High-Performance Self-Consistent Electromagnetic Modeling of Beams

John R. Cary

University of Colorado and Tech-X Corporation

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thanks to the

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New era of computational beam modeling

- Traditional accelerator physics modeling
  - Strong inhomogeneity (strong focusing, cavities, multipactoring)
  - Approximate approaches to self consistency (none, beam-frame electrostatics, beam-beam kicks)
- Traditional plasma modeling
  - Strong self-fields (LWFA, PWFA)
  - Boundaries distant
- New modeling developments combine these capabilities to bring self-consistent modeling of beams in the presence of complex structures.

Parallel computation is making more detailed computations possible

Progression of modeling

Test particles in structures (tracking, multipactoring)

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Wake fields in structures

↓

Beam-frame electrostatics (no structures)

↓

Self-consistent, fully EM in structures

Advances in hardware

↓

Parallel computations

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Accurate parallel algorithms

Basic problem is charged particles moving self-consistently in EM fields

Auxiliary equations

- Maxwell

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

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

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

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

- Particles drive EM

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

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

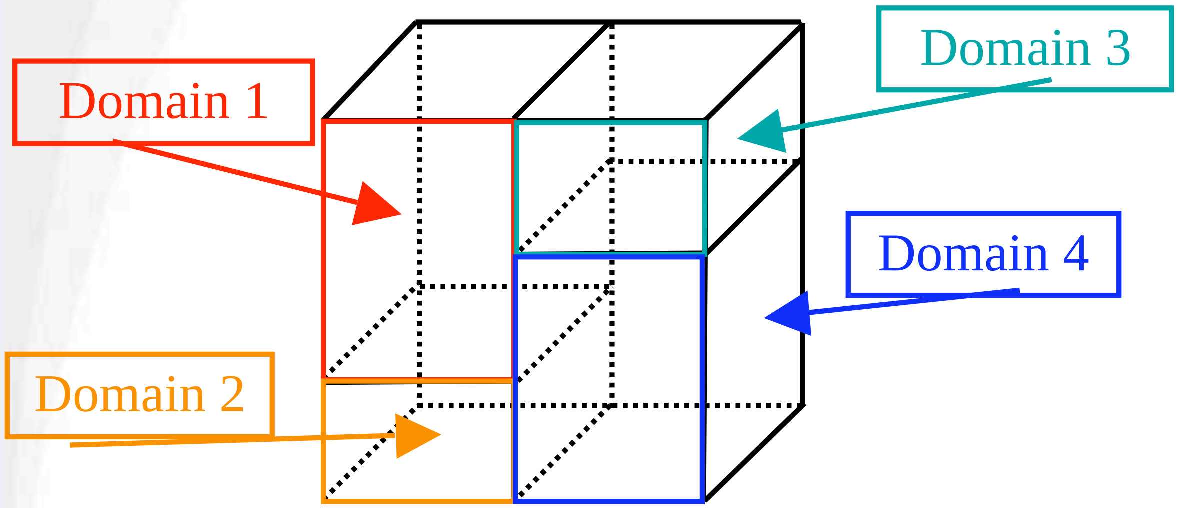
- Particle dynamics from EM

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

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

plus other physics (later)

Parallelism: divide computational responsibilities



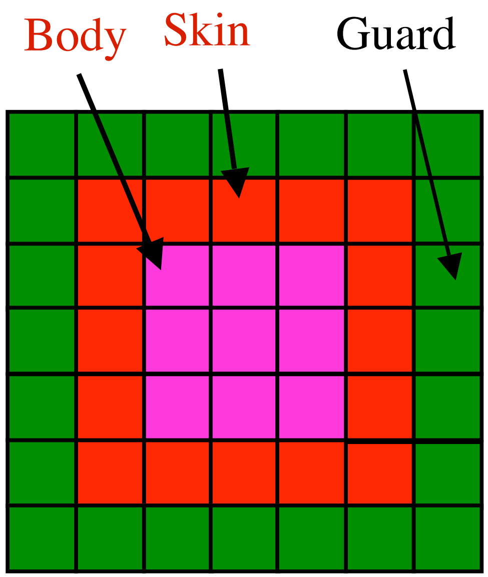
Domain decomposition

Each processor computes fields in one spatial domain
Fastest are LOCAL algorithms, where only boundary information is communicated

- Communication is expensive
- Global communication is really expensive (Poisson solves, global matrix inversion, …)

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 body
  - Receive guard
  - Repeat



<u>Overlap algorithms increase complexity</u>
(threading, asynchronicity, without memory walls, …)
<u>but increase speed</u>
(no loss down to some domain size)

Finite-difference time-domain, particle-in-cell works well for parallel computing

- Simple, second-order accuracy sufficient for beam computations
- Higher-order available when needed
- Naturally includes particles
  - Phase space dynamics
  - Mixing
- LOCAL

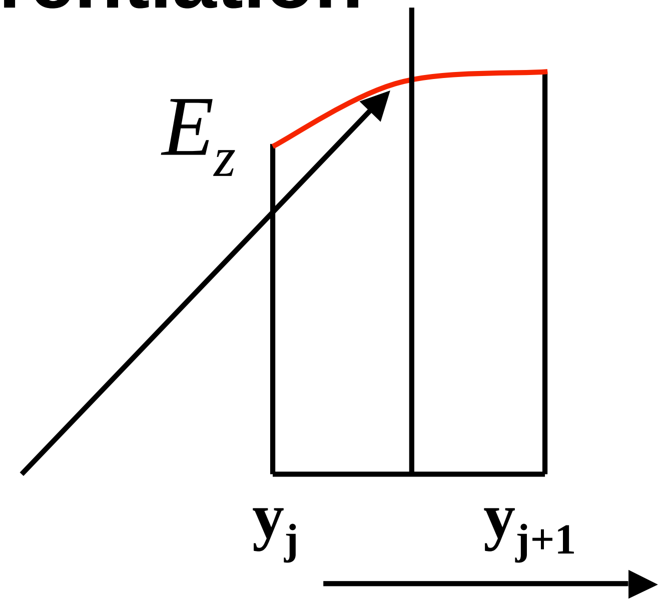
Yee: 2nd order accurate spatial differentiation

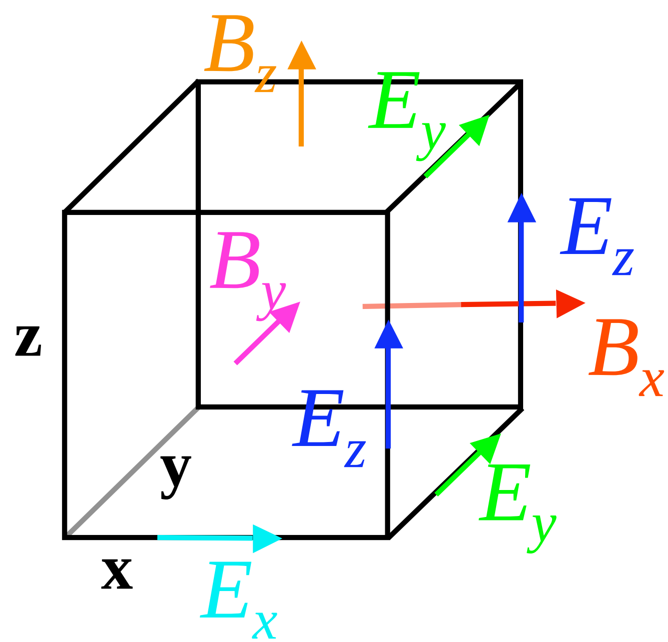
$$\frac{\partial B_x}{\partial t} = -\frac{\partial E_z}{\partial y} + \frac{\partial E_y}{\partial z}$$

