Advances in Self-Consistent Accelerator modeling

John R. Cary

University of Colorado and Tech-X Corporation

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and the VORPAL TEAM

Dan Barnes, David Bruhwiler, Richard Busby, Johan Carlsson, John R. Cary, Dimitre Dimitrov, Eugene Kashdan, Peter Messmer, Chet Nieter, Viktor Przebinda, Nate Sizemore, Peter Stoltz, Raoul Trines, Seth Veitzer, Wen-Lan Wang, Nong Xiang

NSF, the DOE SBIR program

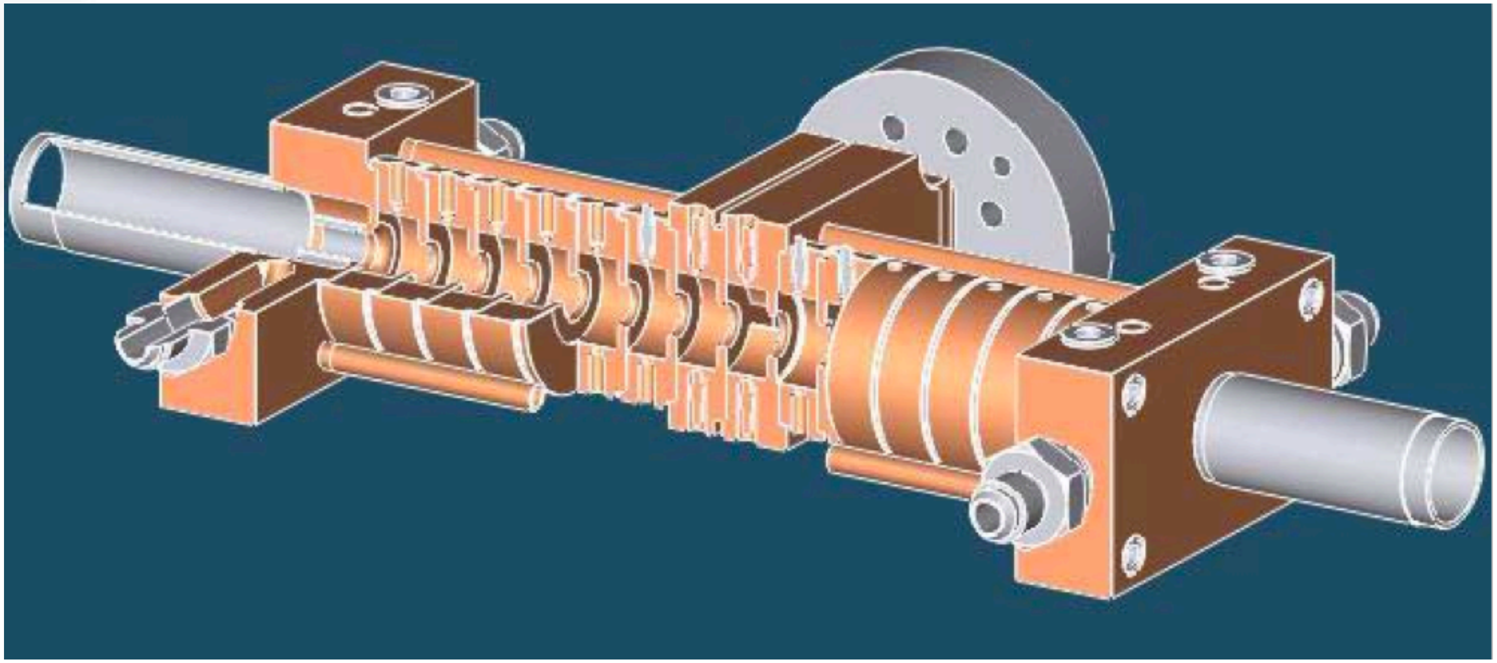
Advances in Self-Consistent Electromagnetic Modeling

- 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

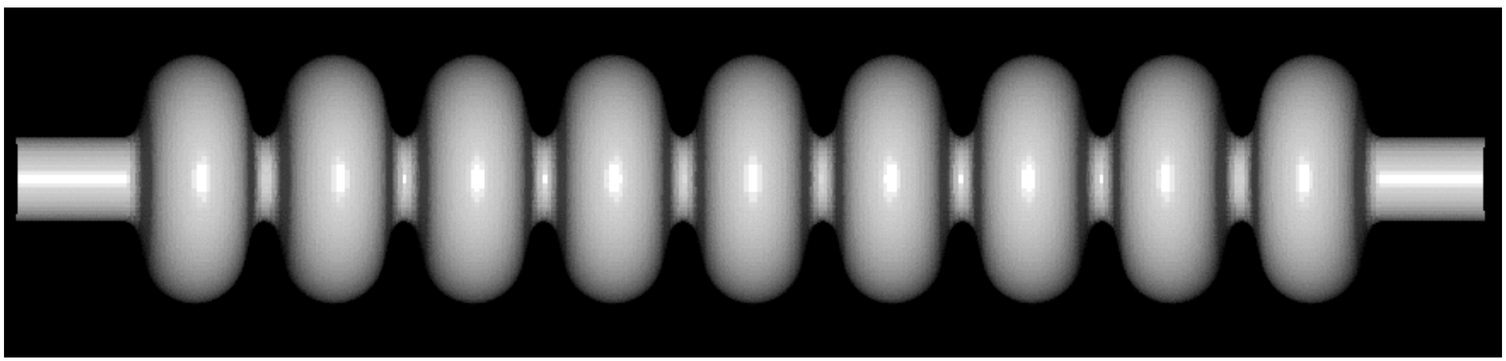
The goals of modeling?

- 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

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

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

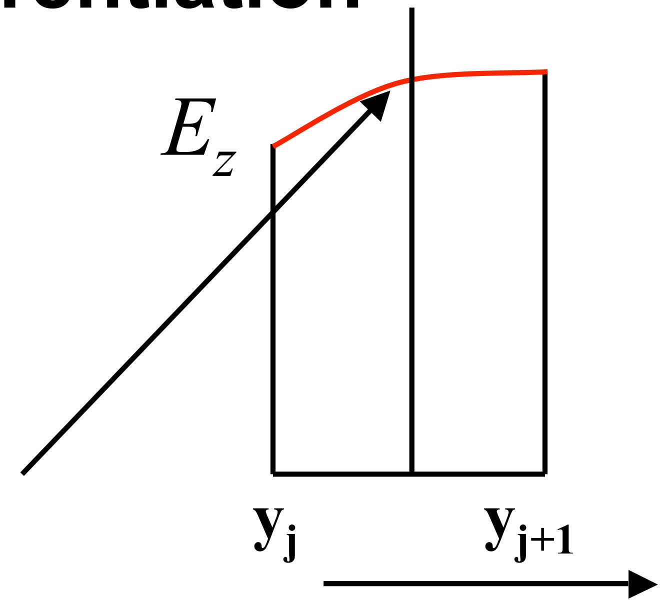
With much other physics added for a complete model

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

ELECTROMAGNETICS

Yee: 2nd order accurate spatial differentiation

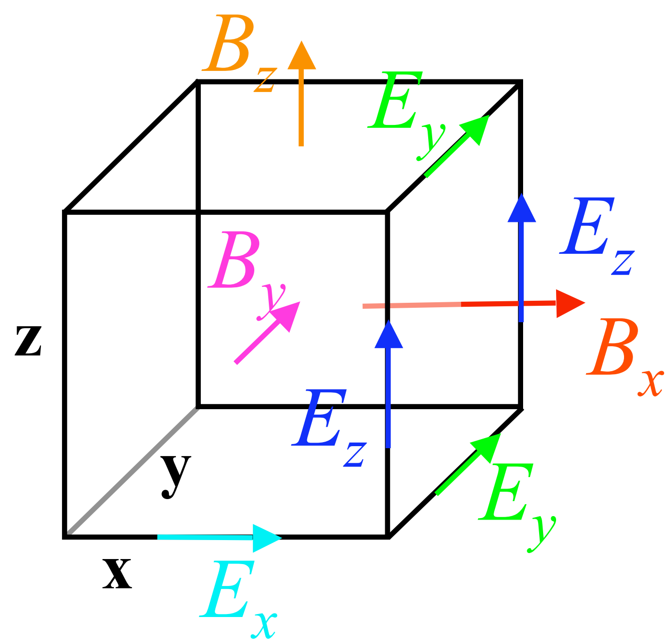
$$\frac{\partial B_x}{\partial t} = -\frac{\partial E_z}{\partial y} + \frac{\partial E_y}{\partial z}$$



