Computations of Complex Dielectric Structures for Accelerators: Algorithms and Applications

- Embedded boundary algorithms: reason, improvements
- Wakefields in photonic crystal structures
- Coupling into photonic crystal waveguides

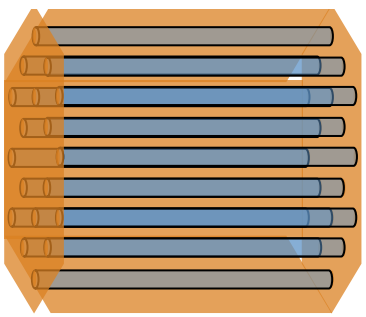
John R Cary
Prof. Physics, U. Colorado
CEO, Tech-X

Greg Werner (CU)
Carl Bauer (CU)
Ben Cowan (Tech-X)

The many different structures proposed for dielectric wave guides are computationally large

STUDY OF HYBRID PHOTONIC BAND GAP RESONATORS FOR PARTICLE ACCELERATORS

M. R. Masullo,[1] A. Andreone,[2] E. Di Gennaro,[2] S. Albanese,[3]
F. Francomacaro,[3] M. Pannielle,[3] V. G. Vaccaro,[3] and
G. / Vol. 48, No. 12, December 2006 DOI 10.1002/mop



TUYB02 Proceedings of IPAC2012, New Orleans, Louisiana, USA

MANUFACTURE AND TESTING OF OPTICAL-SCALE ACCELERATOR STRUCTURES FROM SILICON AND SILICA*

R. J. England, E. R. Colby, R. Laouar, C. M. McGuinness, B. Montazeri, R. J. Noble,
E. A. Peralta, K. Soong, J. Spencer, D. Walz, Z. Wu, SLAC, Menlo Park, CA 94025, USA
M. Qi, C. Lee, Y. Xuan, L. Fan, L. T. Varghese, Purdue Univ., West Lafayette, IN 47907, USA
R. L. Byer, C-M. Chang, K. J. Leedle, Stanford Univ., Stanford CA, USA
B. Cowan, Tech-X, Boulder CO, USA

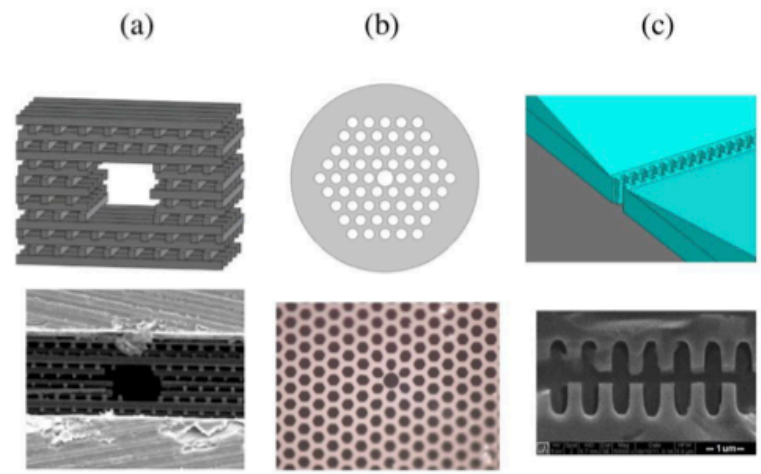


Figure 1: Three dielectric laser accelerator topologies: (a) a 3D silicon photonic crystal structure, (b) a hollow-core photonic bandgap fiber, and (c) a dual-grating structure, showing conceptual illustration (top) and recently fabricated structures (bottom).