- At the midpoint

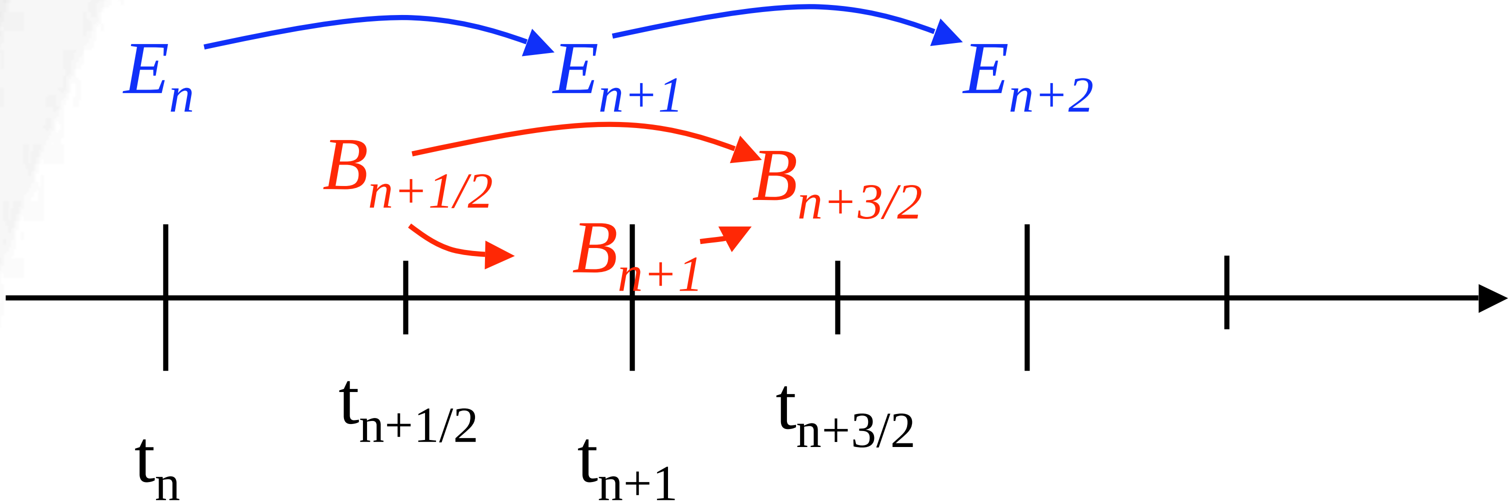
$$\frac{\partial E_z}{\partial y} = \frac{E_{z,j+1} - E_{z,j}}{\Delta y} + O(\Delta y^2)$$

- 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



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

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

- 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
- LOCAL

Computing particle-particle interactions is prohibitive

- Coulomb interaction leads to N_p^2 force computations

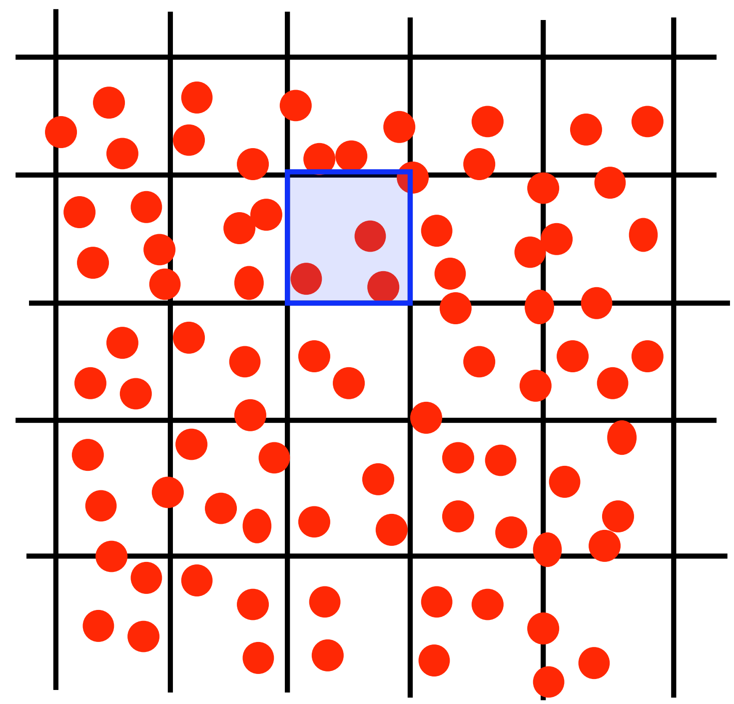
$$\frac{d\gamma_i \mathbf{v}_i}{dt} = \frac{q_i}{\varepsilon_0 m_i} \sum_j q_j \frac{\mathbf{x}_i - \mathbf{x}_j}{\left|\mathbf{x}_i - \mathbf{x}_j\right|^3}$$

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

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

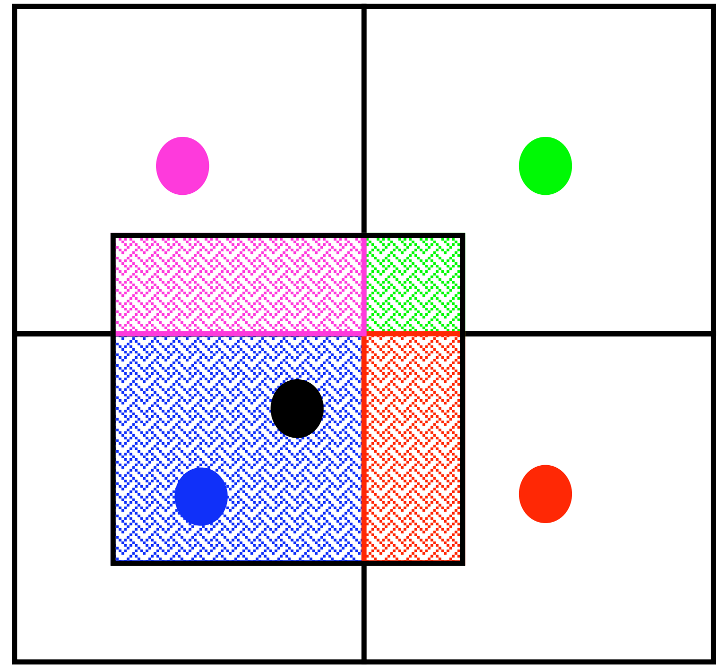
Particle In Cell (PIC) reduces to N_p scaling

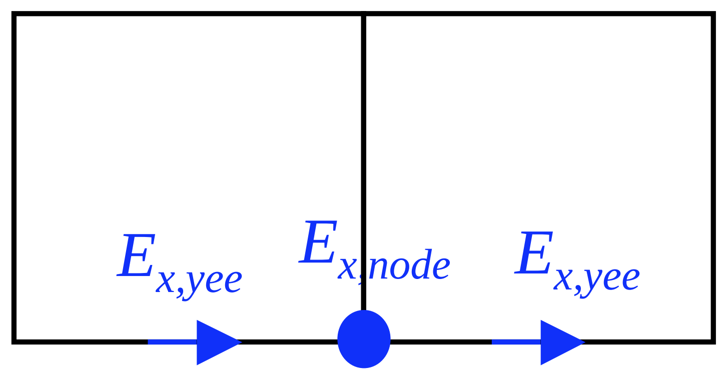
- Particle contributions to charges and currents are added to each cell: $O(N_p)$ operations
- Forces on a particle are found from interpolation of the cell values: $O(N_p)$ operations



