# Computational Modeling of Intense Beams in Electromagnetic Structures

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thanks to
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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 plasma in the presence of complex structures.

# Progression of modeling

Test particles in structures (tracking, multipactoring)

↓

Wake fields in structures

↓

Beam-frame electrostatics (no structures)

↓

Self-consistent, fully EM in structures

Advances in hardware

Parallel computations

Accurate parallel algorithms

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

- Maxwell

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

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

- Particles drive EM

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

- Particle dynamics from EM

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

**Auxiliary equations**

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

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

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

plus other physics (later)

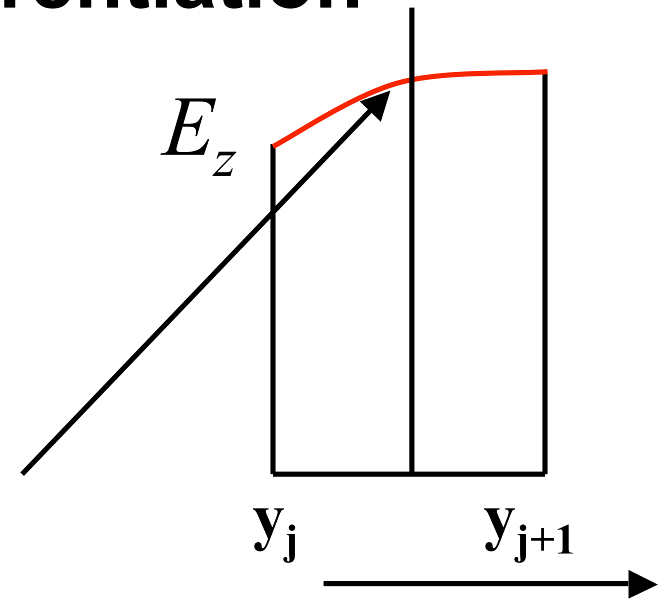
# Yee: 2nd order accurate spatial differentiation

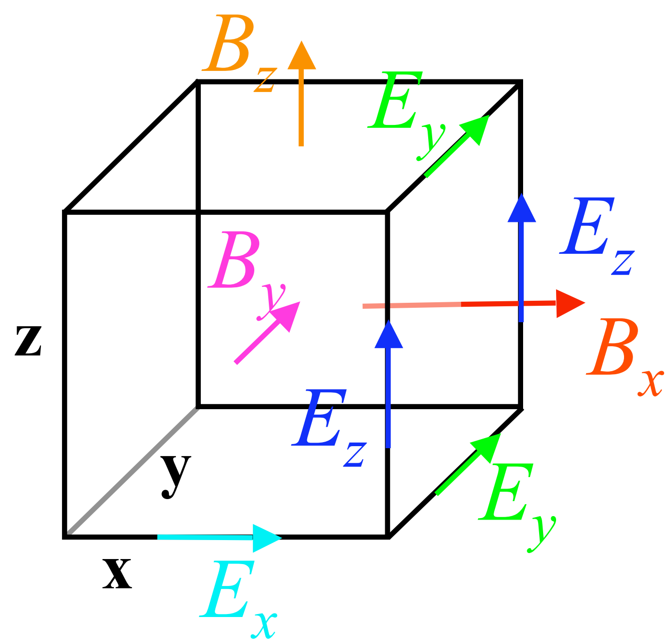
$$\frac{\partial B_x}{\partial t} = -\frac{\partial E_z}{\partial y} + \frac{\partial E_y}{\partial z}$$

- At the midpoint

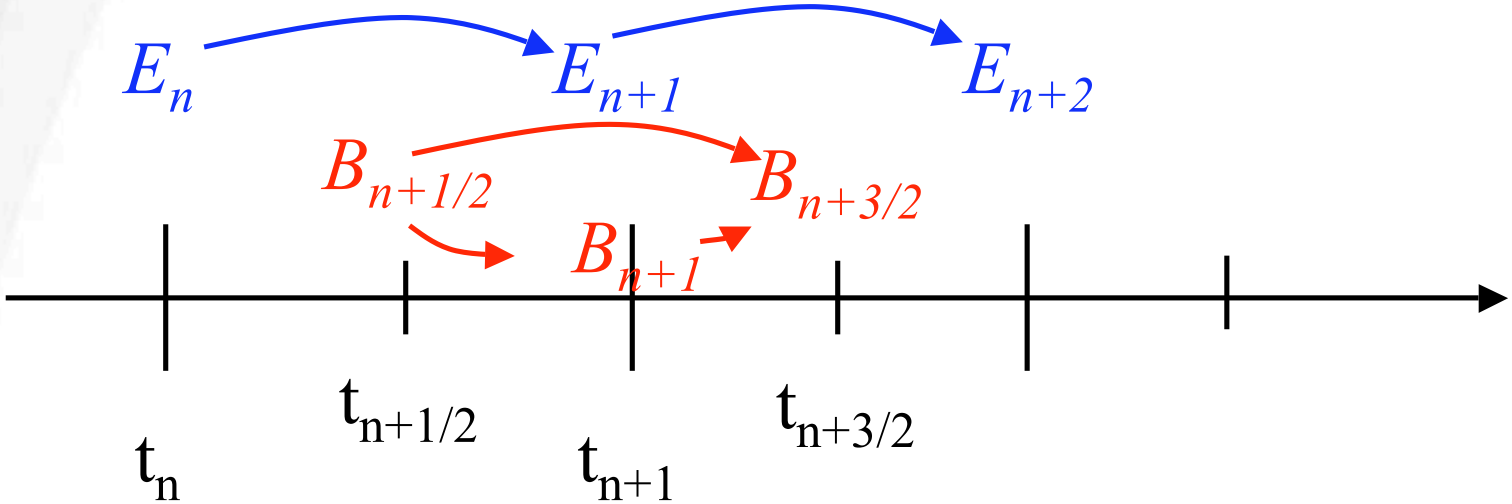
$$\frac{\partial E_z}{\partial y} = \frac{E_{z,j+1} - E_{z,j}}{\Delta y} + O(\Delta y^2)$$

- 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 $\Delta$t
- Can get time-collocated values by half-stepping in B
- Similar for E update, except $c^2$ factor