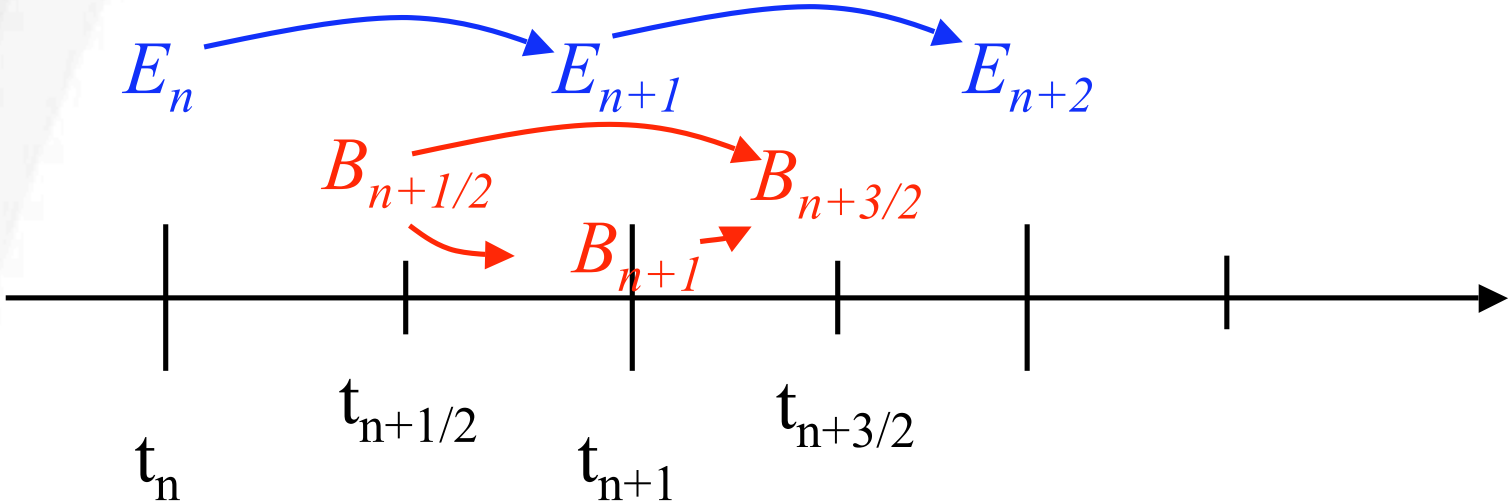
- At the midpoint

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

- 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

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

- 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)
- *Smith, Cary, Carlsson now have implicit, charge-conserving algorithm*

PARTICLES

Computing particle-particle interactions is prohibitive

- Coulomb interaction leads to N_p^2 force computations

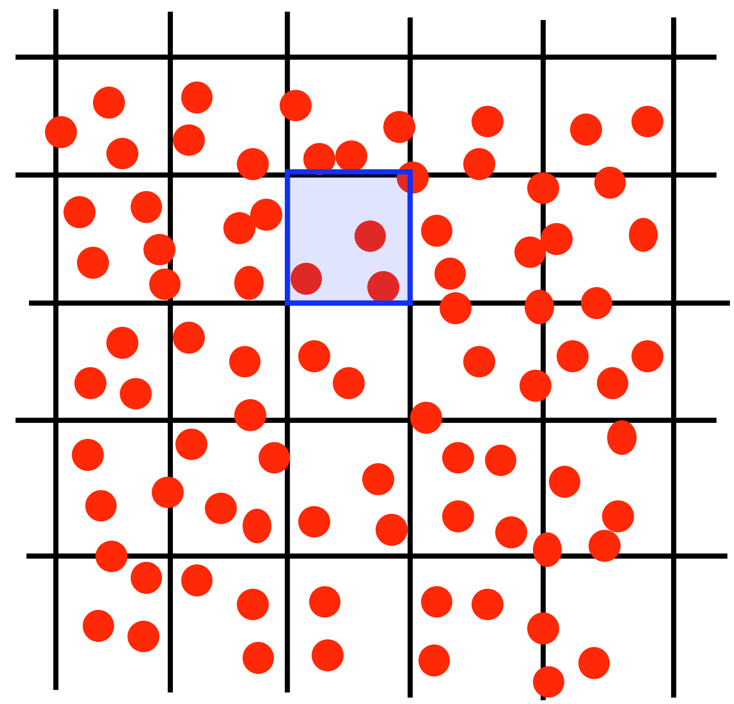
$$\frac{d\gamma_i \mathbf{v}_i}{dt} = \frac{q_i}{\varepsilon_0 m_i} \sum_j q_j \frac{\mathbf{x}_i - \mathbf{x}_j}{\left|\mathbf{x}_i - \mathbf{x}_j\right|^3}$$

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

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

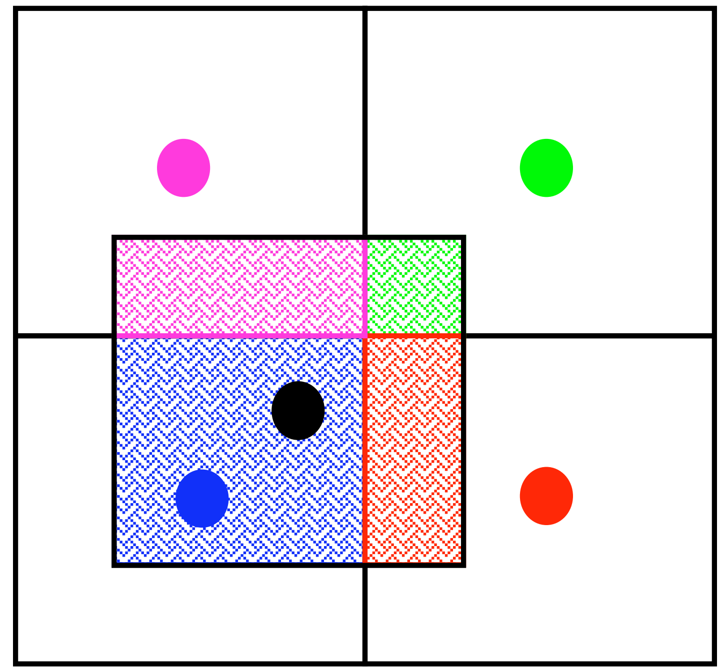
Particle In Cell (PIC) reduces to N_p scaling

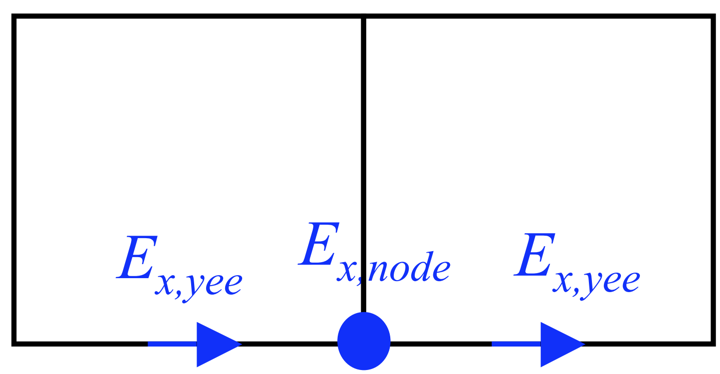
- Particle contributions to charges and currents are added to each cell: $O(N_p)$ operations
- Forces on a particle are found from interpolation of the cell values: $O(N_p)$ operations