Two directions of current photonic cavity research are similar computationally

RF

- Claddings
- 2D rod arrays
  - Metallic
  - Dielectric

Optical

- Dielectric fibers
- 3D structures like woodpiles
- Gratings

Have common goals

- Reduce wake fields (Stable)
- Improve coupling
- Increase breakdown voltage
- …

DLA, DWA modeling presents extreme computational challenges

- Structured mesh (preferably Cartesian) for particles
- Large complexity (parallel) (many layers), so distributed memory computing
- Accurate in both time and frequency domain: embedded boundaries
- Good dispersion for near speed of light

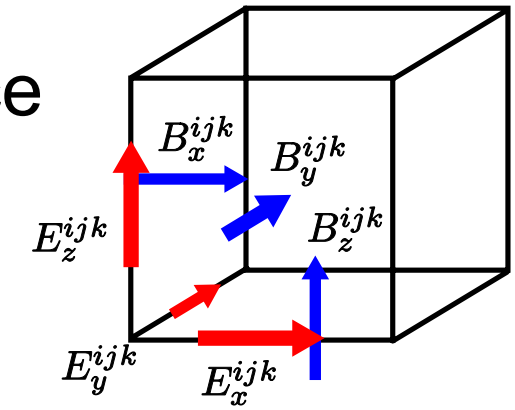
What are the appropriate algorithms?

We have made several algorithm advances

- First 2nd-order accurate embedded boundary algorithm for dielectrics
- Not presented (First scalable frequency domain algorithm for embedded boundary metallics)
- Controlled dispersion for non-cubic cells

Computationally, continuum Maxwell equations become discrete matrix multiplies

- Maxwell discretized by finite difference



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

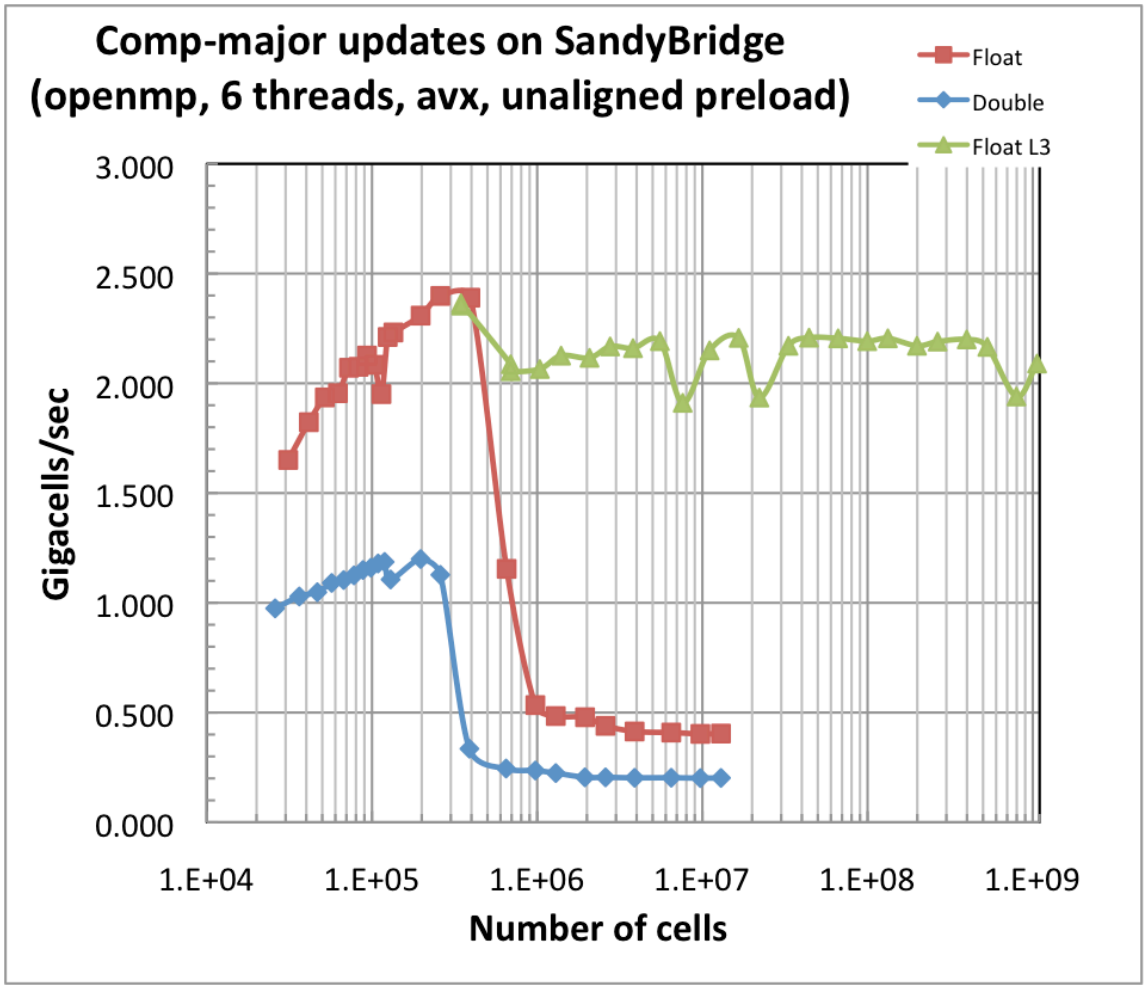
$$\frac{\partial \mathbf{E}}{\partial t} = c^2 \left[\nabla \times \mathbf{B} - \mu_0 \mathbf{j} \right]$$