# Computing particle-particle interactions is prohibitive

- Coulomb interaction leads to $N_p^2$ force computations

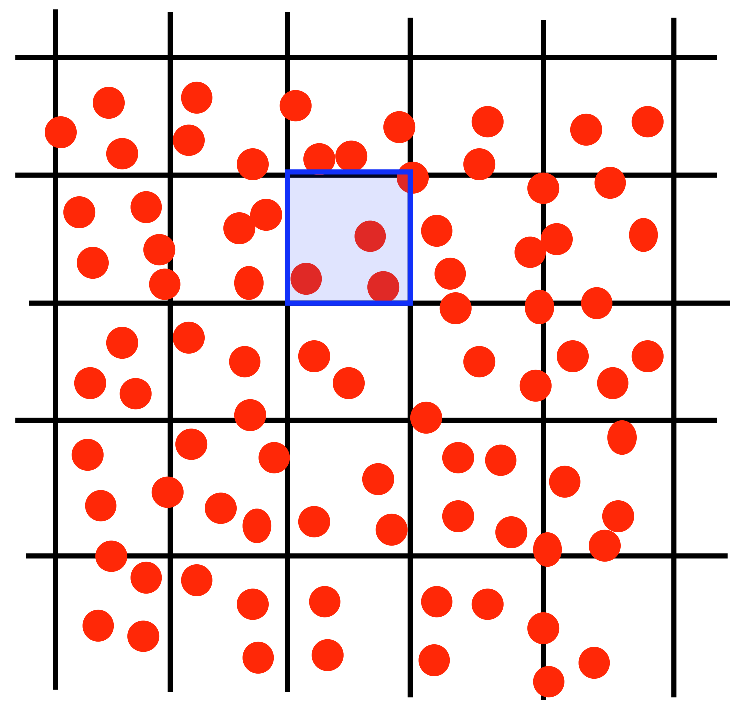
$$\frac{d\gamma_i \mathbf{v}_i}{dt} = \frac{q_i}{\varepsilon_0 m_i} \sum_j q_j \frac{\mathbf{x}_i - \mathbf{x}_j}{\left|\mathbf{x}_i - \mathbf{x}_j\right|^3}$$

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

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

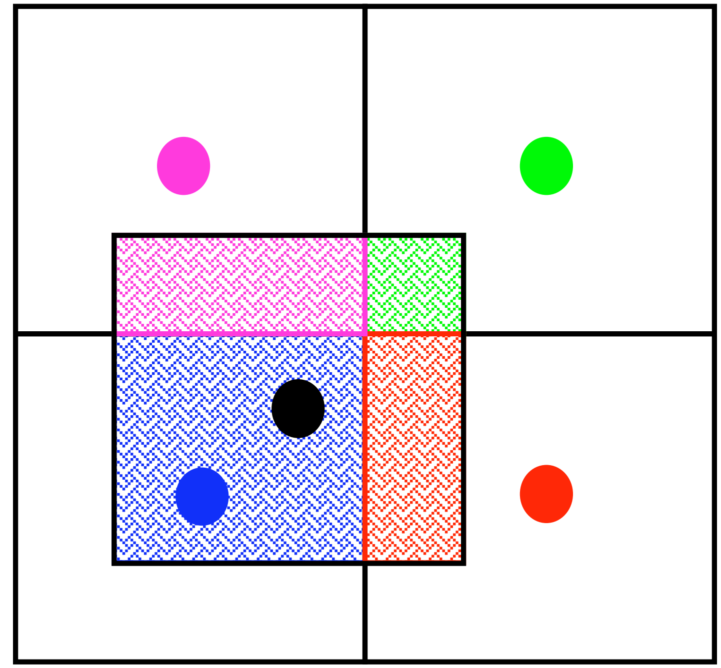
# Particle In Cell (PIC) reduces to $N_p$ scaling

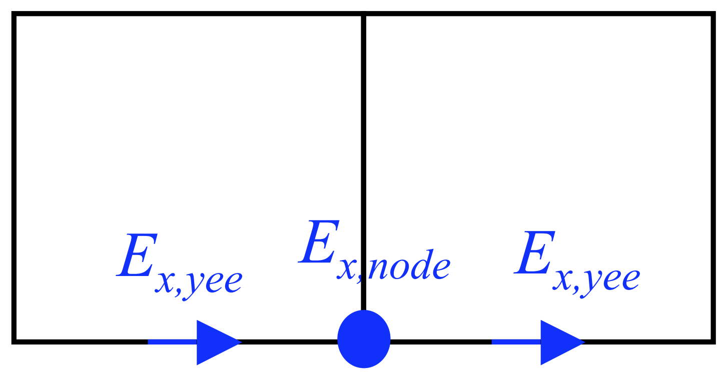
- Particle contributions to charges and currents are added to each cell: $O(N_p)$ operations
- Forces on a particle are found from interpolation of the cell values: $O(N_p)$ operations



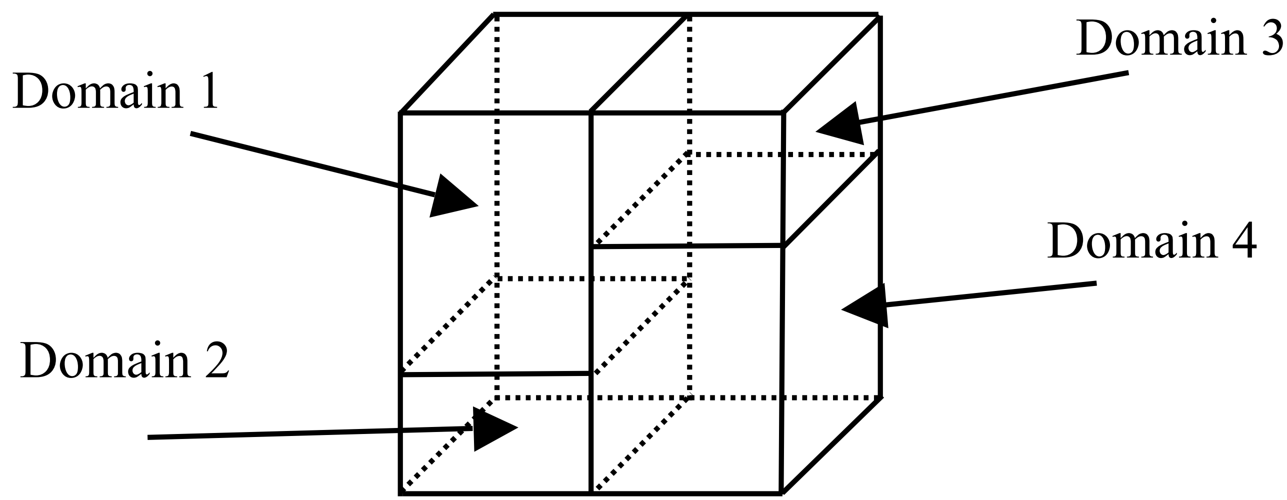
# Finding the force: interpolation (gather)