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





Efficiency

Avoiding Poisson

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

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

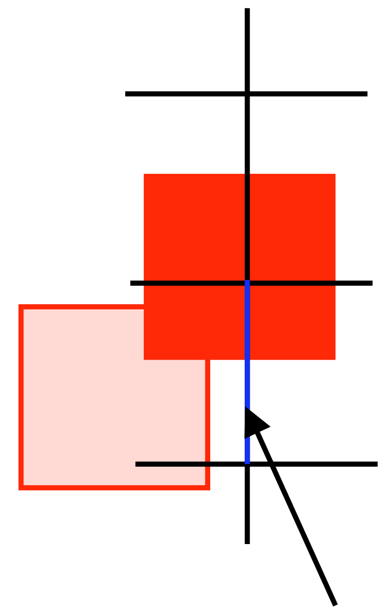
and

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

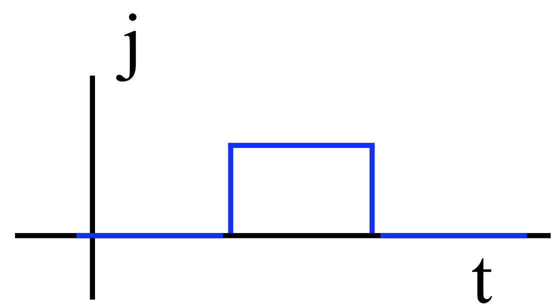
$$\frac{\Delta \rho}{\Delta t} = -\frac{\Delta j_x}{\Delta x} + \frac{\Delta j_y}{\Delta y} + \frac{\Delta j_z}{\Delta z}$$

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

P.J. Mardahl [1], J.P. Verboncoeur

Cory Hall Box 173, Department of Electrical Engineering and Computer Science, University of California, Berkeley, CA 94720-1770, USA

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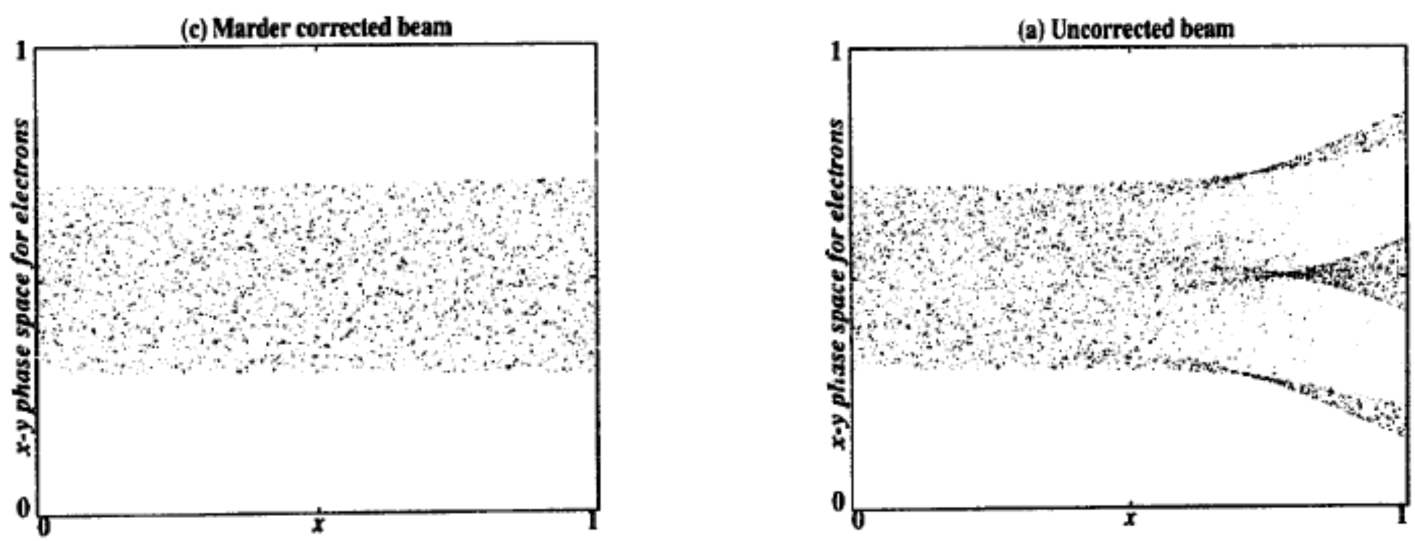
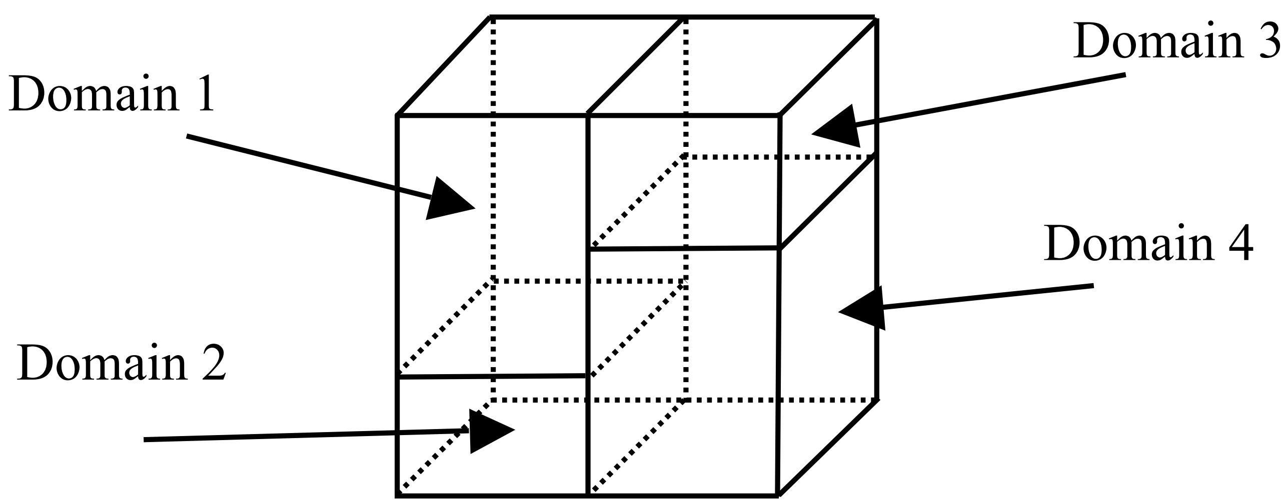


Parallelism: domain decomposition

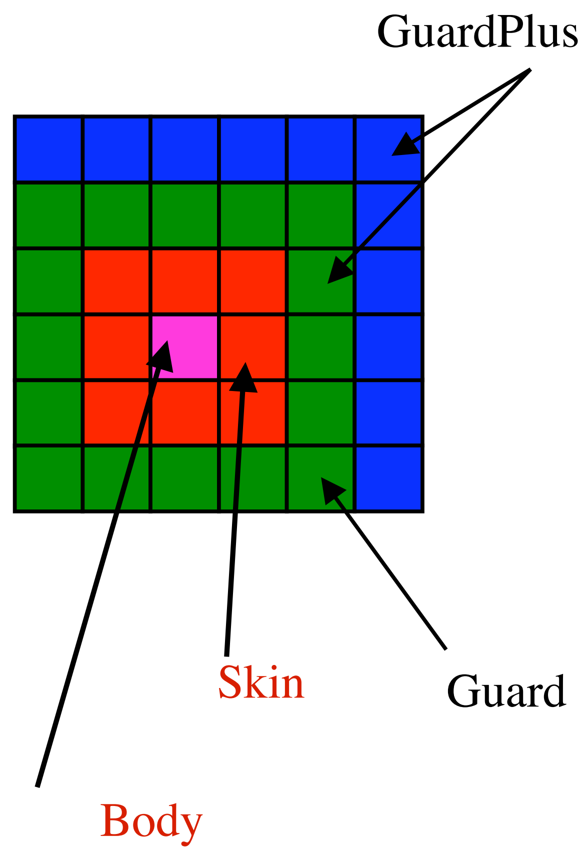


Parallelism rules of thumb

- Communication is expensive
- Global solves are really expensive

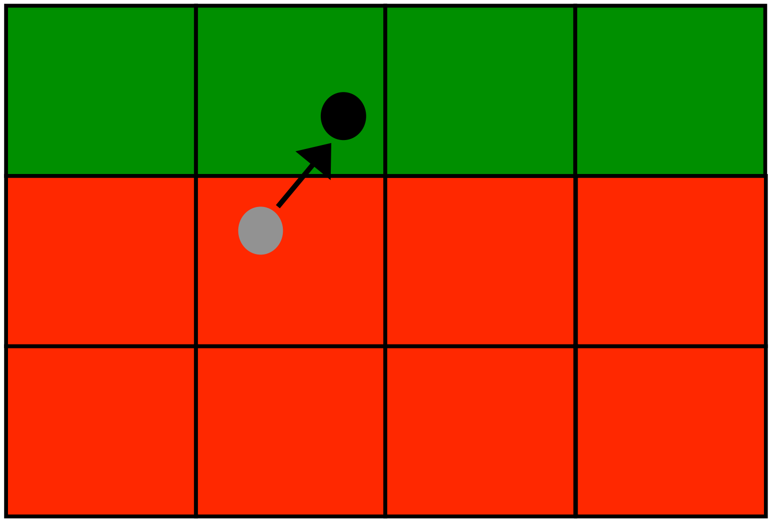
Overlap of communication and computation needed for speed