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

- Same for E
- Regularly structured data is desired
  - Best for access, esp on modern architectures
  - Works well (only?) with particles if rectilinear
- But then, conformal (curved) surfaces are represented by embedded boundaries

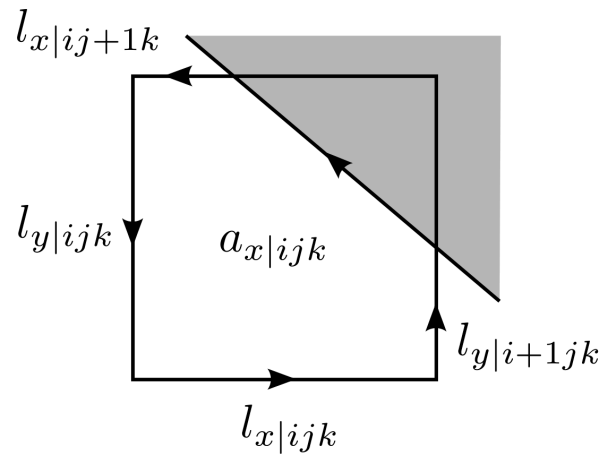
Cache-optimized update blazingly fast

- Previous tanks at 300k cells = 170^3
- Now arbitrarily large systems
- Billion cells at 1 step/s on one cpu
- Not yet in Vorpal, but planned this year
- Dielectrics: perhaps 50%
- GPU Speed
- Not yet at theoretical limit



