High-accuracy embedded boundary algorithms for electromagnetics

ELECTROMAGNETICS COMPUTATIONS ON THE YEE MESH ARE VERY FAST, WITH A CELL UPDATE REQUIRING LESS THAN 3 CORE-NS ON SANDYBRIDGE HARDWARE. HOWEVER, IN THE PRESENCE OF NON-GRID-ALIGNED DIELECTRICS OR CONDUCTORS, WITH STAIR-STEPPED BOUNDARIES, THE ERROR RISES TO O(DX). FOR CONDUCTORS, DEY-MITTRA EMBEDDED BOUNDARIES REDUCE THE ERROR TO O(DX^2), WITH O(DX^3) ERROR AVAILABLE THROUGH RICHARDSON EXTRAPOLATION. AS SHOWN HERE, SIMILAR ACCURACY IN EIGENMODE FREQUENCIES CAN NOW BE OBTAINED FOR DIELECTRICS WITH NON-GRID-ALIGNED SURFACES, AND SURFACE FIELDS ARE OBTAINED ACCURATELY AS WELL. FINALLY, THE PROPER DEFINITION OF THE MAGNETIC FLUX DIVERGENCE FOR THE CONDUCTOR-CUT BOUNDARY CELLS IS FOUND. SUBTRACTING ITS GRADIENT FROM THE CURL-CURL OPERATOR LEAVES A POSITIVE DEFINITE OPERATOR THAT CAN BE INVERTED USING A MULTI-LEVEL PRECONDITIONER.

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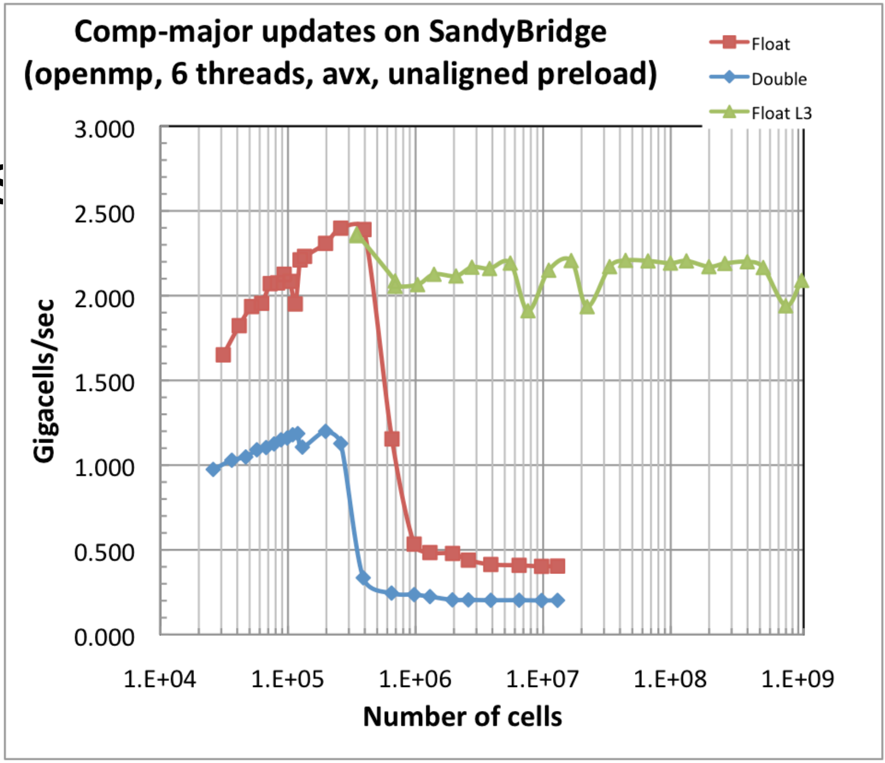
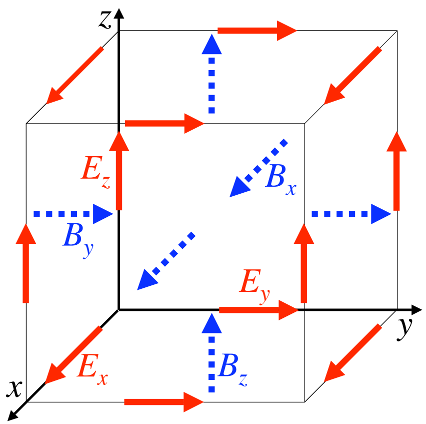
Today: embedded boundary methods, fast accurate, scalable: dielectrics and metals