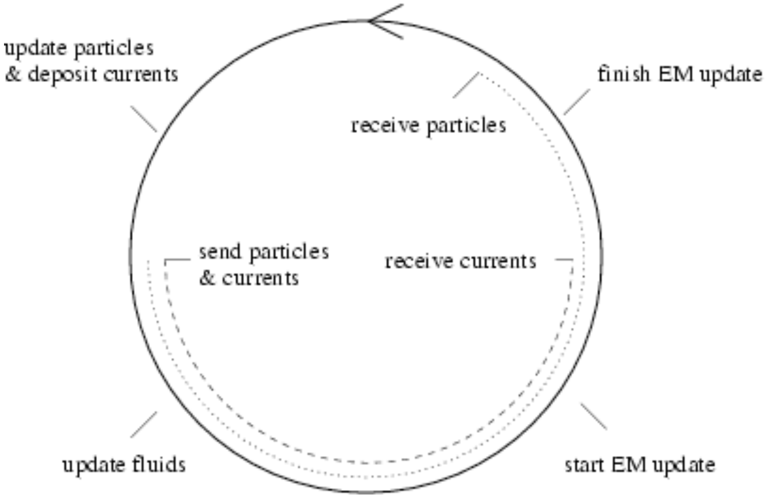
- Non overlap algorithms:
  - Compute domain
  - Send skin (outer edge)
  - Receive guard
  - Repeat
- Overlap algorithms
  - Compute skin
  - Send skin
  - Compute interior
  - Receive guard
  - Repeat



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





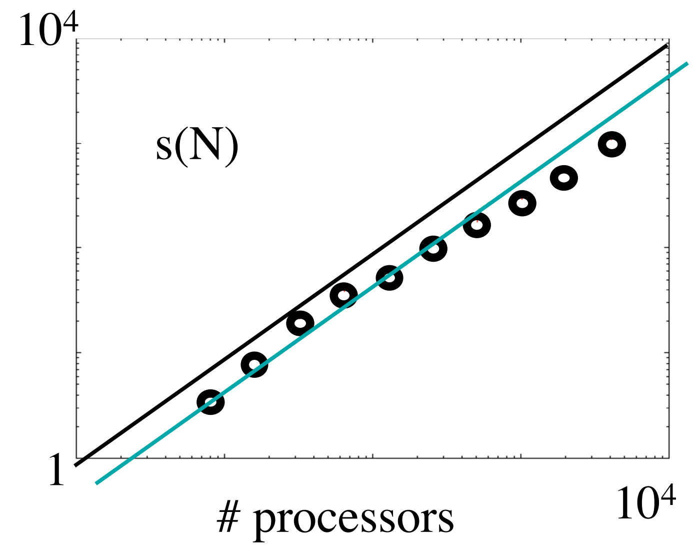
Without charge conserving current deposition, further costly global solve

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)

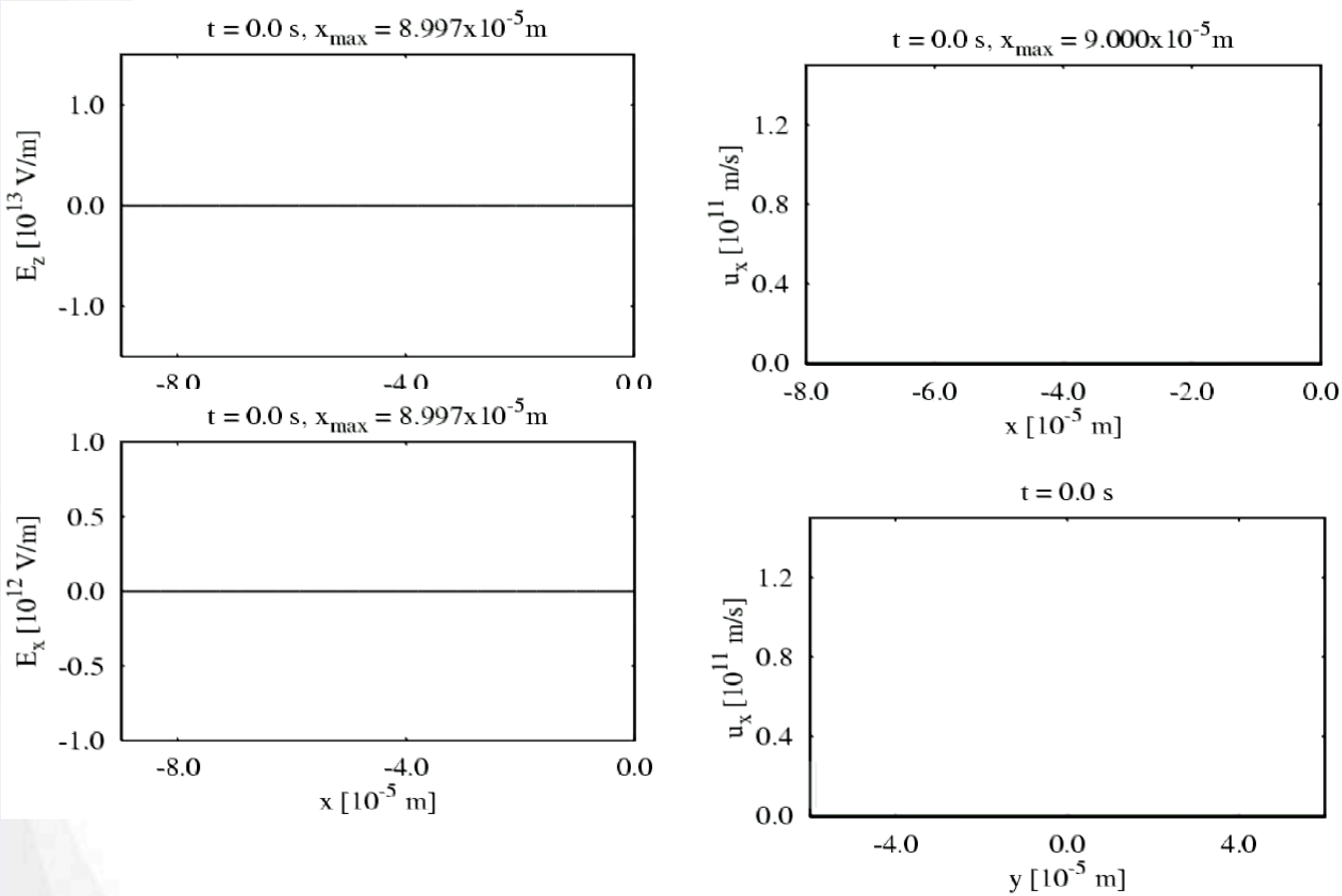


VORPAL scales well to 1,000’s of processors (strong scaling)

