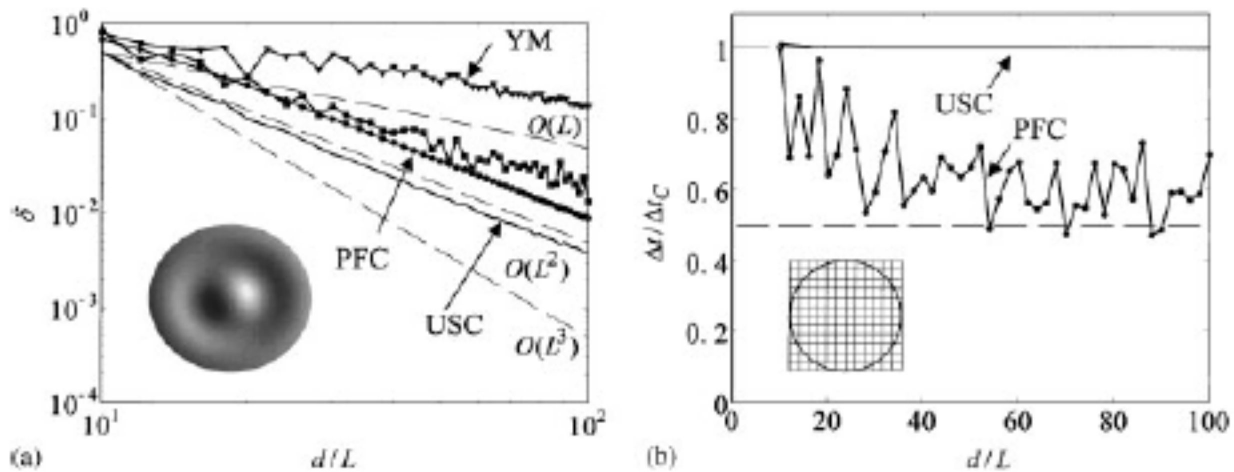


Improvement on cut-cell recently discovered

INTERNATIONAL JOURNAL OF NUMERICAL MODELLING: ELECTRONIC NETWORKS, DEVICES AND FIELDS
Int. J. Numer. Model. 2003; 16:127–141 (DOI: 10.1002/jnm.488)

A uniformly stable conformal FDTD-method in Cartesian grids

I. A. Zagorodnov*†, R. Schuhmann and T. Weiland



- New method gives error lower than Dey-Mittra
- Does not have reduction of stable Δt
- Favorable properties re particle introduction
- Now being implemented

Regular, structured grids allow for self-consistent integration of particles

Wakefield for Tesla cavities computed by VORPAL in 3D

Future?

- More accurate EM integrators with boundaries and particles? Wish list:
  - Absolutely stable, getting slow solution correct for large time steps, conserving divergence
  - No global solves
- More accurate particle deposition not requiring higher order in all directions
- Conformal boundaries with
  - Surface resistance
  - Dark currents
  - And more and more physics