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.

Carl A Bauer, Greg R Werner, U. Colorado
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CEO, Tech-X
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

- Upward differencing = $\mathbf{C}$
- Downward differencing = $\mathbf{C}^T$

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

\[\epsilon_0 = \mu_0 = 1 \text{ vacuum}\]

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- (Unpublished) derivation exists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

\[ \frac{\partial^2 B}{\partial t^2} = -A^{-1} CLC^T B \]

\[ \frac{\partial^2 \left( A^{1/2} B \right)}{\partial t^2} = -A^{-1/2} CLC^T A^{-1/2} \left( A^{1/2} B \right) \]

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)


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

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

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

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

\[ \omega^2 \mathbf{B} = \nabla \times \nabla \times \mathbf{B} = \nabla \nabla \cdot \mathbf{B} - \nabla^2 \mathbf{B} = -\nabla^2 \mathbf{B} \]

Stencil reaches outside boundary
Removal of grad-div relies on geometric interpretation

- Know curl curl in Dey-Mitra
- \( \text{del}^2 \) 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 \( \text{del}^2 \)

\[
\psi_{ijk} \equiv (\nabla \cdot \mathbf{B})_{ijk} = \frac{B_{x i+1,jk} - B_{xijk}}{\Delta x} + \ldots
\]

\[
= \frac{B_{x i+1,jk} a_{x i+1,jk} - B_{xijk} a_{xijk}}{V_{ijk}} + \ldots
\]

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

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

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Getting volume right crucial to rapid convergence

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

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<th>$\epsilon$</th>
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<th>Error from Eq. 27</th>
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Frequency now always converges as $O(Dx^2)$
Fields appear to converge nearly as $O(Dx^2)$.
Algorithmic progress in other areas as well

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

- Regular convergence
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