Simplest algorithm allows complex computations

- Example: formation of beams in laser-plasma interaction

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

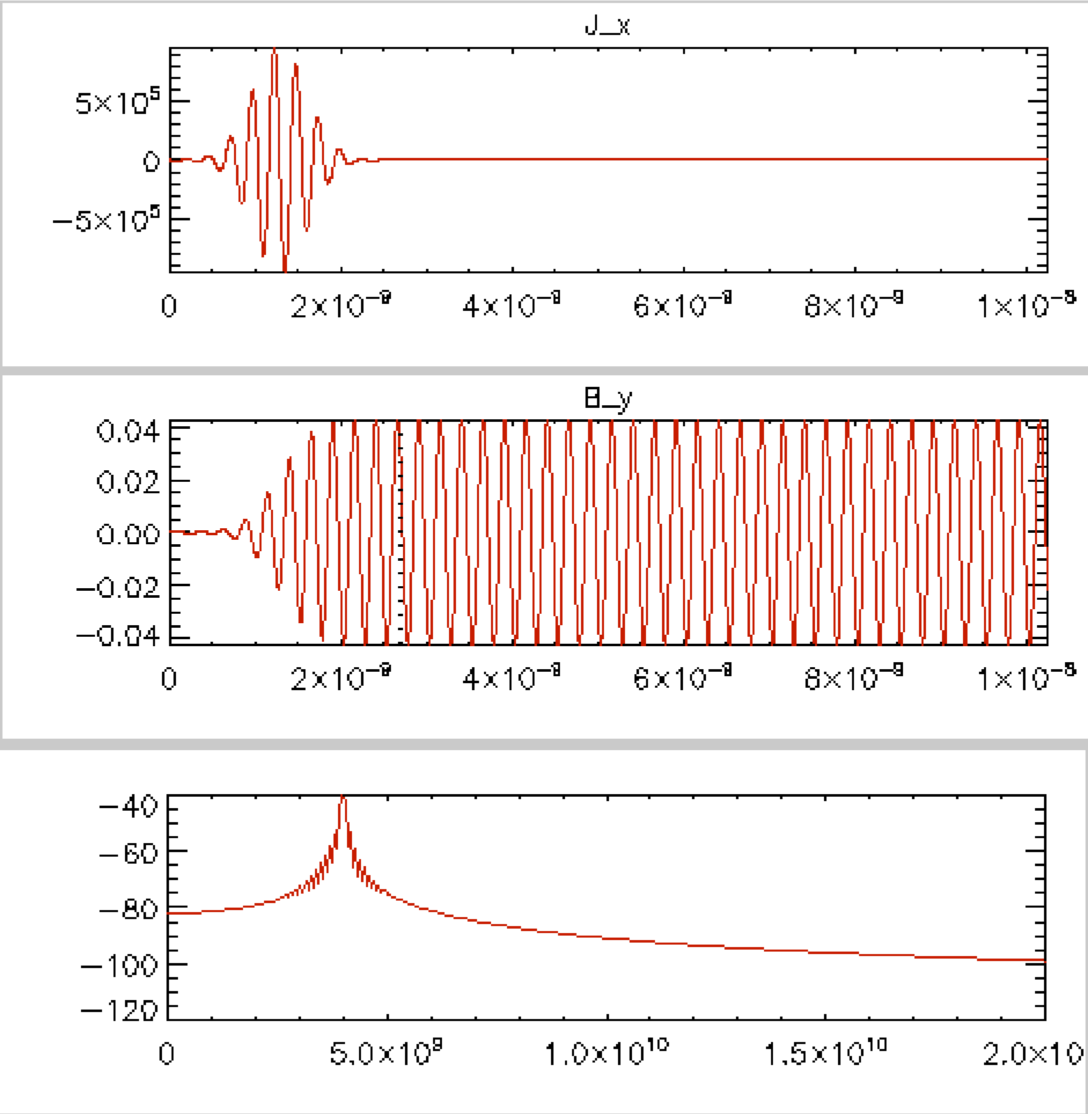


Simulations have found the hosing problem

Complications: boundaries

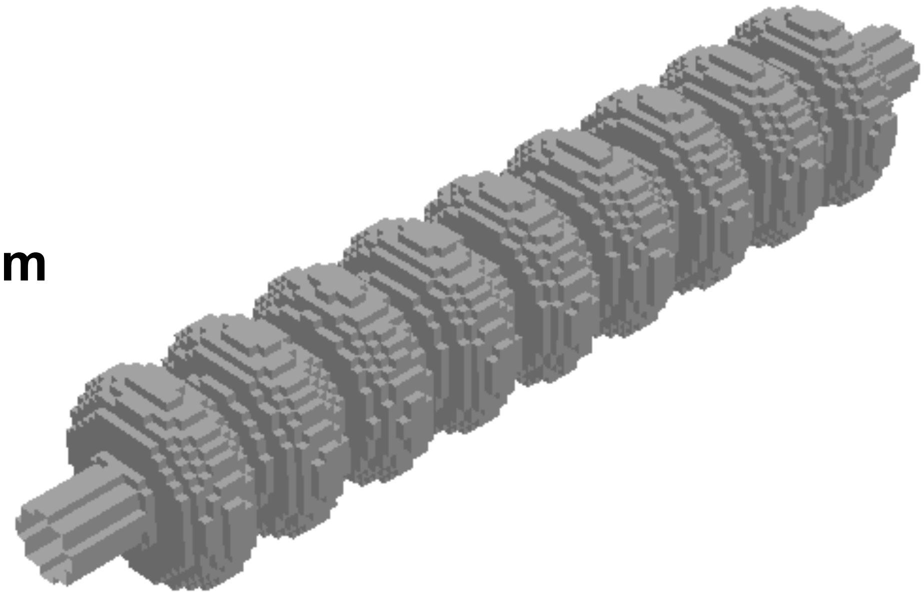
Modes computed with combination of FFT and fitting

- Spherical cavity
- Resonant current driver
- FFT measurement of frequency, for accuracy by fitting



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

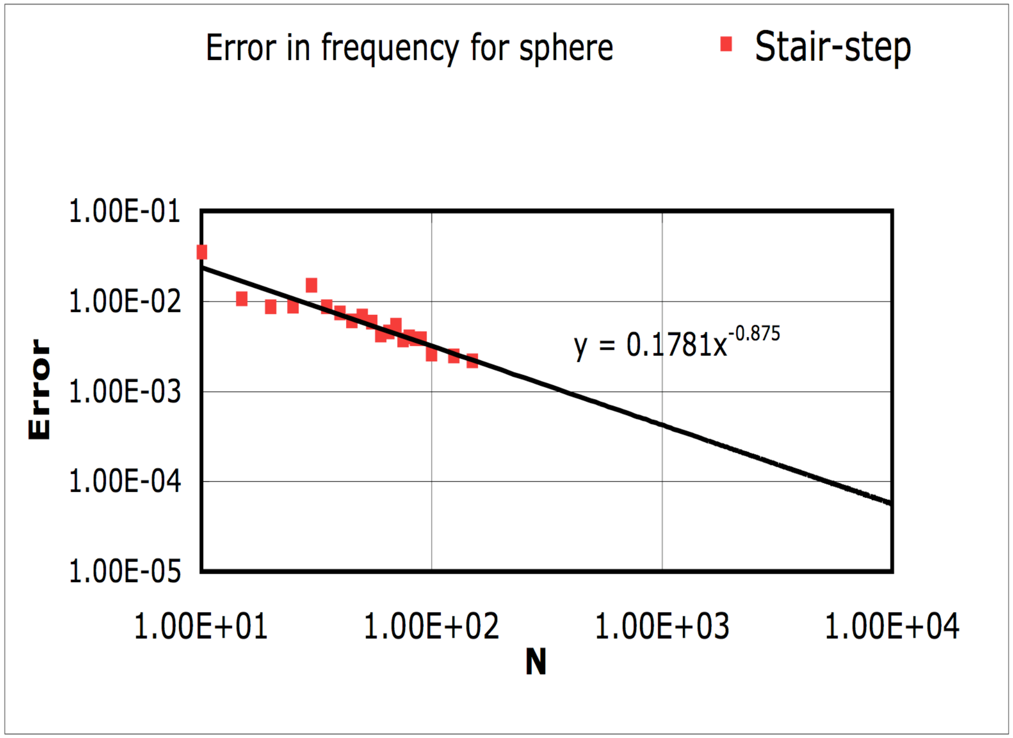
120x24x24 = 71,424 cells
= 215,000 degrees of freedom



- 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 = $N^2(\Delta x/L)^3 = O(1/N)$

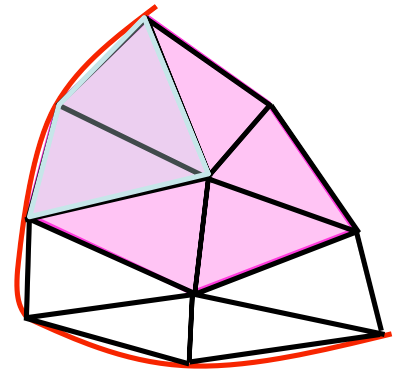
Convergence studies confirm result, indicate modeling problem