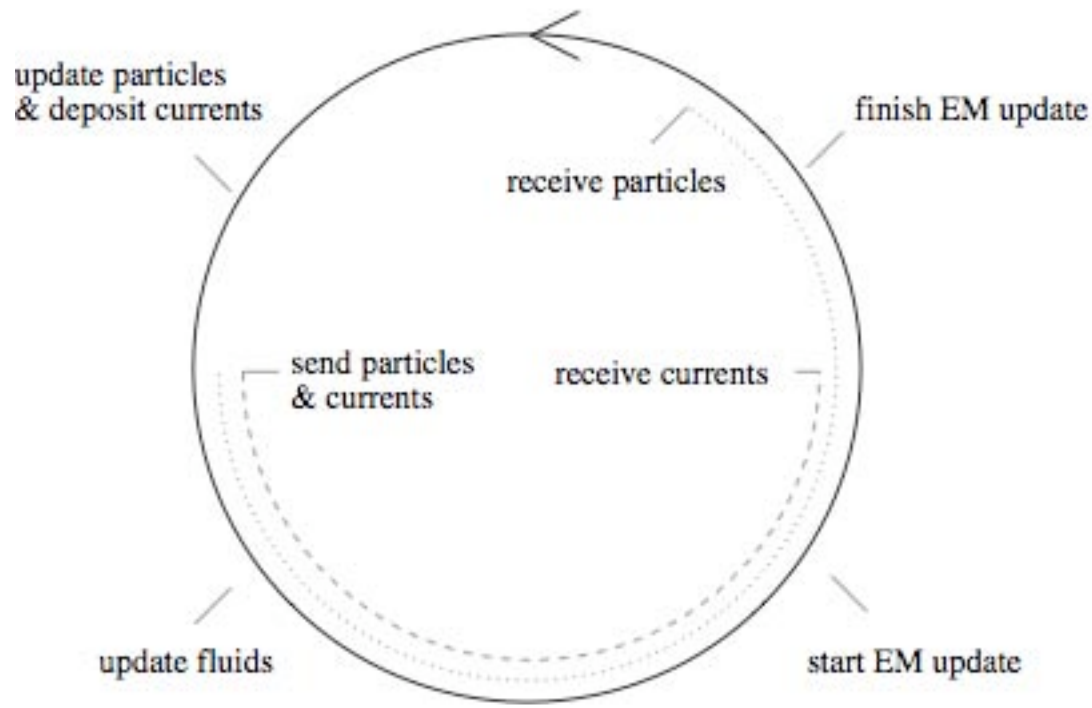
Finding the force: interpolation (gather)

- 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
- LOCAL





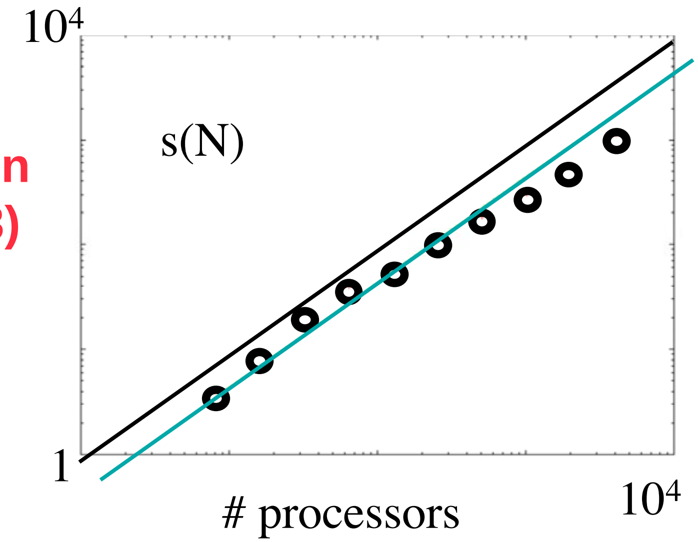
Important to overlap communication and computation



- Break EM update into two parts
- Do current-free part prior to reception of particle currents
- Do remainder after

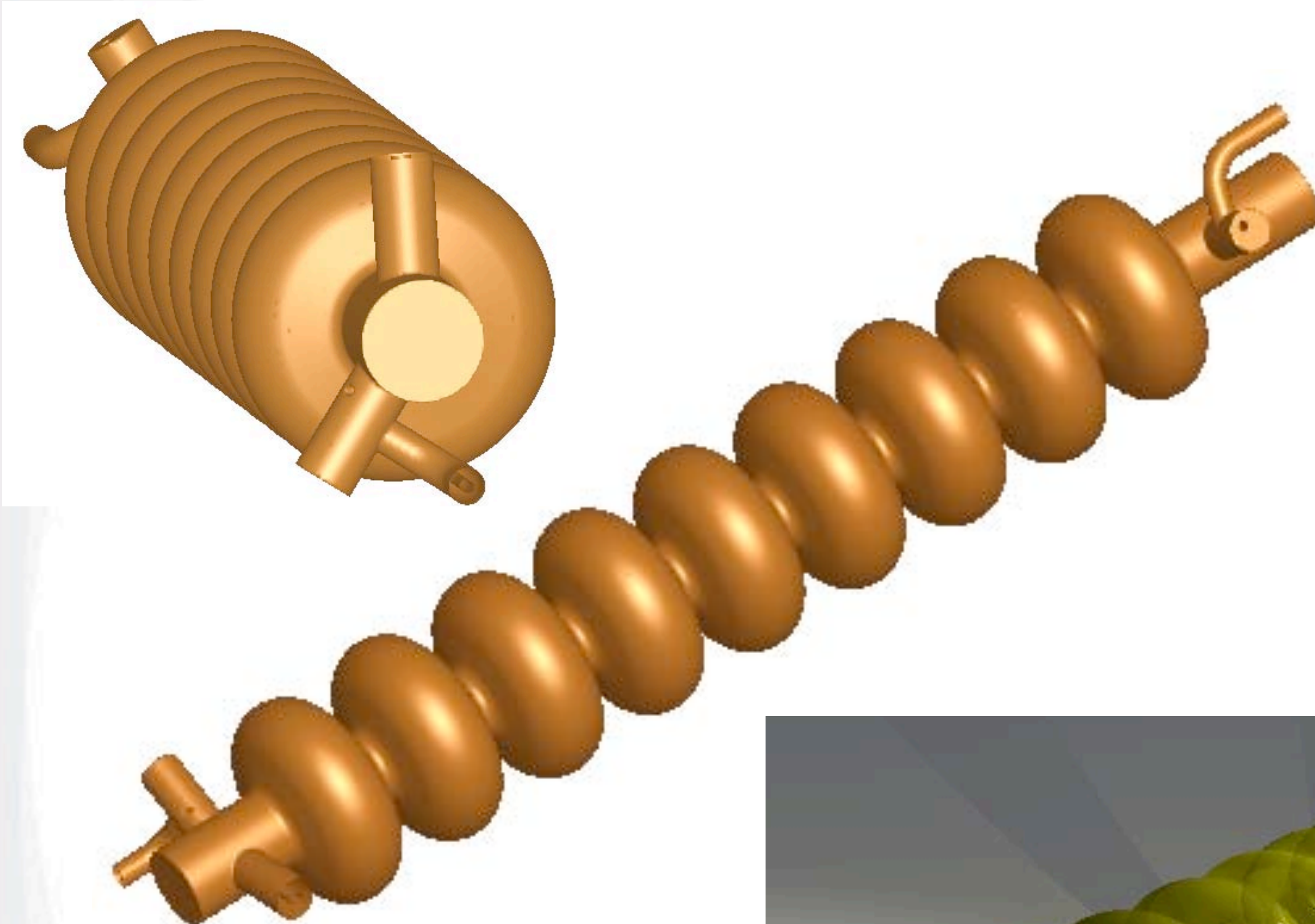
Local update algorithms scale very well to large numbers of processors

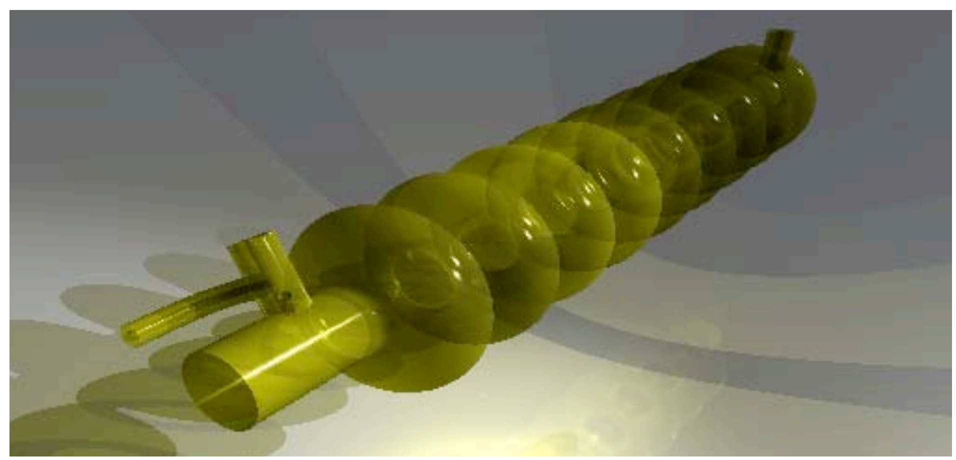
VORPAL scaling on Seaborg (IBM SP3)