- Historical finite difference inaccurate, but metallic embedded boundary methods recover accuracy
- Improve frequencies with eigenvalue solver but
  - Need Poissonish operator
  - Need to subtract gradient of divergence in partial cells
- Fields also improved
- Dielectrics improved



Standard Yee update can be written in matrix form



Vector calculus	FD Matrix
$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E}$	$\frac{\partial B}{\partial t} = -CE$
$\frac{\partial \mathbf{D}}{\partial t} = \nabla \times \mathbf{H}$	$\frac{\partial D}{\partial t} = C^T E$

$e_0 = m_0 = 1$

vacuum

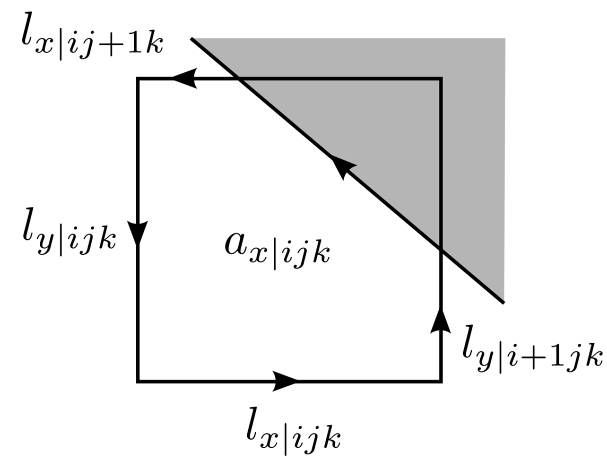
- Upward differencing = C
- Downward differencing = C^T

$$\frac{\partial^2 B}{\partial t^2} = -CC^T B$$

K. Yee, IEEE Trans. Ant. and Prop. 14, 302 (1966).

Precise Dey-Mittra boundary conditions give local O(Dx), global O(Dx^2)

- DM use integral form of Faraday
  - Multiply E by lengths
  - Divide by area
- DM not derived but heuristic
  - only Faraday changed
  - B no longer centered so how further differenced?
- (Unpublished) derivation exists
- Gustafson "theorem"
- Modifies matrix form



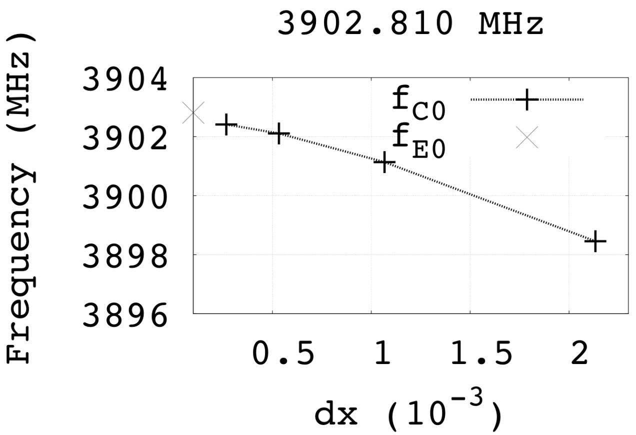
$$\frac{\partial^2 B}{\partial t^2} = -A^{-1} C L C^T B$$

$$\frac{\partial^2 \left(A^{1/2} B\right)}{\partial t^2} = -A^{-1/2} C L C^T A^{-1/2} \left(A^{1/2} B\right)$$

B. Gustafsson, Math. Comput. 29, 396 (1975).

Modified CFL condition for Dey-Mittra BCs gives transition to O(Dx)