- 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





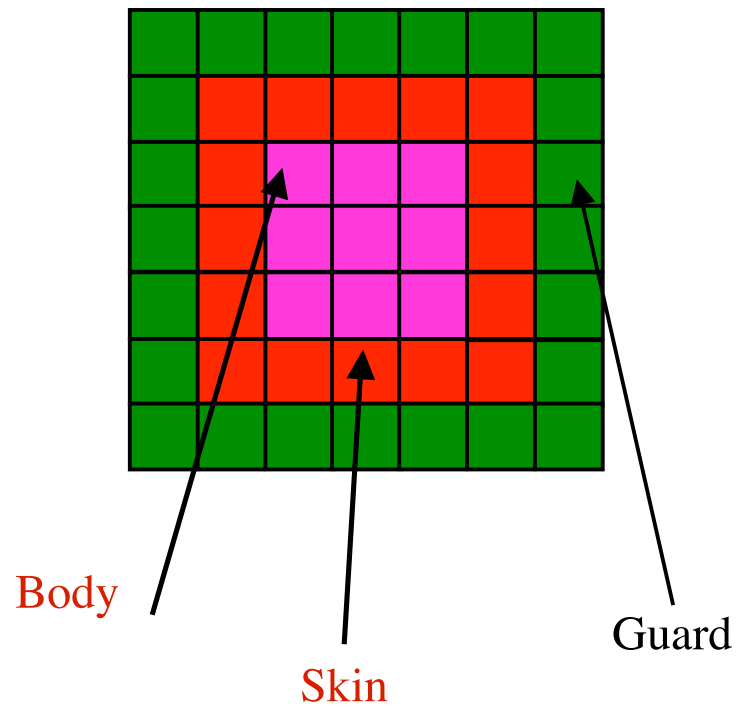
# Parallelism: domain decomposition



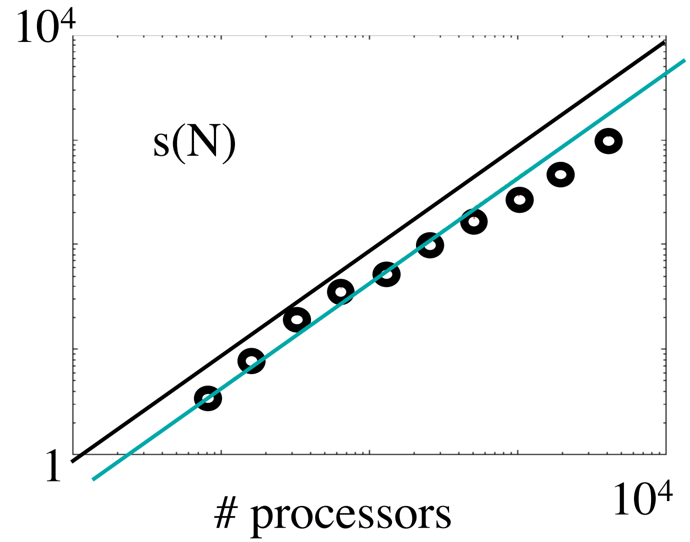

- Communication is expensive
- Global communication is really expensive

# Overlap of communication and computation needed for speed

- Non overlap algorithms:
  - Compute domain
  - Send skin (outer edge)
  - Receive guard
  - Repeat
- For local algorithms,overlap
  - Compute skin
  - Send skin
  - Compute body
  - Receive guard
  - Repeat



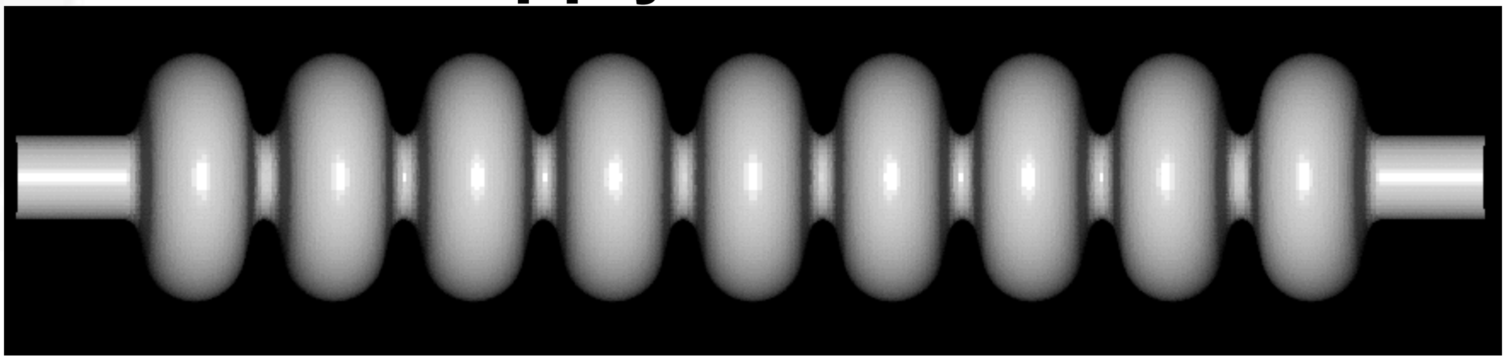
# Local update algorithms scale very well to large numbers of processors



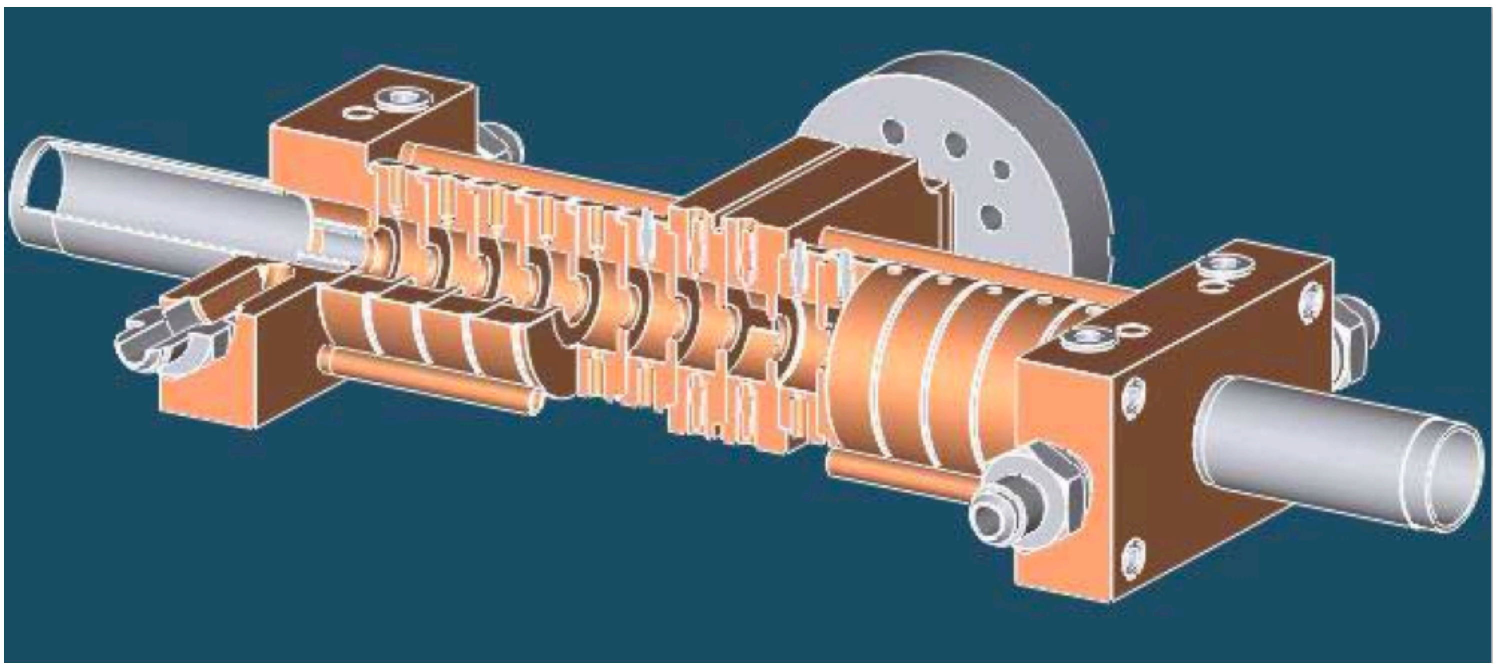

VORPAL scaling on Seaborg (IBM SP3)