- Strong scaling, 10,000x400 continually subdivided
- Similar behavior on 1,500x300x300
  - (135M cells, 0.5 B particles)
- Resolution of sub-micron (laser)
- Propagation to 1 mm (20,000 steps) in 30-40 hours with 2000 POWER III or 400 POWER V.
- Parallelism depends on surface to volume ratio
- All computations for recent LWFA were of this type
- 2×10^{13} particle-time-steps or 10^{14} cell-time-steps (no particles) routine

Boundaries lead to increasingly complex modeling



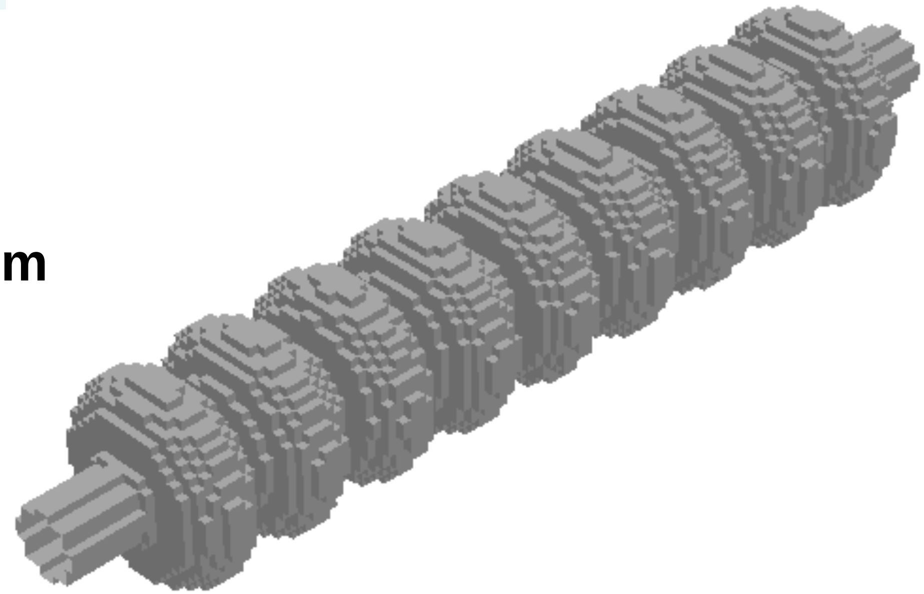


How can we apply ***massive*** computation to complex shapes?

- Local algorithms (no Poisson solves, no global matrix inversions)
- Accurate for complex shapes

Early, *stair-step* boundary conditions gave unacceptable computational errors

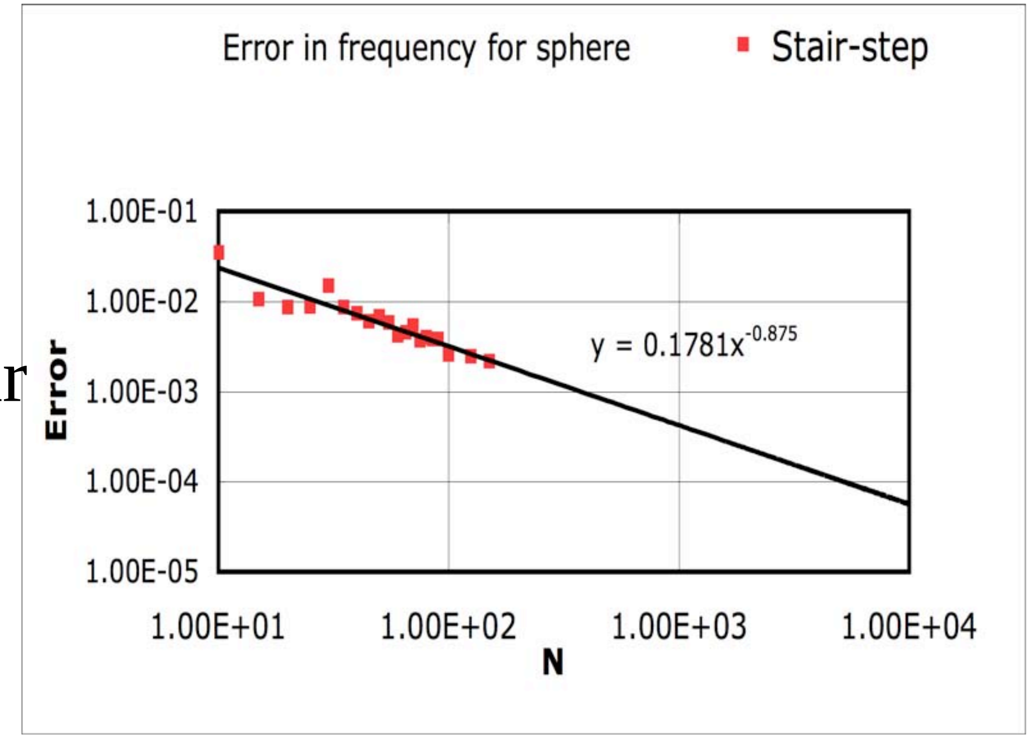
120x24x24 = 71,424 cells
= 215,000 degrees of freedom



- 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^{-4} 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

Resurgence of regular grids: cut cells at surface retain accuracy of volume

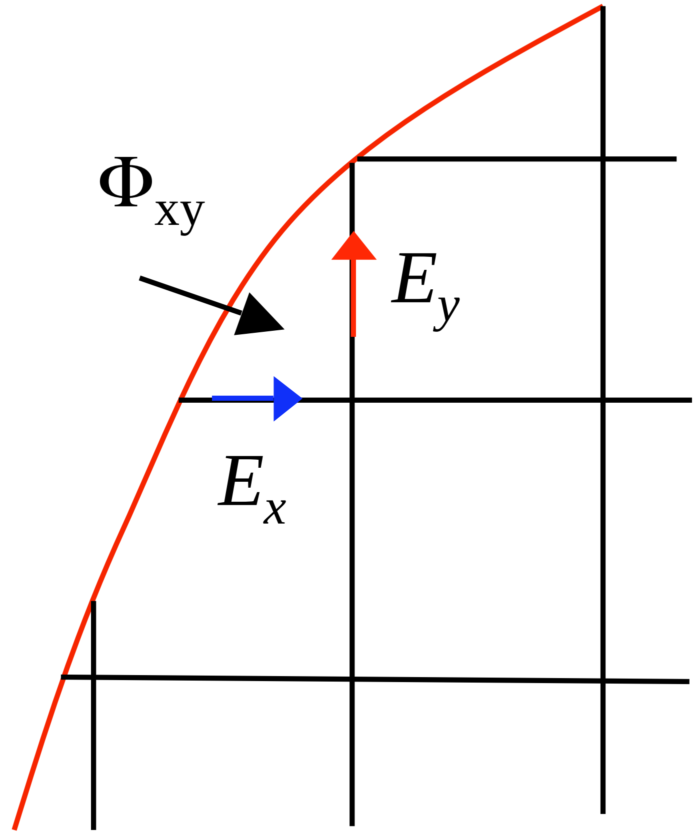
- For cells fully interior, use regular update
- For boundary cells:
  - Store areas and lengths
  - Update fluxes via

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

  - Update fields via

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

- Dey-Mittra
- Gustafson



Dey-Mittra has some reduction of stable time step

- Spatial discretization takes continuum equations to coupled linear ODEs. One vector component for each cell face.
- Temporal discretization (leap frog) - time step limited by maximum eigenvalue
- Gershgoren theorem estimates maximum eigenvalue
- Ignore cells that are too small