- Stair-step error is 10^{-3} at 5000 cells per dimension, error linear with cell size
- 10^{11} 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

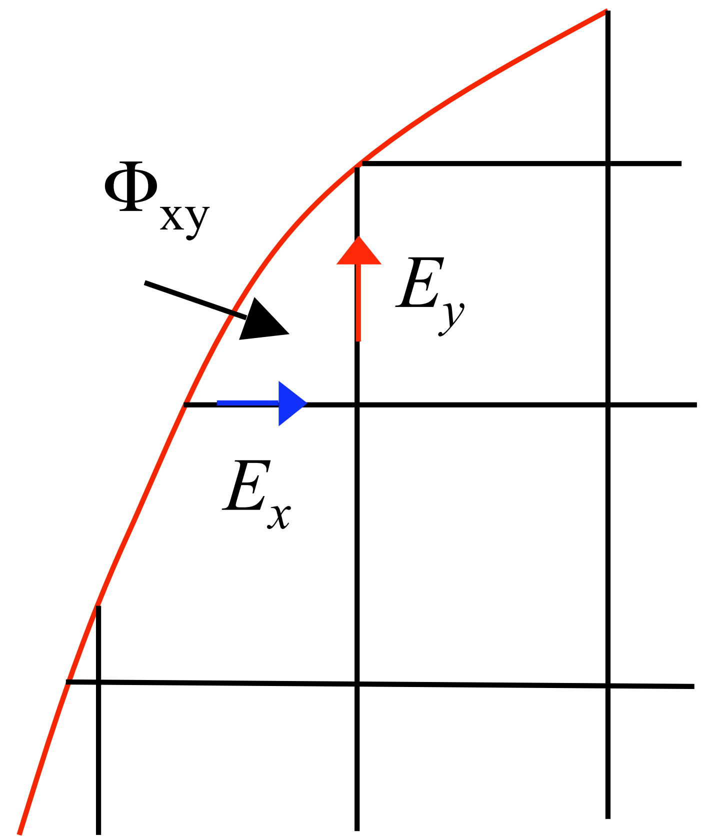
Resurgence of regular grids: cut cells give same accuracy as finite elements

- For cells fully interior, us regular update
- For boundary cells:
  - Store areas and lengths
  - Update fluxes via

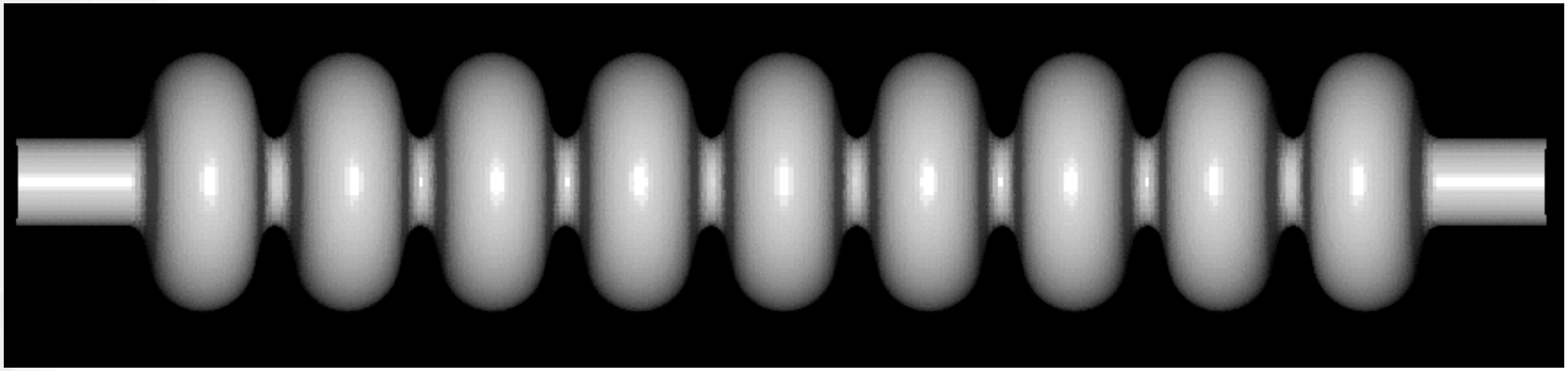
    $$\dot{\Phi}_{xy} = -E_x \ell_x - E_y \ell_y$$