- Strong scaling, 10,000x400 continually subdivided
- Similar behavior on 1,500x300x300
  - (135M cells, 0.5 B particles)
- Propagation to 1 mm (20,000 steps) in 30-40 hours with 2000 SP3 or 400 POWER V.
- Parallelism depends on surface to volume ratio
- All computations for recent LWFA were of this type
- $2{\times}10^{13}$ particle-time-steps or $10^{14}$ cell-time-steps (no particles) routine

# To investigate without construction, need to apply methods to



ILC (Tesla)



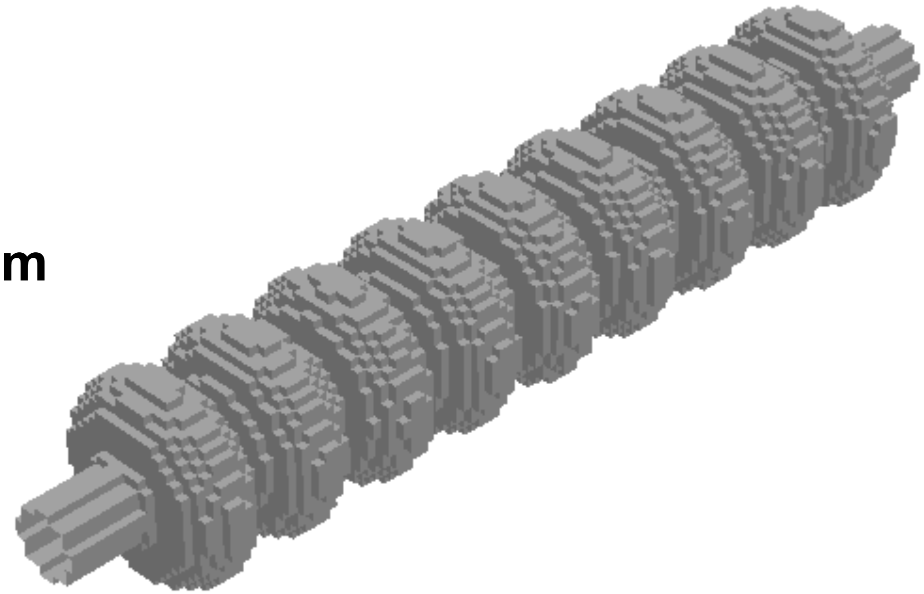
High-gradient

# 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

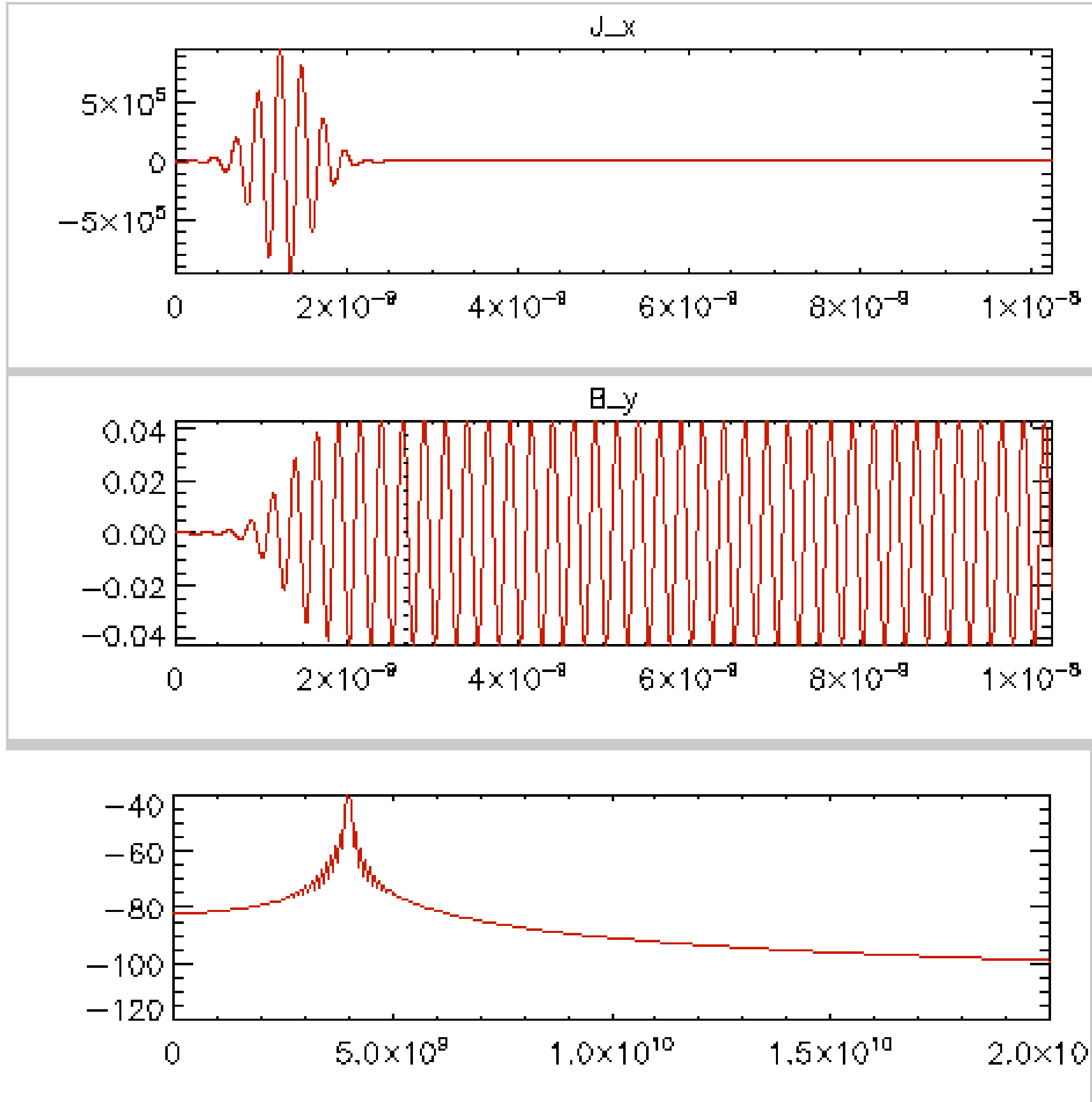
**120x24x24 = 71,424 cells**
**= 215,000 degrees of freedom**