Guaranteed stability

$$-\frac{\partial^2 B}{\partial t^2} = c^2 \nabla \times \nabla \times B$$

$$-\frac{\partial^2 V}{\partial t^2} = M \bullet V$$

$$\max eigenvalue(M)\Delta t^2 < 4$$

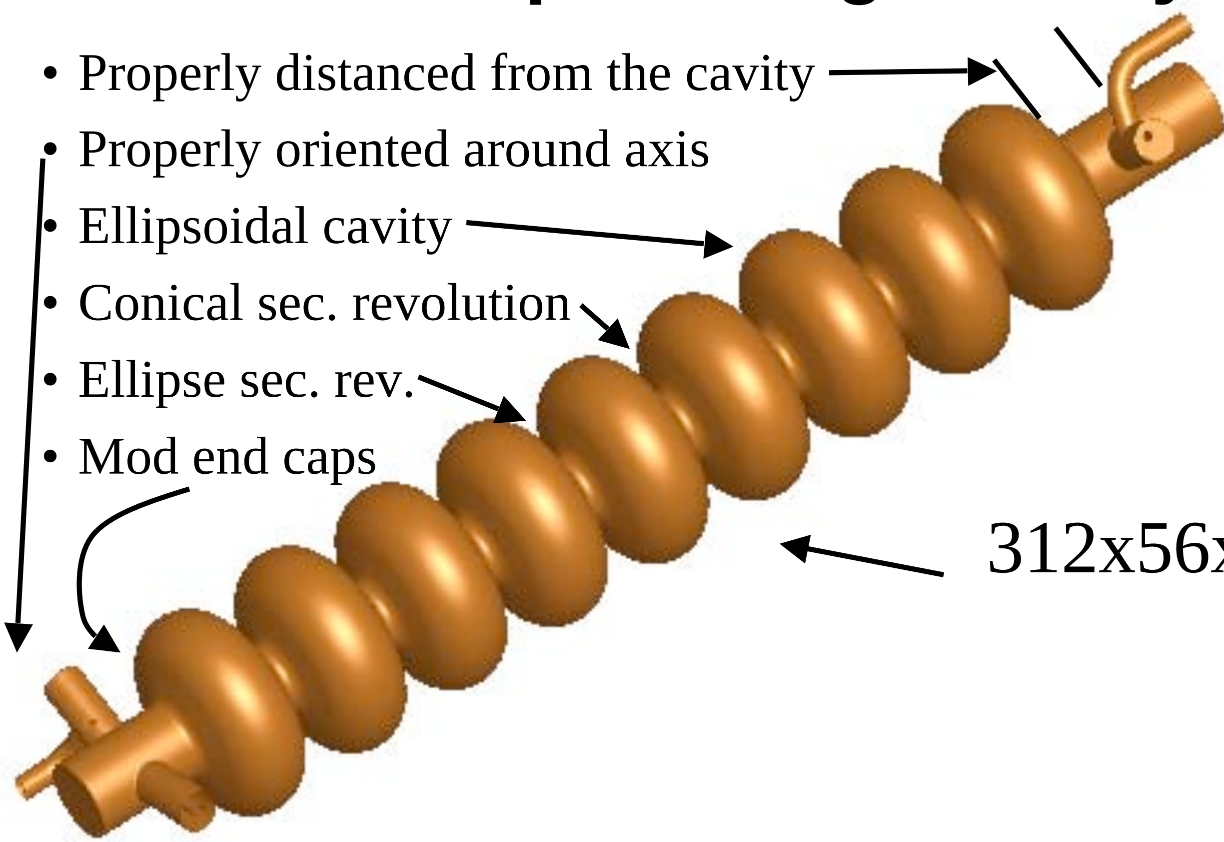
$$\lambda < \max_i \sum_j \left| M_{i,j} \right|$$

$$\Delta t = f_{DM} \Delta t_{CFL}$$

$$keep \sum_j \left| M_{i,j} \right| f_{DM}^2 \Delta t_{CFL}^2 < 1$$

Cut-cell boundary conditions accurately represent geometry

- Properly distanced from the cavity
- Properly oriented around axis
- Ellipsoidal cavity
- Conical sec. revolution
- Ellipse sec. rev.
- Mod end caps



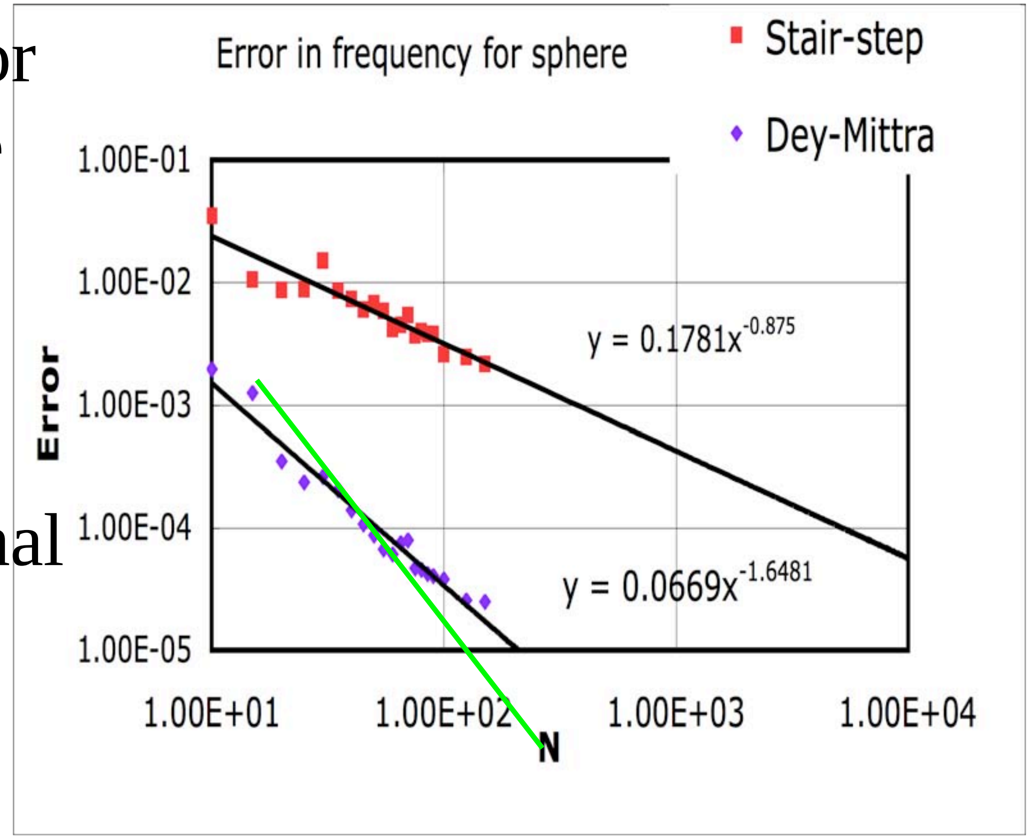
312x56x56 cells

<u>Rapid meshing</u>

- Parallelizes well, since only boundary cells computed
- < 2 m on 16 proc

Dey-Mittra (1997) cut-cells provide 10^{-5} accuracy

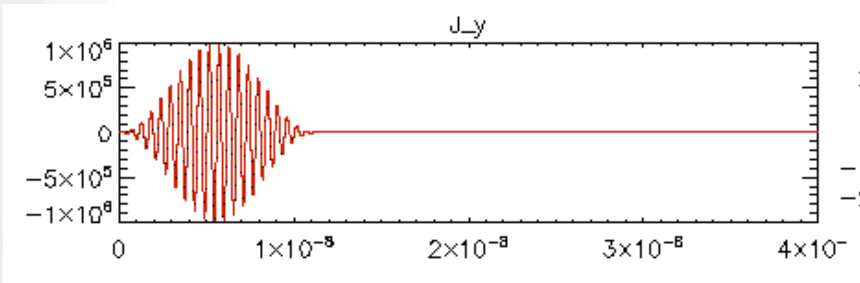
- Fewer than 10^7 cells for cavity modeling at one part in 10^5
- Implementation exists now in VORPAL
- No significant additional computational cost