- Cut-cell matrix elements scale as L/A
- L/A can be vanishingly small
- Time domain then requires face dropping
  - Pick CFL acceptable CFL reduction (Dey-Mittra fraction)
  - Use Gershgorin circle theorem to drop faces
- Result is lower accuracy at high resolution (still get parts in 10^5 through Richardson)



T. M. Austin, J. R. Cary, S. Ovtchinnikov, G. R. Werner, and L. Bellantoni, Comput. Sci. Disc. 4 015004 doi: 10.1088/1749-4699/4/1/015004 (2011).

Frequency extraction: G. R. Werner and J. R. Cary, J. Comp. Phys. 227, 5200-5214 (2008), http://dx.doi.org/10.1016/j.jcp.2008.01.040.

Frequency solver would eliminate transition, but want multigrid friendly operator

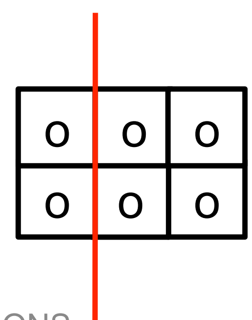
- Curl-curl: coupled vector components
- Shift invert requires solving
- Not amenable to multigrid solves
- Direct solvers not scalable
- Vector calculus gives Laplacian, but
  - reaches outside simulation
  - unknown for Dey-Mittra

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

$$\omega^2 B_x = \frac{\partial}{\partial y}\left[\frac{\partial B_y}{\partial x} - \frac{\partial B_x}{\partial y}\right] - \frac{\partial}{\partial z}\left[\frac{\partial B_x}{\partial z} - \frac{\partial B_z}{\partial x}\right]$$

$$= -\frac{\partial^2 B_x}{\partial y^2} - \frac{\partial^2 B_x}{\partial z^2} + \frac{\partial^2 B_y}{\partial x \partial y} + \frac{\partial^2 B_z}{\partial x \partial z}$$

$$\omega^2 \mathbf{B} = \nabla \times \nabla \times \mathbf{B} = \nabla \nabla \bullet \mathbf{B} - \nabla^2 \mathbf{B} = -\nabla^2 \mathbf{B}$$



Stencil reaches outside boundary

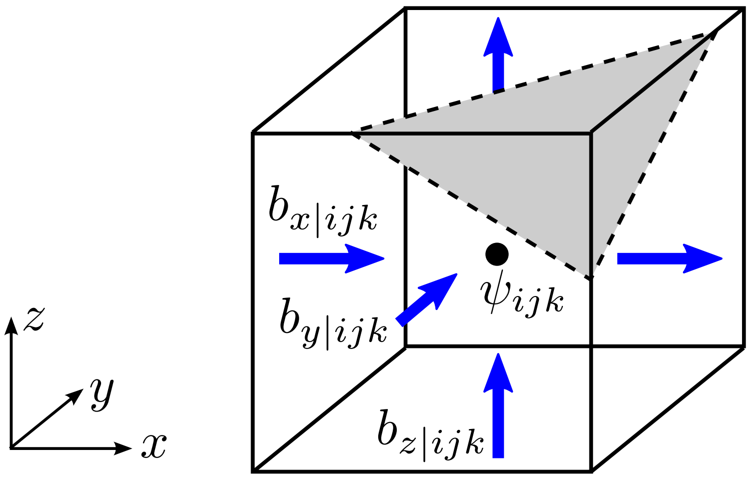
Removal of grad-div relies on geometric interpretation

- Know curl curl in Dey-Mittra
- -del^2 comes from subtracting off grad-div
- div can be written in terms of cell face areas and volumes
- Use that to get the Dey-Mittra -del^2

$$\psi_{ijk} \equiv (\nabla \bullet \mathbf{B})_{ijk} = \frac{B_{xi+1\,jk} - B_{xijk}}{\Delta x} + \ldots$$

$$= \frac{B_{xi+1\,jk} a_{xi+1\,jk} - B_{xijk} a_{xijk}}{V_{ijk}} + \ldots$$

$$\omega^2 B = A^{-1} C L C^T B - D^T V^{-1} D A$$



CA Bauer, GR Werner, JR Cary, *A fast multigrid-based electromagnetic eigensolver for curved metal boundaries on the Yee mesh*, xarchive.