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

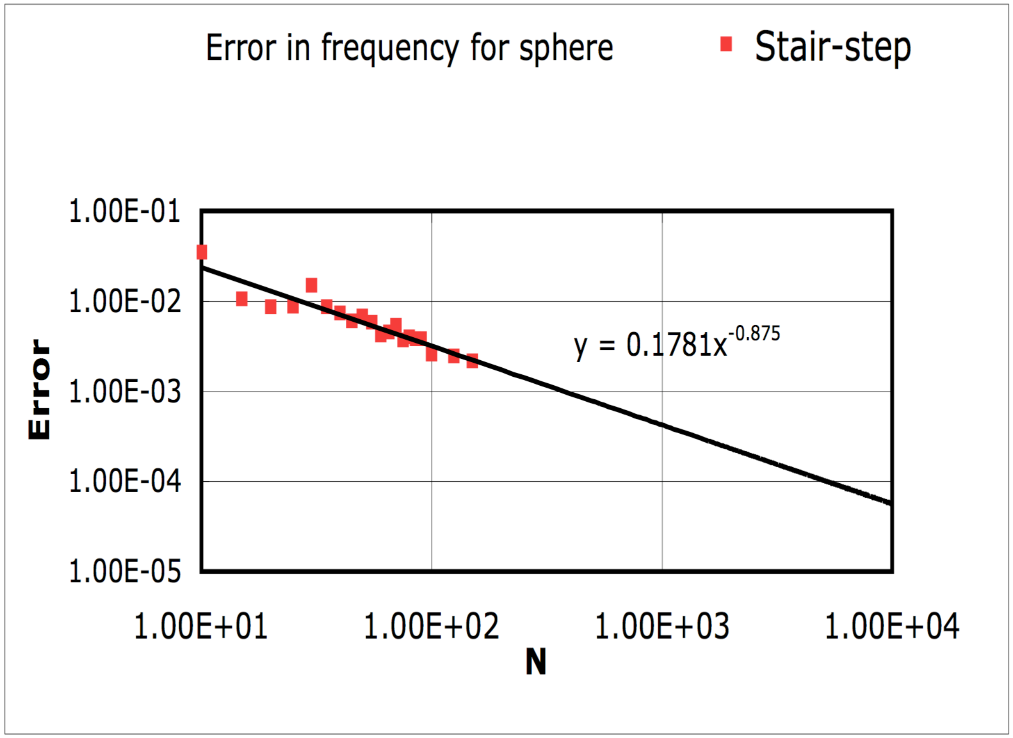
# Modes computed with combination of FFT and fitting

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



# 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

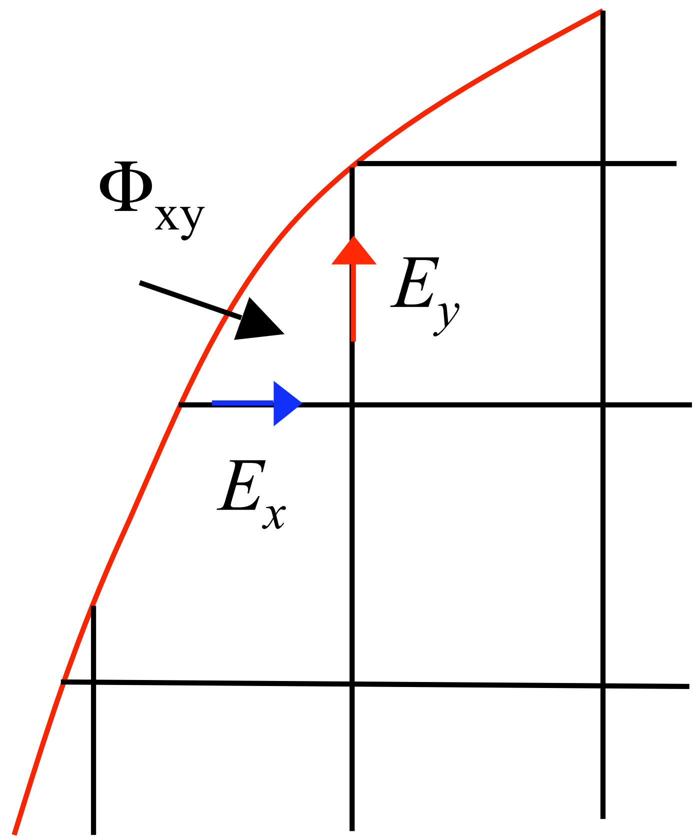
# Resurgence of regular grids: cut cells give same accuracy as finite elements

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

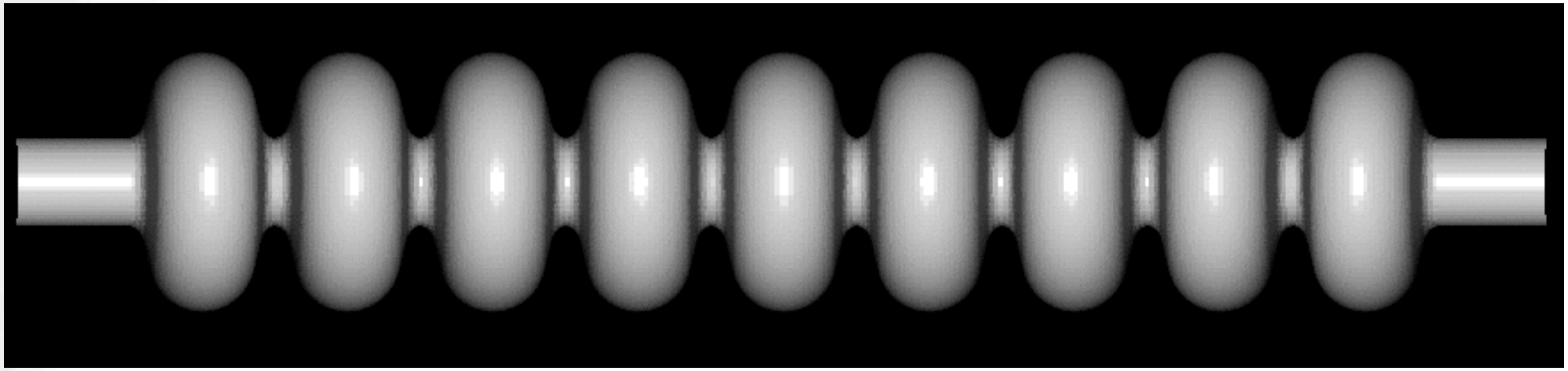
$$\dot{\Phi}_{xy} = -E_x \ell_x - E_y \ell_y$$