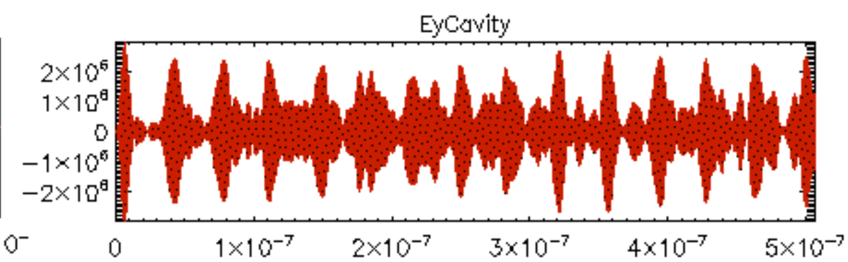


Richardson extrapolation does even better, 10^{-5} accuracy with 60 cells across (for self-similar meshes)

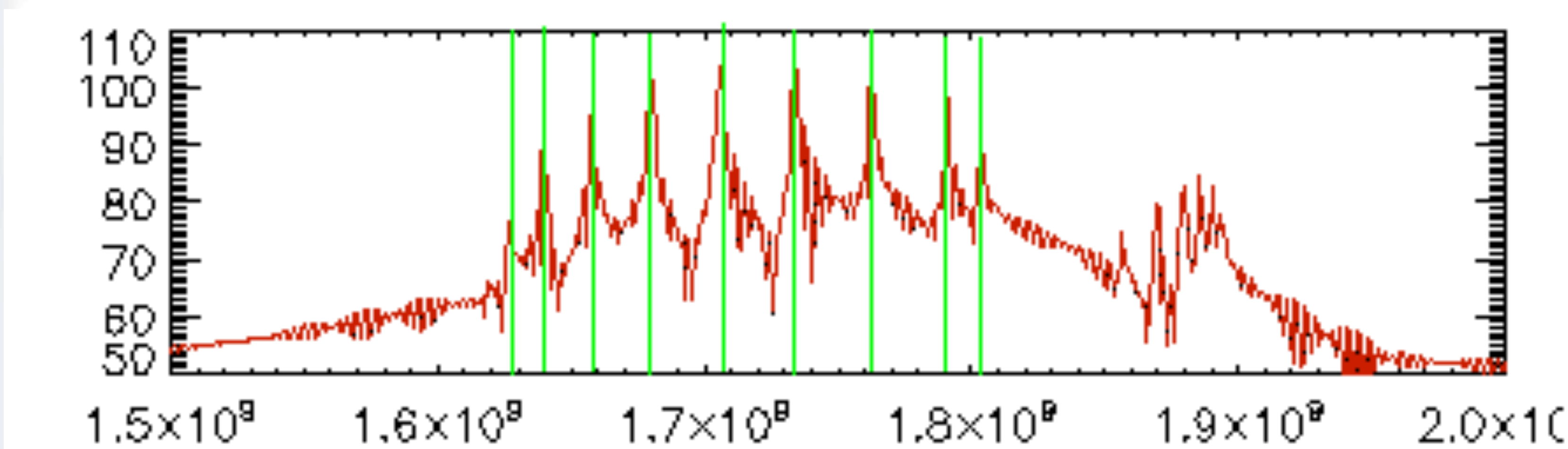
Obtain all modes through broad band excitation of end cell

- Wide-band TE excitation of end cavity leads to all modes being generated.