Found rapid convergence for inversion

- Trilinos ML with GMRES
- Embedded boundary conversion as fast as grid aligned

	Cube			Sphere		
Component count	11,520	95,232	774,144	7,224	53,160	405,876
Avg. iteration count	8.0	8.5	9.6	7.0	8.0	8.5
Convergence rate	0.18	0.20	0.24	0.14	0.18	0.20
Multigrid levels	4	4	4	3	4	4
Multigrid complexity	4.1	4.6	4.9	3.6	4.5	4.9
Domain decomposition	1x1x1	2x2x2	4x4x4	1x1x1	2x2x2	4x4x4

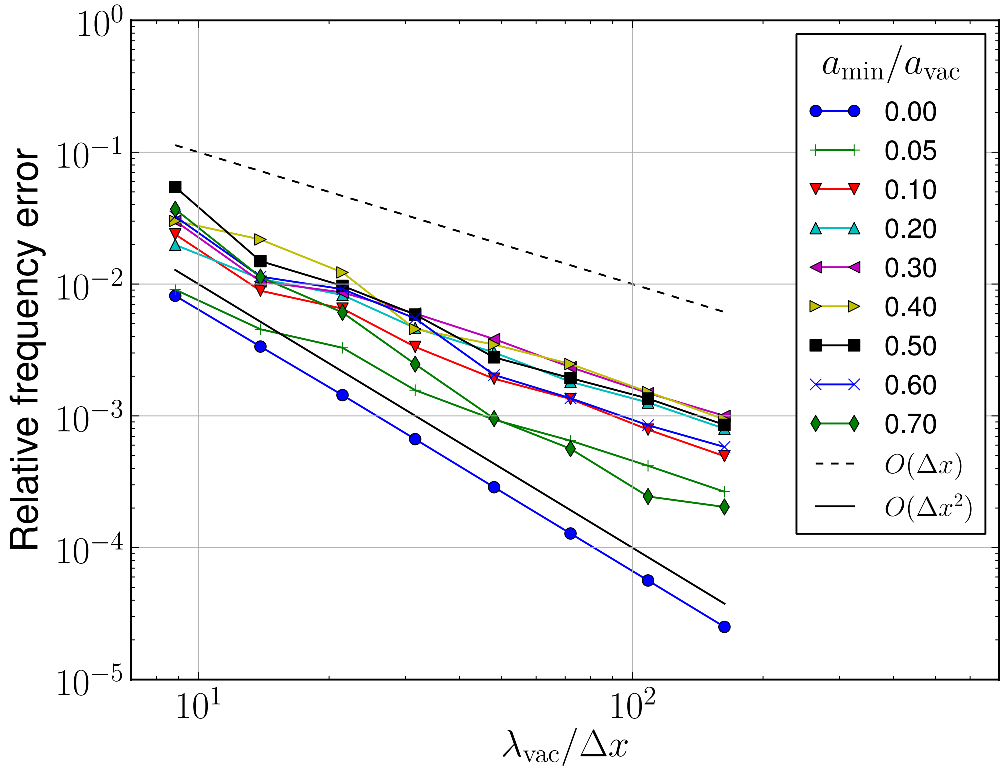
Getting volume right crucial to rapid convergence