  - Update fields via

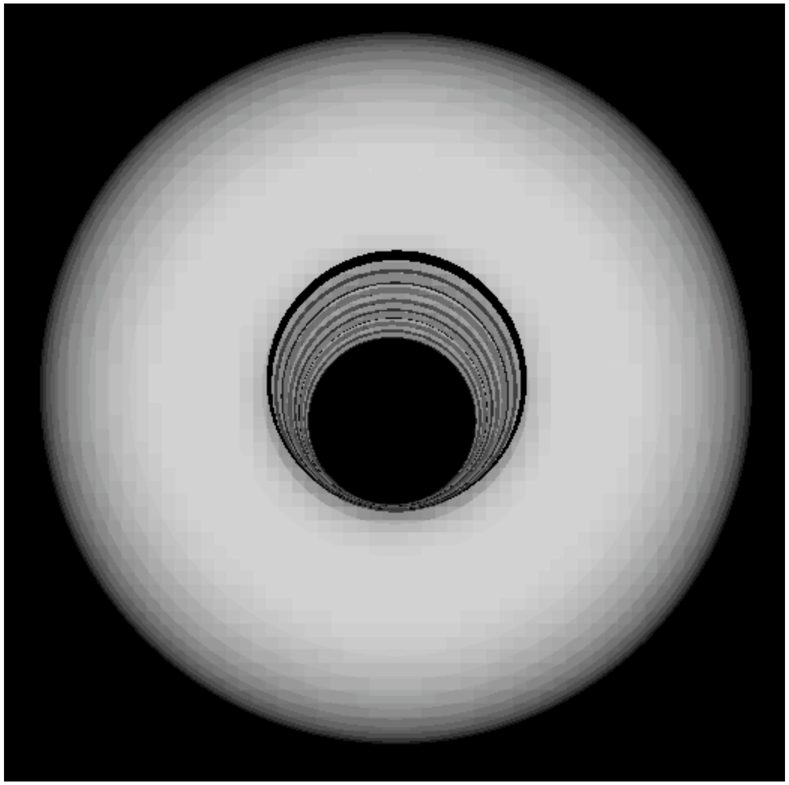
$$B_z = \Phi_{xy} / A_{xy}$$



# Cut-cell boundary conditions accurately represent geometry

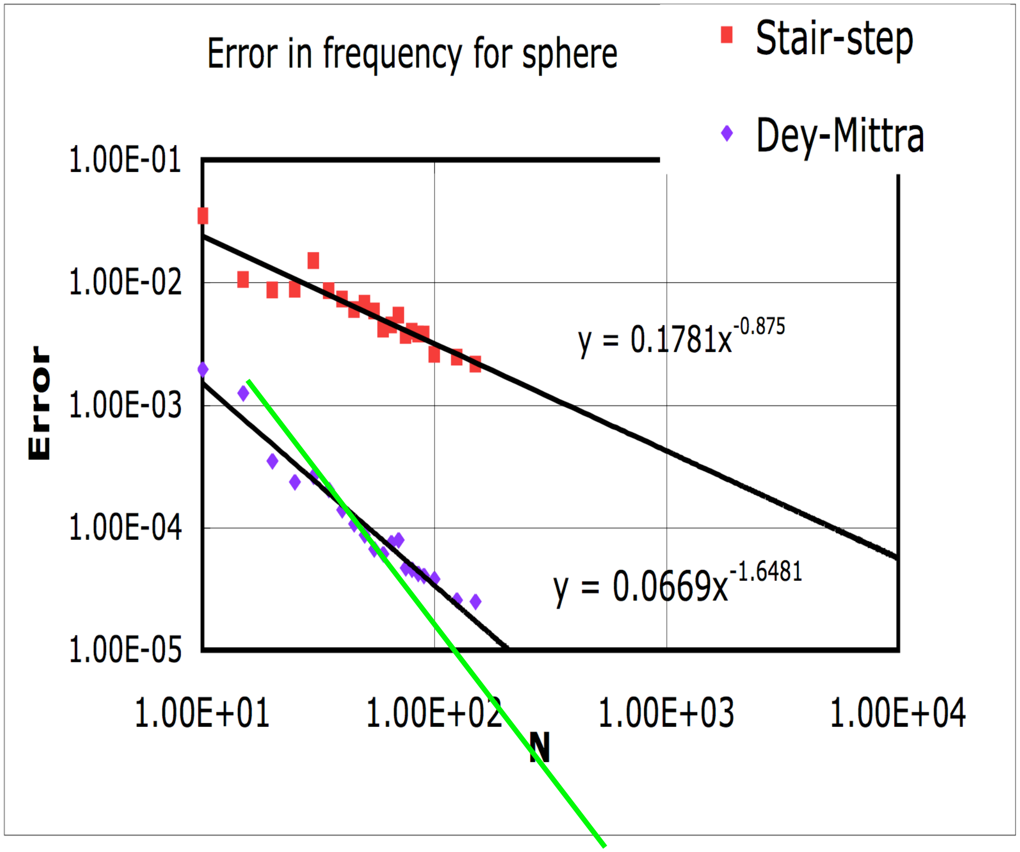


- Tesla 2000 cavities
- 312x56x56 ($10^6$) cells



# Dey-Mittra (1997) cut-cells allow $10^{-5}$ 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

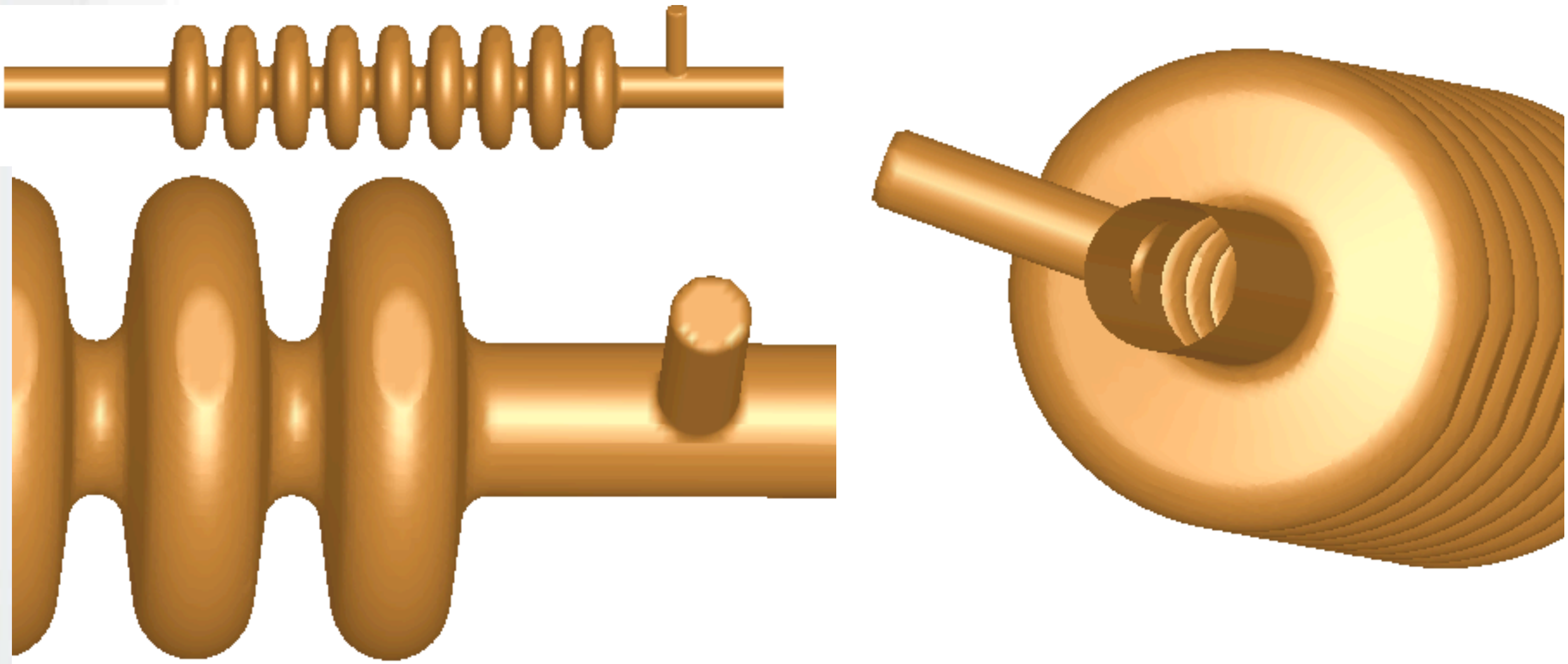
# Cut-cell methods allow us to model accelerator systems self-consistently and electromagnetically