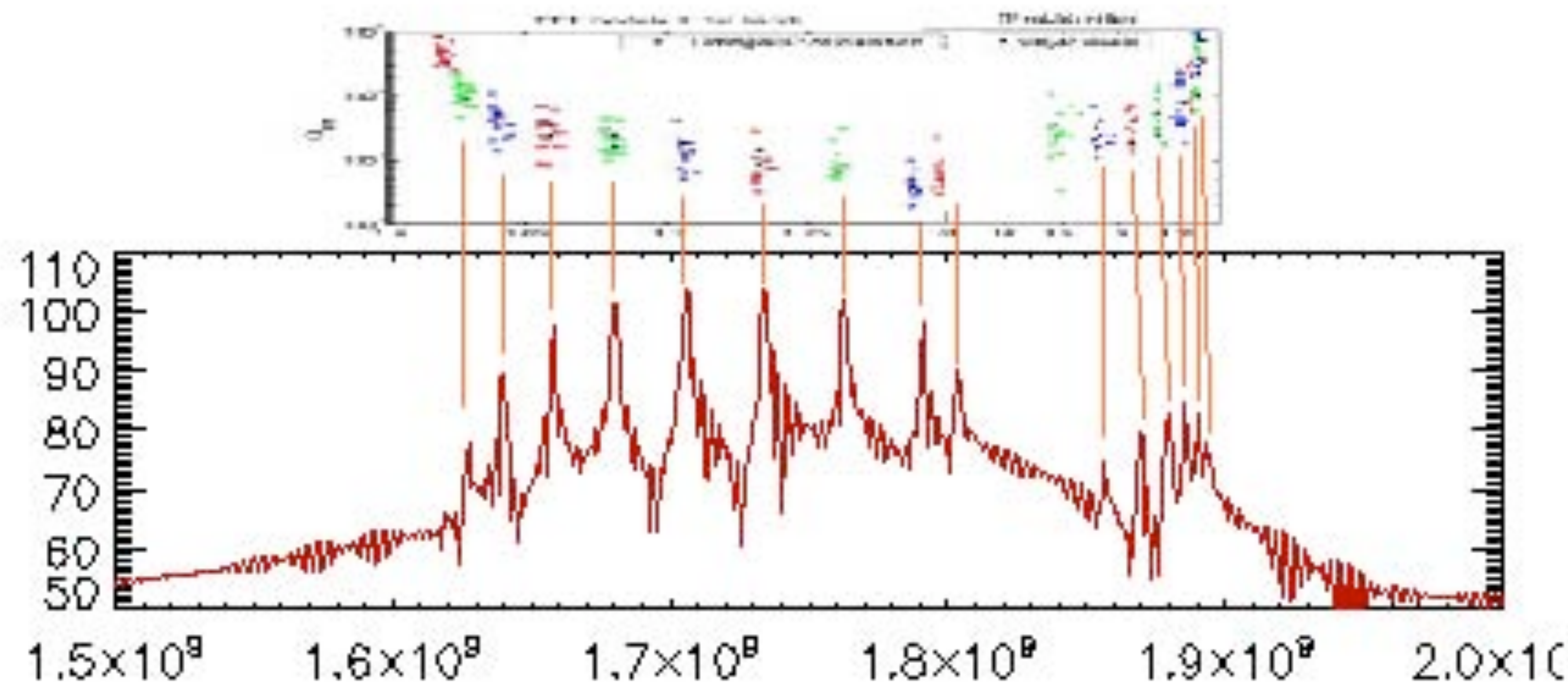


- FFT after 500 nanoseconds shows TE mode spectrum



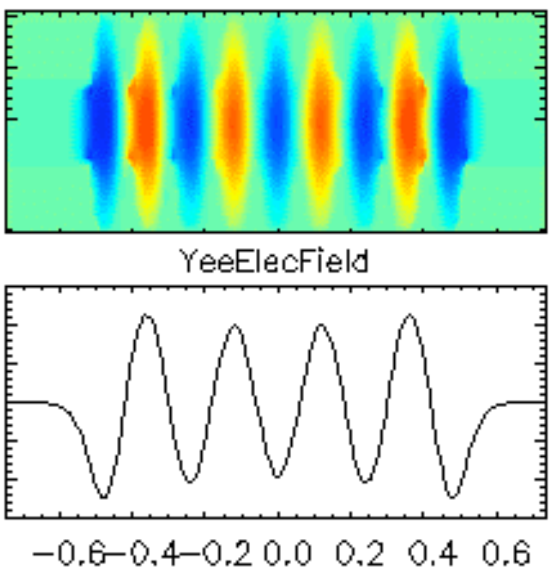
- Accurate modes obtained by fitting

Compares well with measurements

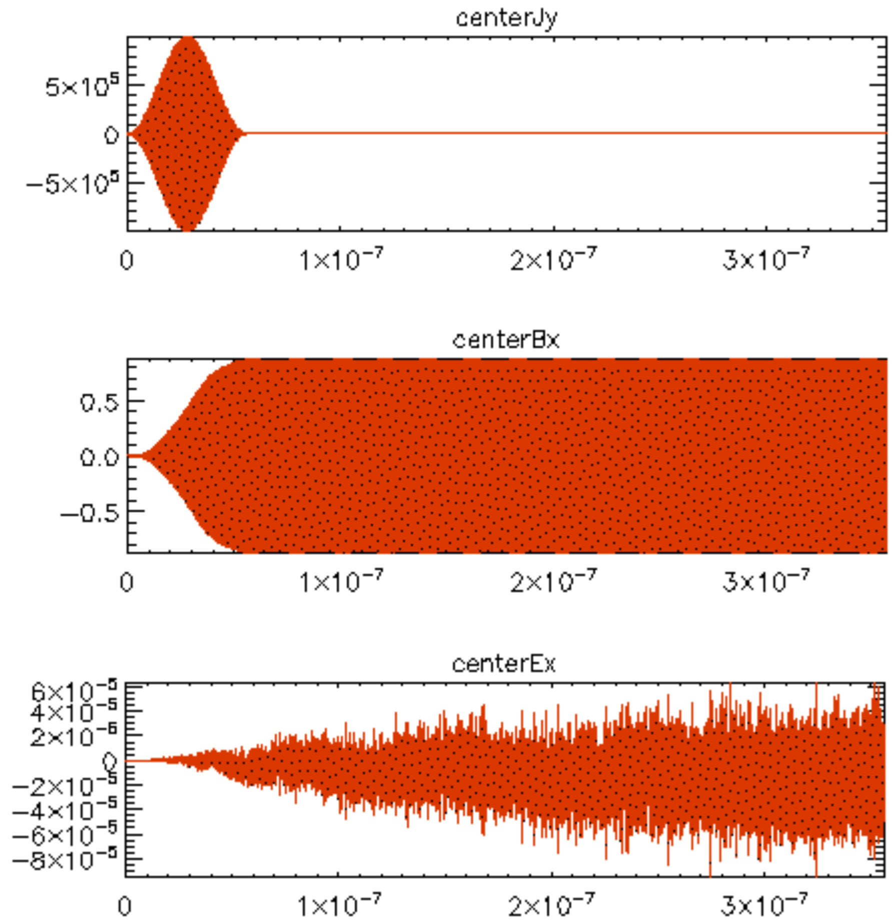


Obtain precise single mode through narrow band excitation

- no HOM
- 100,000 steps, 520 periods
- Stable & Pure



TM

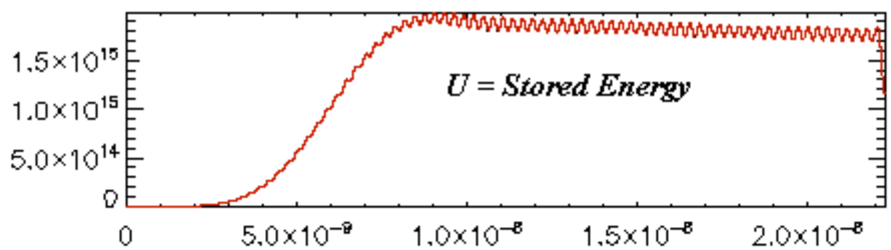


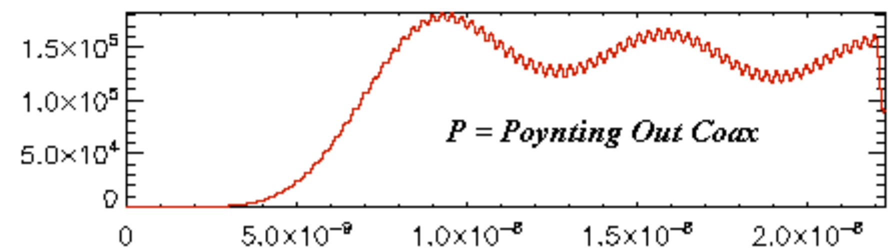
TE

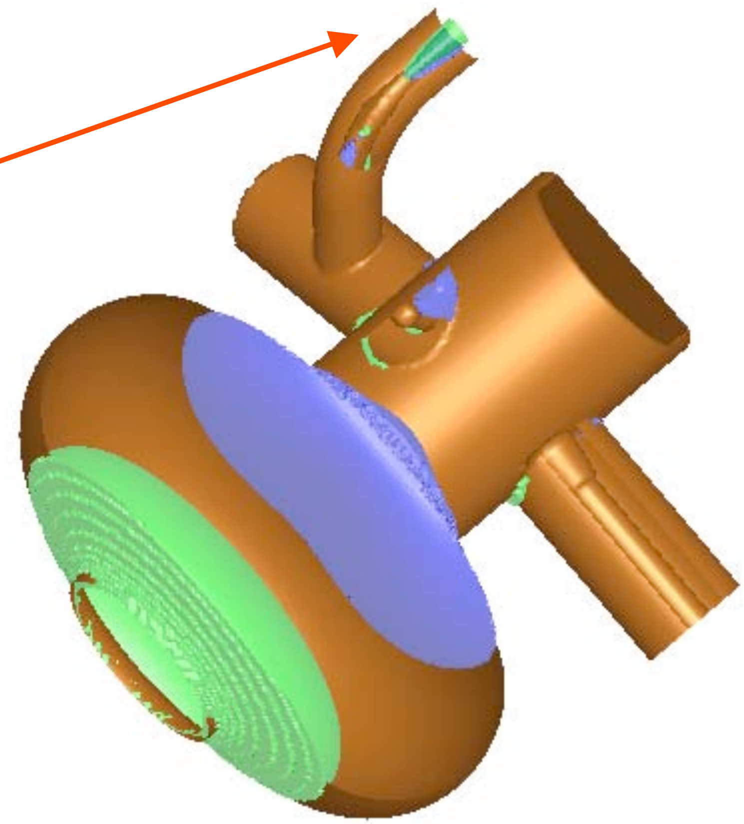
Growth of real-symmetry-excluded mode at numerical limit. Diffusive, not unstable.

Outgoing wave BC, power from measuring Poynting flux

- Measure:
  - P = Poynting flux exiting coax
  - U = Stored Energy
- Calculate: $Q = \omega U/P$