1. Random relative errors in volumes
2. Random errors in volumes (e.g., from subsampling)

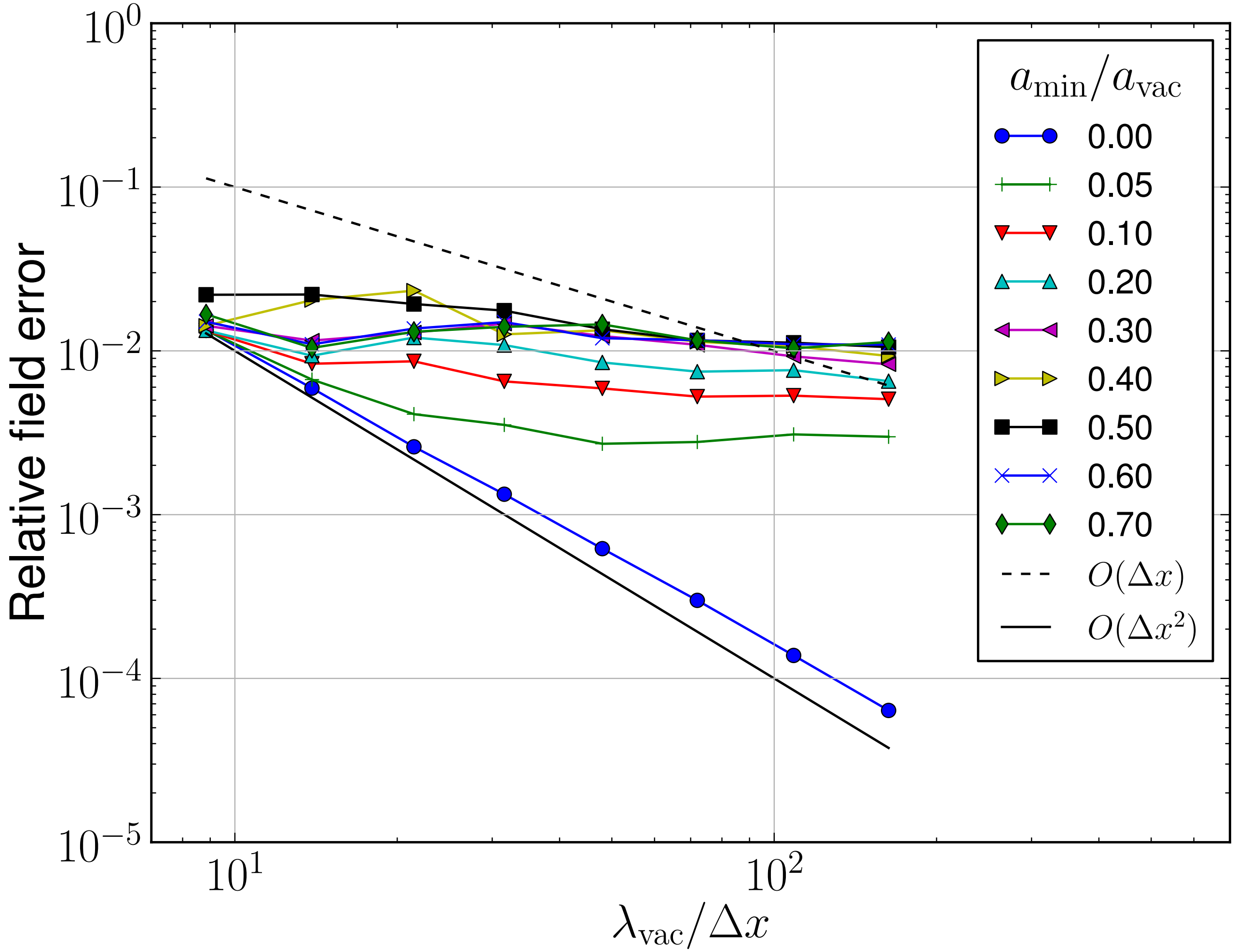
Error from Eq. 26						
ϵ	0.2	0.3	0.5	1	2	3
Avg. iteration count	8	9	12	21	63	212

Error from Eq. 27			
$\Delta v / v_{\mathrm{vac}}$	10^{-5}	10^{-4}	10^{-3}
Avg. iteration count	8	37	200

Frequency now always converges as O(Dx^2)



Fields appear to converge nearly as O(Dx²)