- SRF accelerating cavities, crab cavities, etc.
  - Before: compute wake fields, get impedances, apply engineering rules
  - Now: model the full, multi-bunch problem
- SRF guns
  - Before: field is composed of rf mode (ignore others) and self-fields, ignore wake fields
  - Now: model to full cavity problem

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

**Wakefield for Tesla cavities computed by VORPAL in 3D**

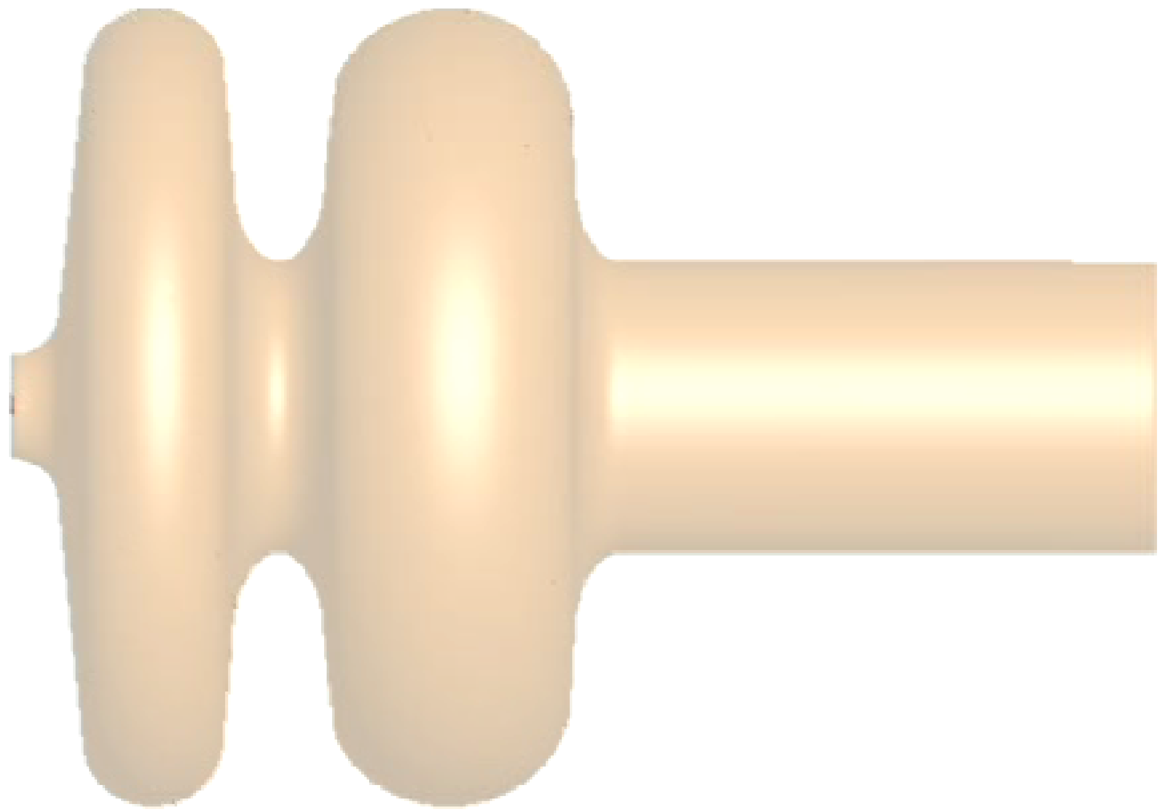
# Crab cavity generation, visualization, computation of splitting



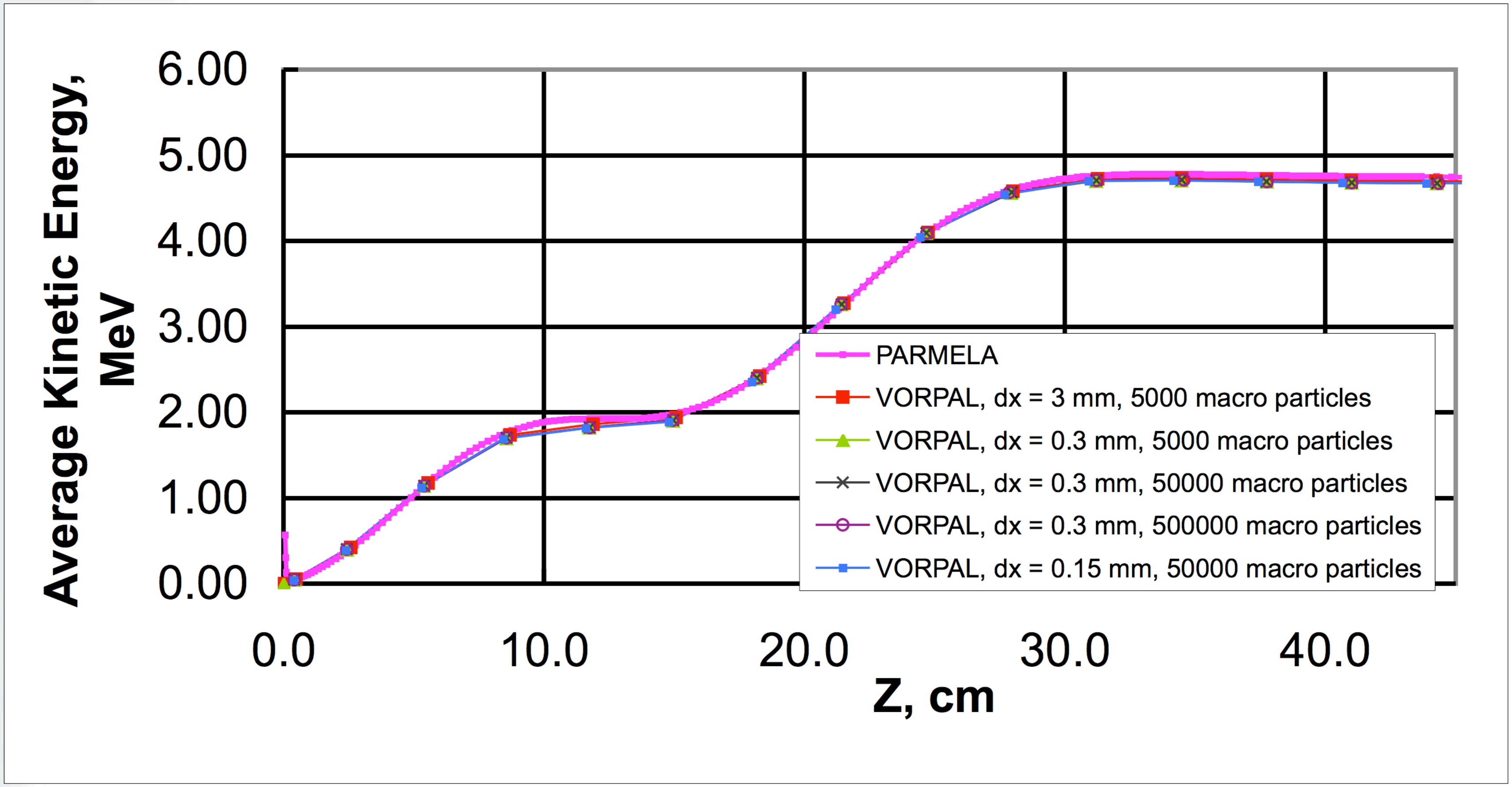
- CAD representations
- Python coding of shapes