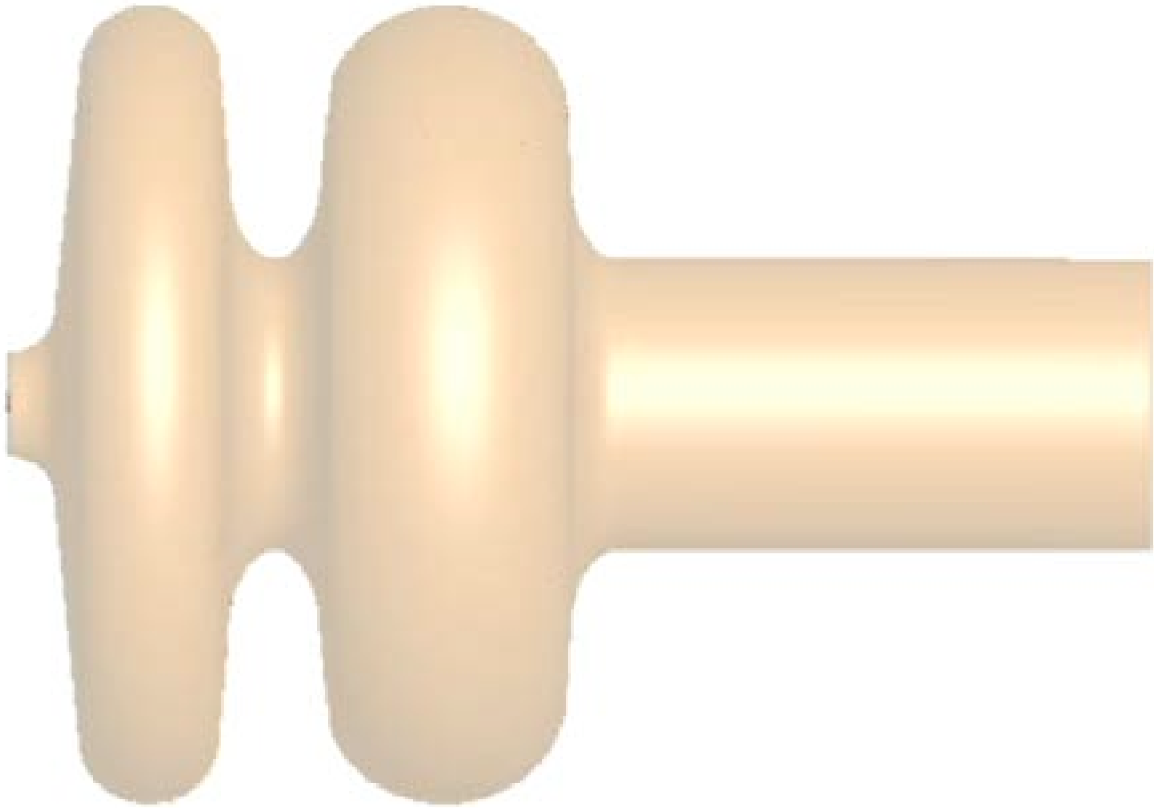
Mur and PML both present

Wakefields obtained without summing modes

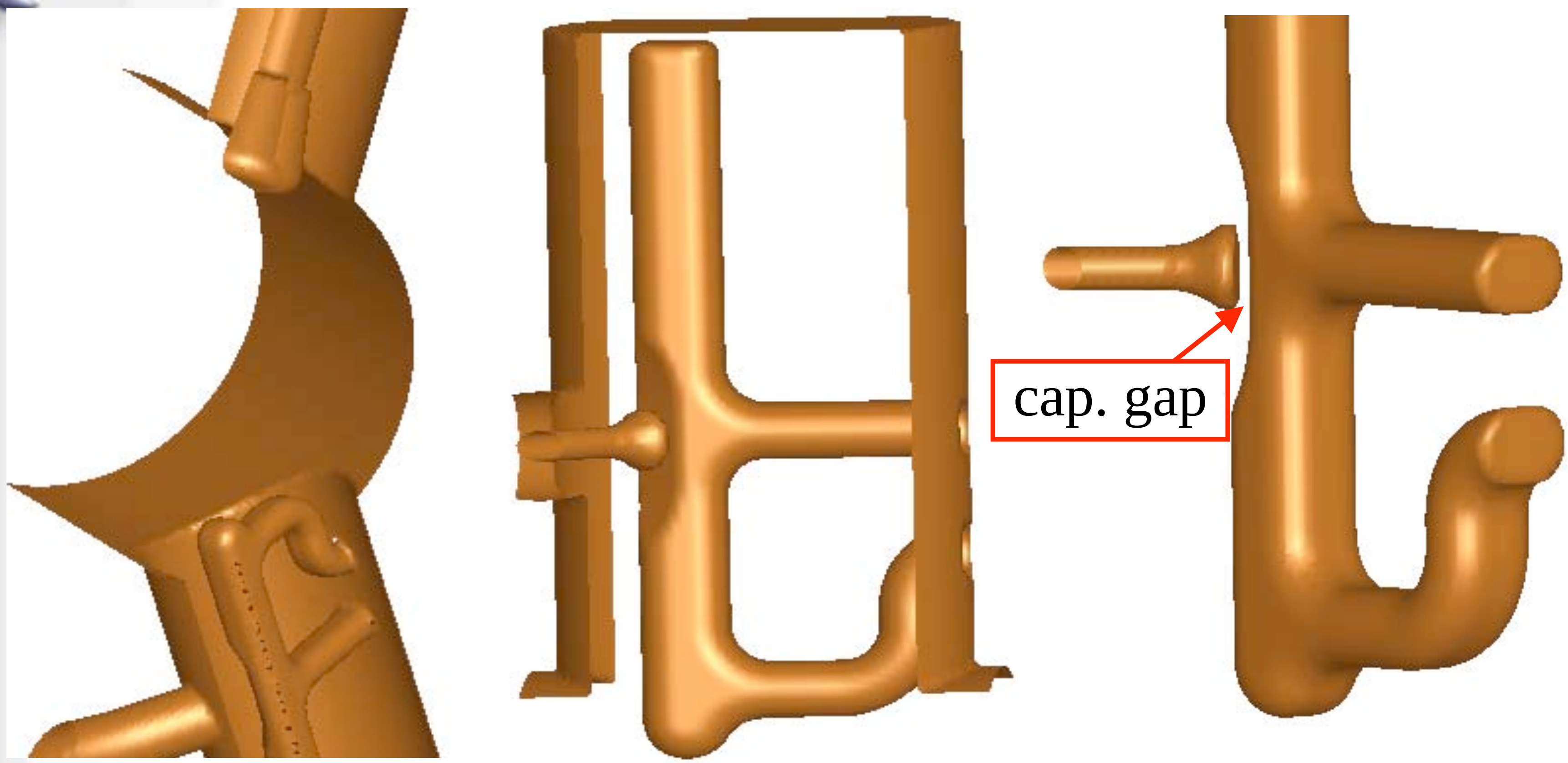
Wakefield for Tesla cavities computed by VORPAL in 3D

Self-consistent EM gun simulations in complex cavities now possible

- Image charges during beam emission
- Wakes from constrictions
- Wake fields influencing final emittance



Next challenges - including capacitive gaps



- HOM capacitive coupler gap is significantly smaller than grid necessary to resolve other features (gap is exaggerated in this figure).
- Full sim is 1283.4 x 222 x 222 mm^3 = 63.25×10^6 mm^3
- Resolving 0.35 mm gap to 0.1 mm requires 6.3×10^{10} cells
- Possible to "brute-force" but algorithm development will allow use of computing power elsewhere

SciDAC will allow us to provide advanced capability for this problem

- FDTD methods permit stable computations for millions of time steps, thus permitting direct study of multi-bunch dynamics
- New implicit solver (sparse matrix inversion in one step) will allow large time steps with fine resolution
- Capacitive gap model will allow large simulations with less resolution per cavity
- Parametric representation of geometry make addition of errors easy

New studies inspire capability, requests

- Laser-plasma: self-consistency, parallelism
  - Higher-order particle shapes
  - Reduced models
- Accelerating cavities: shape modeling
  - Higher-order field to particle near walls
  - Resistive walls for complex shapes
  - Implicit EM solvers, variable grids
- Electron guns, cavities, high-gradient
  - Better emission models, esp. for conformal boundaries
  - Multipactoring
  - Heat deposition computations
  - Microphonics!
- Dielectric systems
  - Complex photonic band-gap systems
- Beam quality
  - Collisions
- Crab cavities
  - Notch filters, LOM couplers
  - Variable grids
- Error analysis (python scripting capability)

ILC end-to-end presents incredible challenges

- Transverse ratio = 10 cm/10 nm = 10^7
- Longitudinal ratio = 20 km long/1 mm = 2×10^7
- Courant limit would give $T/\Delta t = 2\times10^{11}$
- Multiply by number (1000) of bunches by 300
- Composite of 2.4×10^{38} cell-time-steps (10^{14} is routine)
- Need to overcome disparity of 3×10^{24}

<u>But there is a plan</u>

- Implicit solvers increase Δt by 10^6
- Reduced model buys 300
- Variable grid gives 10^8
- Moving window gives another factor of 2×10^4
- Savings of $6\text{x}10^{20}$

Possible with combined improvements in

<u>Hardware, Algorithms, Addition of models</u>

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