  - Update fields via

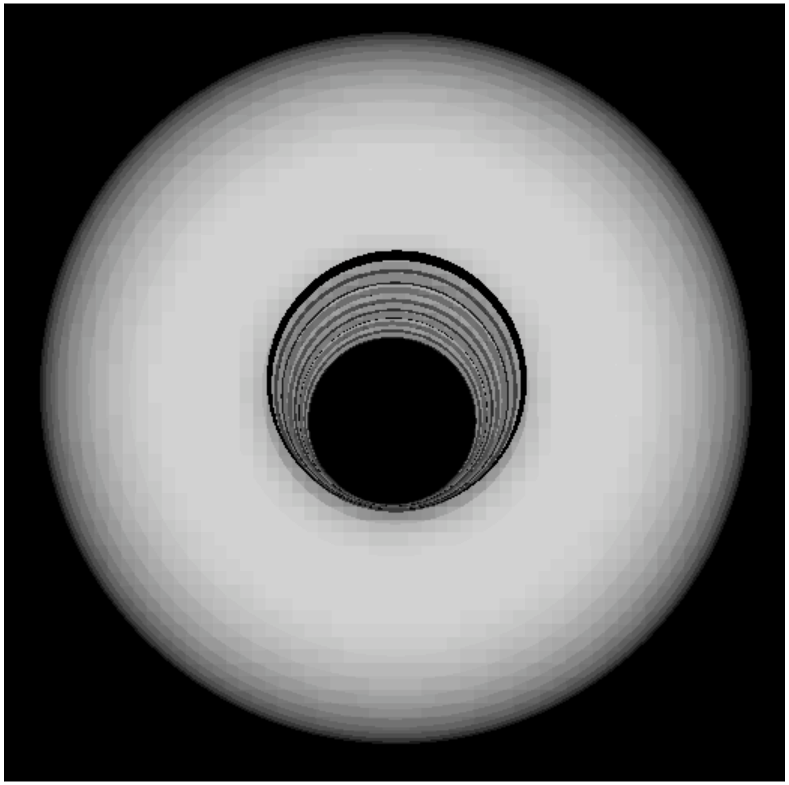
    $$B_z = \Phi_{xy} / A_{xy}$$



Cut-cell boundary conditions accurately represent geometry

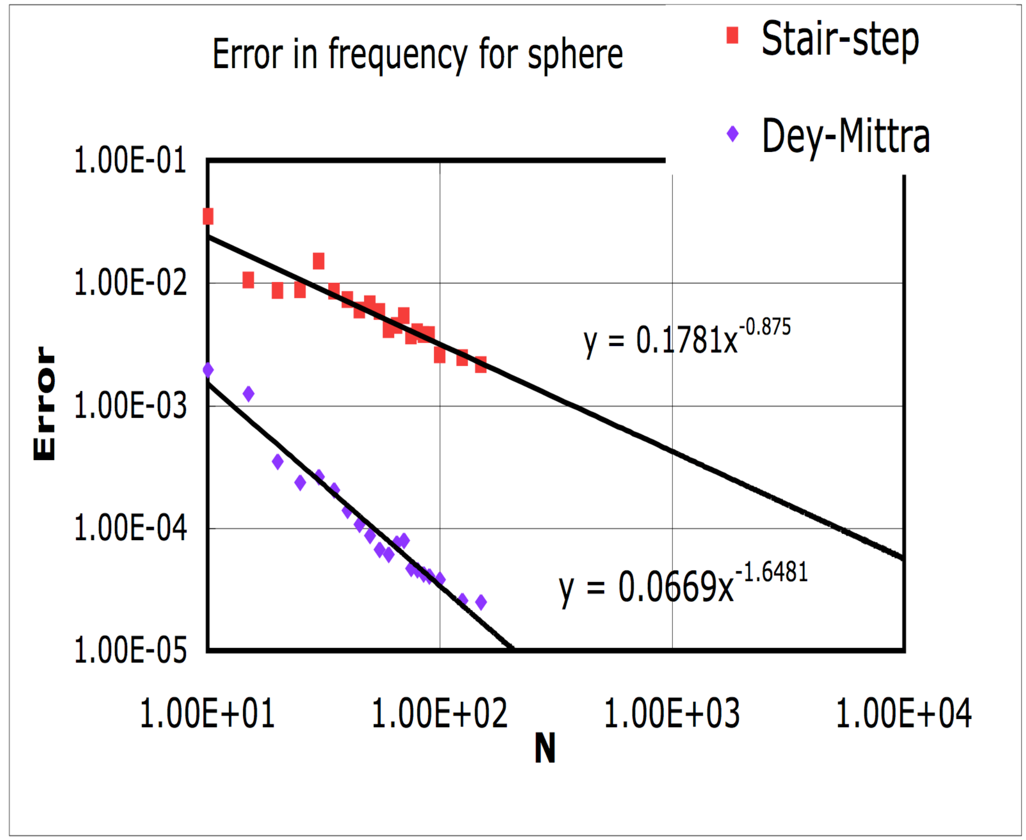


- Tesla 2000 cavities
- 312x56x56 (10^6) cells



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

- Fewer than 10^7 cells for cavity modeling at one part in 10^5
- Implementation exists now in VORPAL
- No significant additional computational cost



Beam problems provide motivation for further work

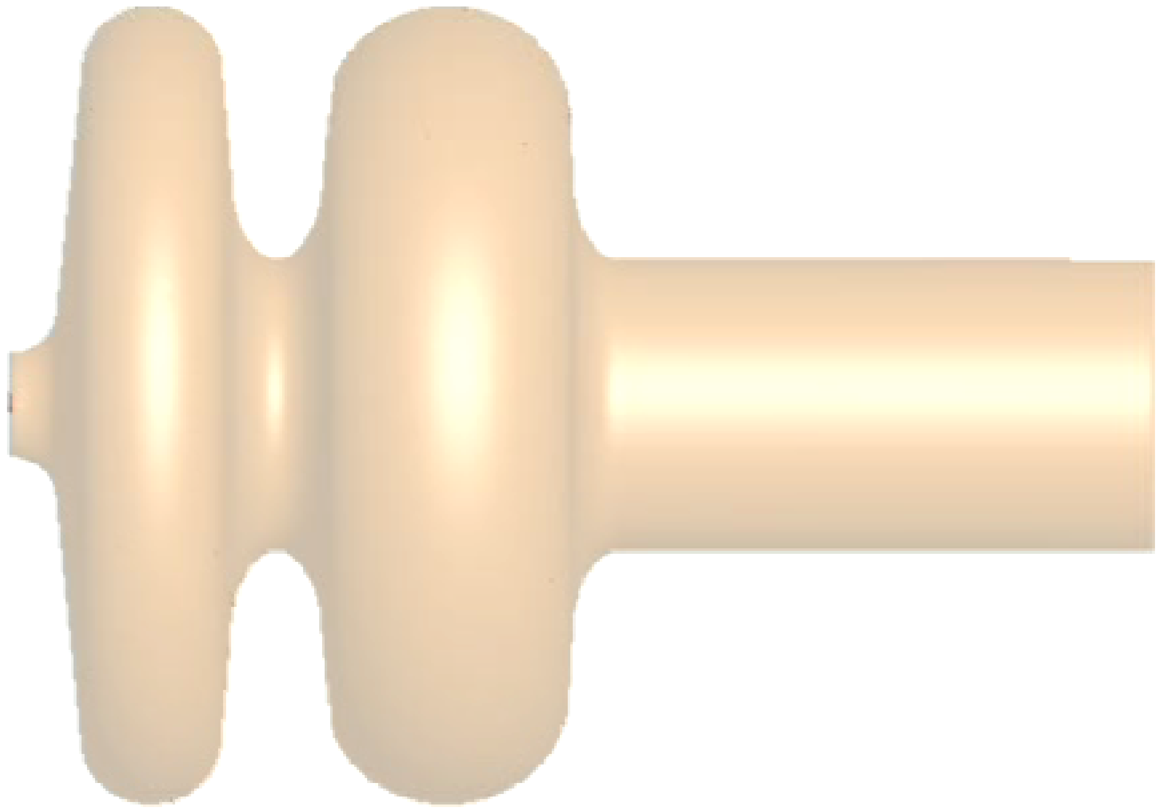
- SRF accelerating cavities
- SRF guns
- Crab cavities

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

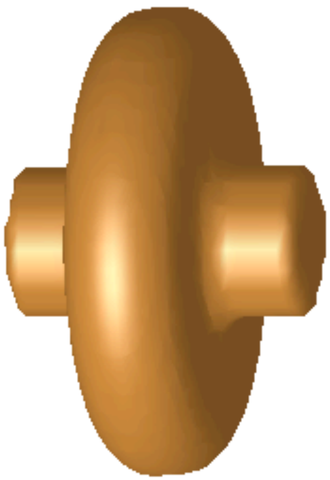
Wakefield for Tesla cavities computed by VORPAL in 3D

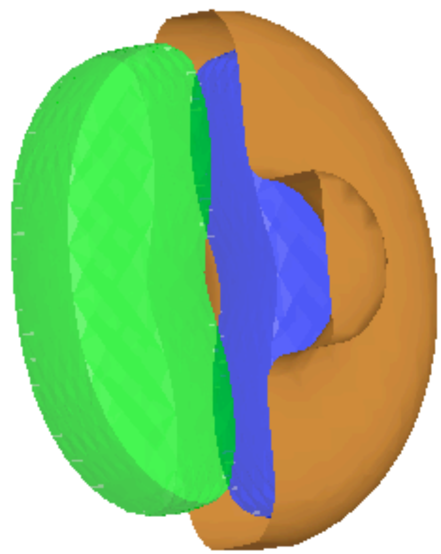
Self-consistent EM gun simulations in complex cavities

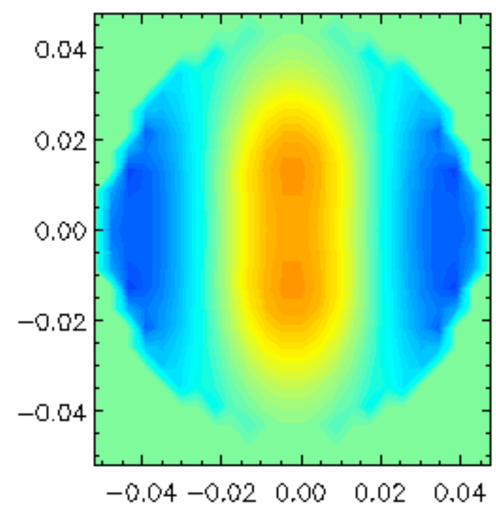
- Emitted beam
- Wakes from constrictions



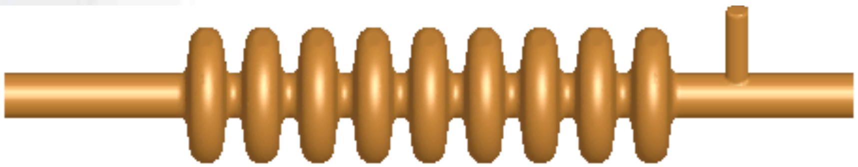
Now simulating dipole modes in symmetric cavities