# Self-consistent EM gun simulations in complex cavities

- Image charges during beam emission
- Wakes from constrictions

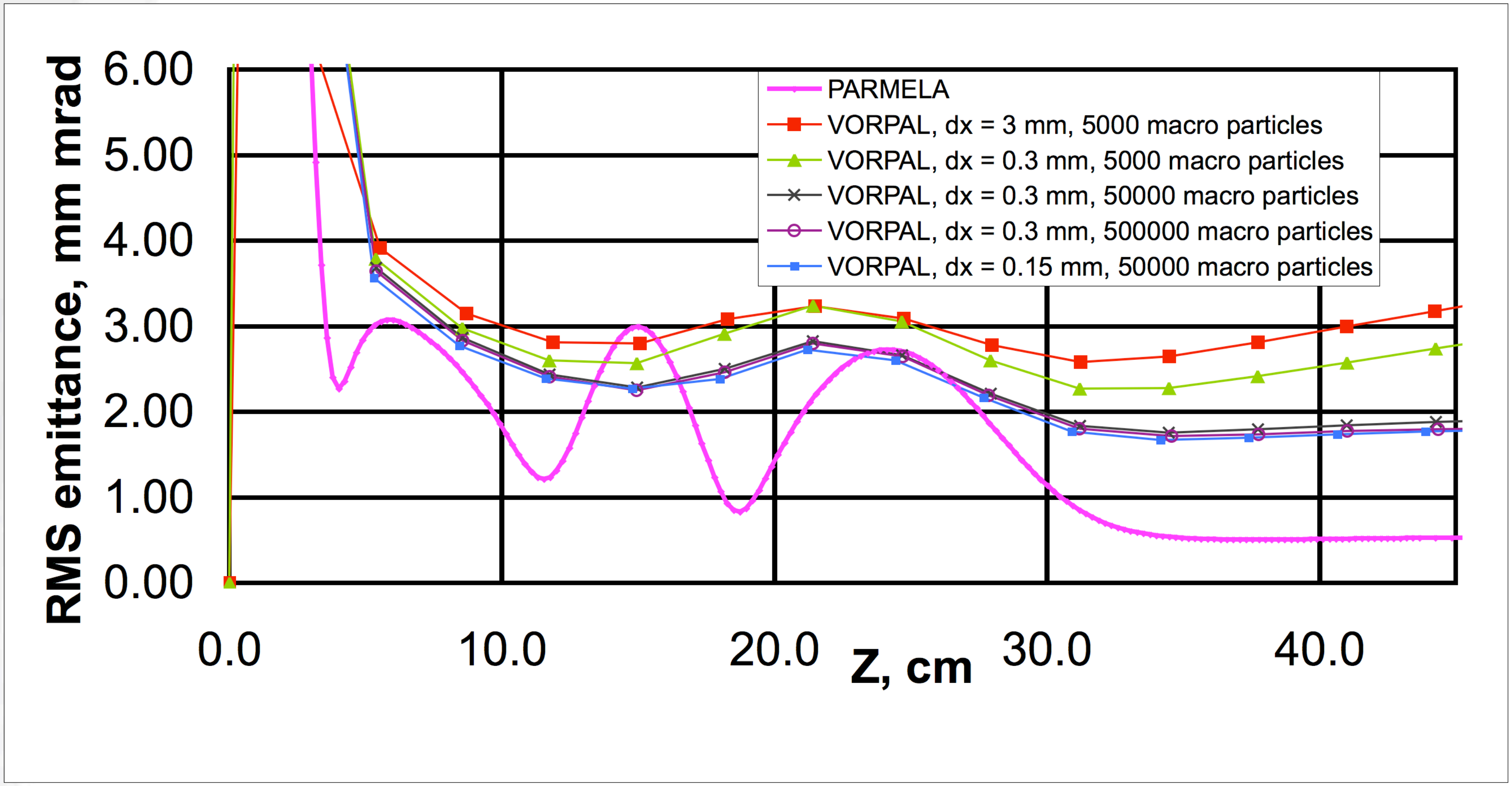


# Verification by comparison of beam energy with Parmela shows consistency




- D. Dimitrov (Tech-X), D. Kayran (BNL) + collaborators
- Parmela has beam-frame electrostatics
- VORPAL is fully electromagnetic, 3300x180x180, 100M cells

# Simulation results indicate electromagnetics playing a role in emittance




- VORPAL results converged
- 200M cell runs completed

# Each new study inspires capability, brings 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

# ILC end-to-end presents incredible challenges

- Transverse ratio = 10 cm/10 nm = $10^6$
- Longitudinal ratio = 20 km long/1 mm = $2\times10^6$
- Courant limit would give $T/\Delta t = 2\times10^6$
- Multiply by number of bunches by 300
- Composite of $1.2\times10^{27}$ cell-time-steps ($10^{14}$ is routine)
- Need to overcome disparity of $4\times10^{13}$

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

- Implicit solvers increase $\Delta t$ by $10^5$
- Reduced model buys 300
- Moving window gives another factor of $2\times10^4$
- Still need increase by 100 in capability: doable

# 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 (GUI's?)
  - Defines cavity shapes
  - Define particle beams