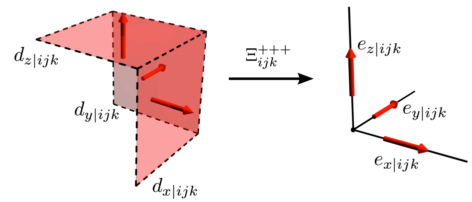


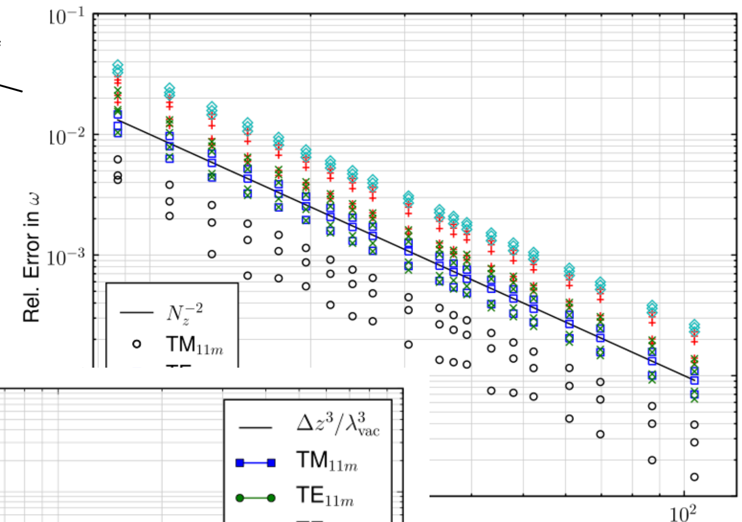
Algorithmic progress in other areas as well

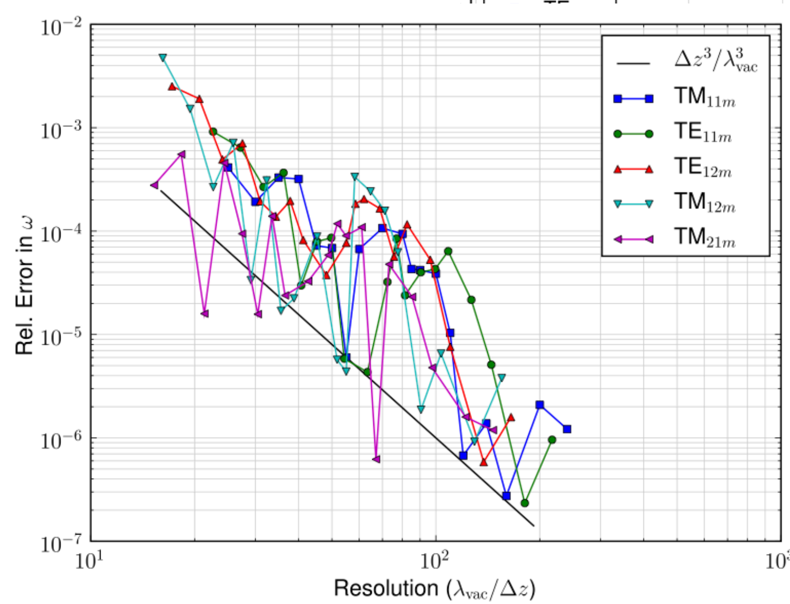
- New, finite difference dielectric algorithm gives 2nd order error
- New beam launcher method reduces simulation volume