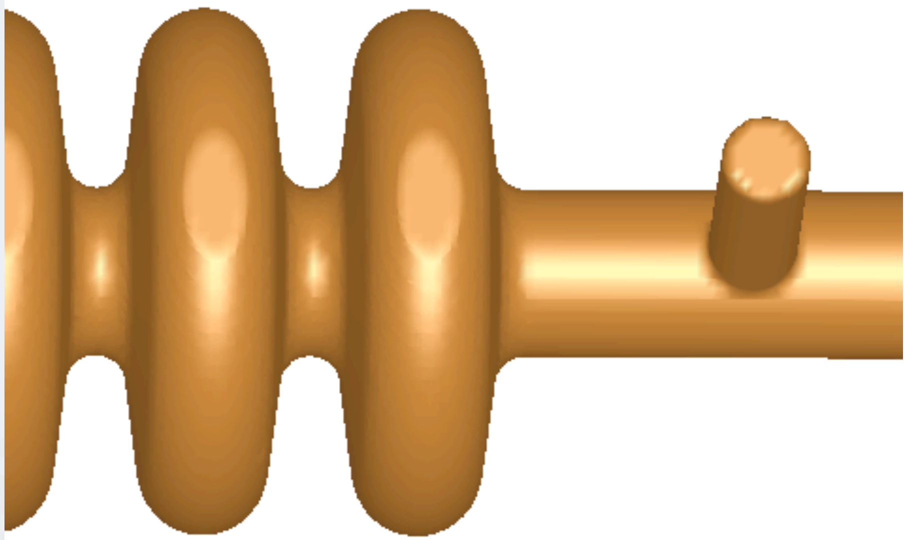


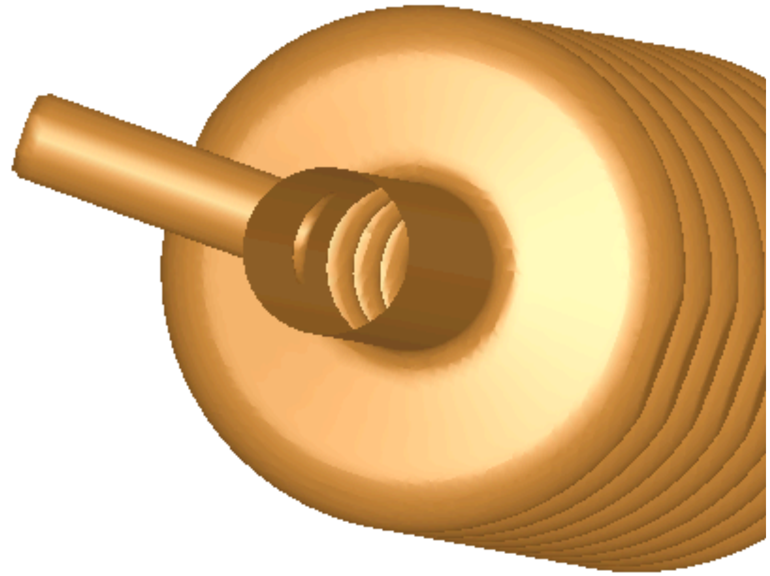




Crab cavity generation, visualization, computation of splitting



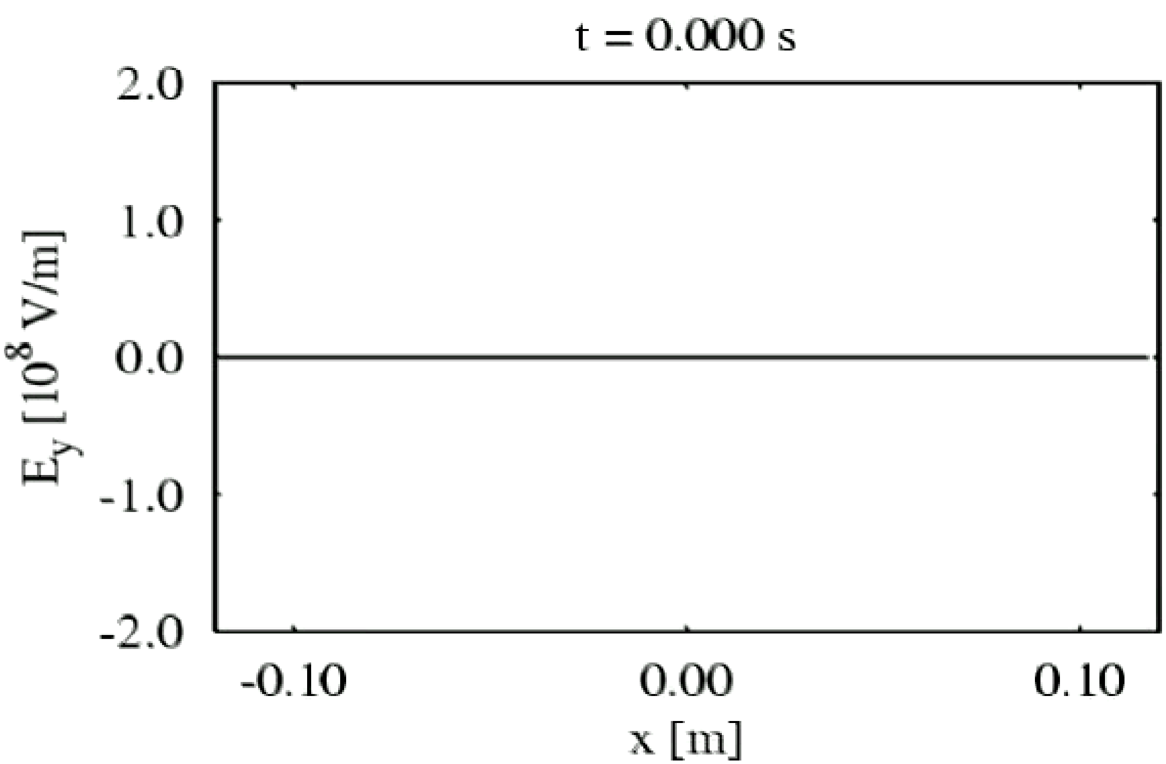




- CAD representations
- Python coding of shapes

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

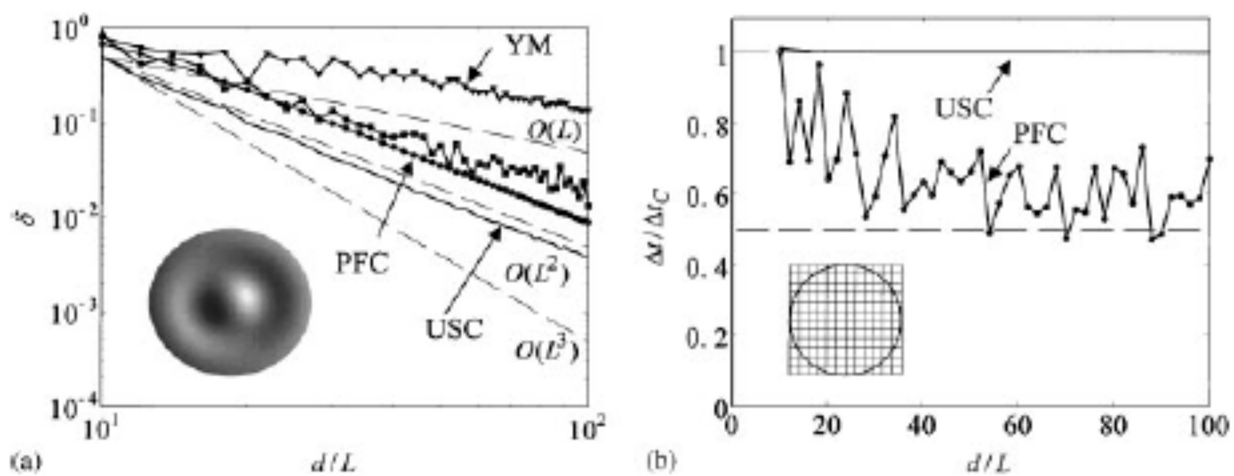


Improvement on cut-cell recently discovered

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

Each new study inspires capability, brings requests

- Laser-plasma: self-consistency, parallelism
  - Higher-order particle shapes
- Accelerating cavities: shape modeling
  - Higher-order field to particle near walls
  - Resistive walls for complex shapes
  - Implicit EM solvers
- Electron guns
  - Better emission models
- Crab cavities
  - Notch filters, LOM couplers

Summary

- Self-consistent EM modeling has progressed
  - High-performance, self-consistent computations
  - Accurate treatment of boundaries
  - Secondary emission
  - Absolutely stable charge-conserving algorithm
- Remain algorithm needs
  - Conformal resistive walls
- Remain implementation needs
  - Surface resistance
  - Dark currents
  - Photonic emission
  - Absolutely stable charge-conserving algorithm
- Remains work in simulation setup
  - Defines cavity shapes
  - Define particle beams