New, finite difference dielectric algorithm gives 2nd order error

- Regular convergence

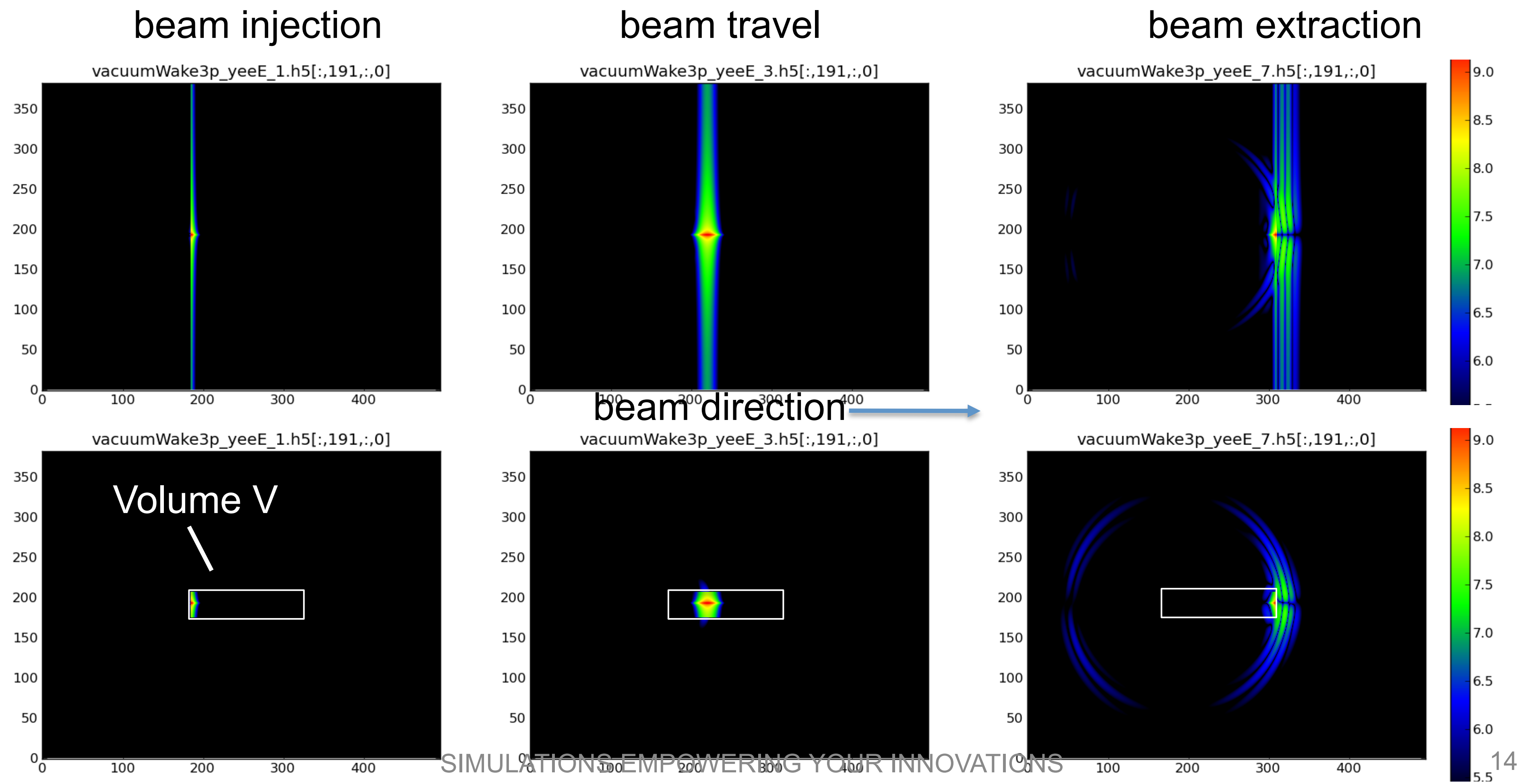






Equivalent surface currents method greatly reduces size of simulated region

The fields inside the volume V are the same in both simulations. The top simulation injects current along an entire plane; it has to simulate a large region to capture the waves emitted from all that current. The bottom simulation has no currents outside V; current on the surface of V produces the same waves (inside V) that the entire plane would produce. Here, the transverse electric field is shown.



Progress in finite difference algorithms for metallic and dielectric structures and

- Metallic embedded boundaries: can now use multigrid as a preconditioner
- Dielectric structures: high-order convergence seen
- Computational region for wake field calculations for infinite systems greatly reduced in size