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

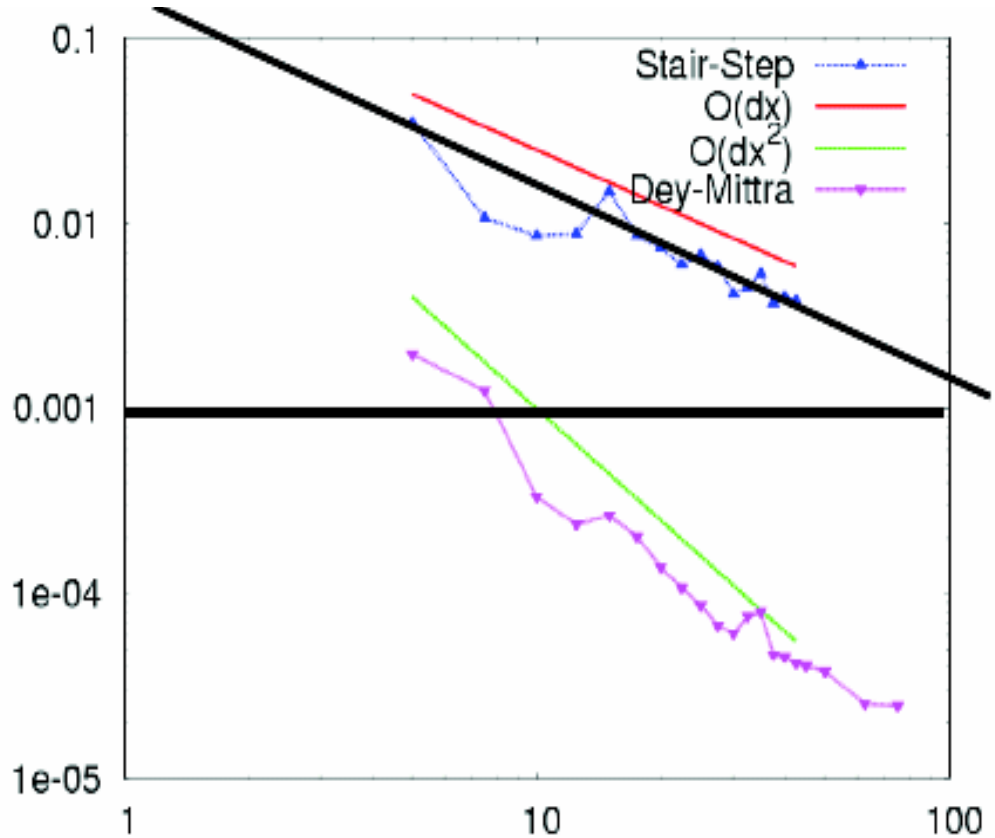


$$\frac{\partial^2 B}{\partial t^2} = -A^{-1} C L C^T B$$

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

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

Embedded mettalic boundary (conformal, cut-cell, Dey-Mittra, PBA) computations more accurate



Stair-step boundary condition (MAGIC, MAFIA, OOPIC) has first-order error.

Dey-Mittra (1997) technique has the second-order error.

30x improvement in accuracy at 10 cells/scale length

Embedded boundary algorithm for dielectric conformal surfaces just developed

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A second-order 3D electromagnetic algorithm for curved interfaces between anisotropic dielectrics on a Yee mesh

Carl A. Bauer[a,*], Gregory R. Werner[a], John R. Cary[a,b]

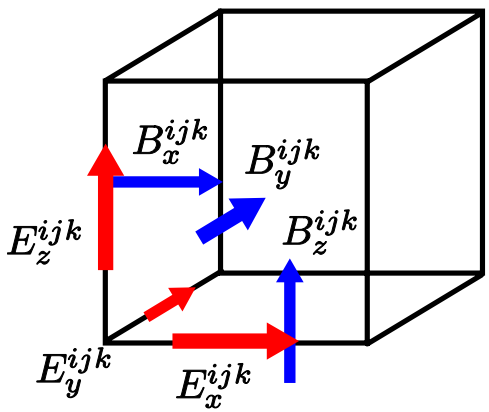
[a] *Department of Physics and the Center for Integrated Plasma Studies, University of Colorado, Boulder, Colorado 80309*

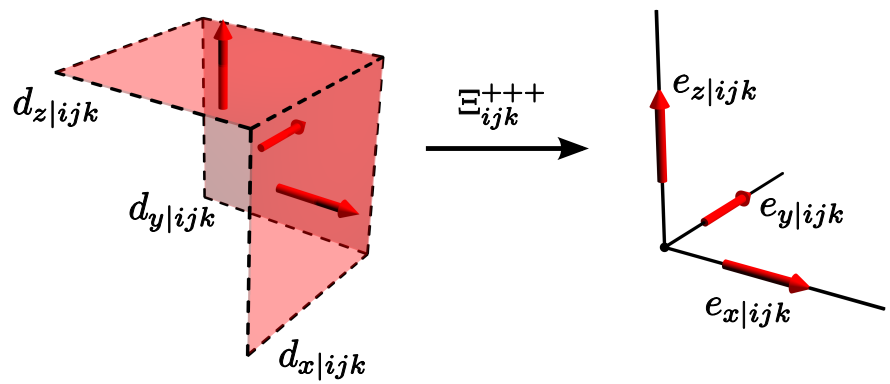
[b] *Tech-X Corporation, Boulder, Colorado 80303*

Abstract

A new frequency-domain electromagnetic algorithm is developed for simulating curved interfaces between anisotropic dielectrics embedded in a Yee mesh with second-order error in resonant frequencies. The algorithm is systematically derived using the finite integration formulation of Maxwell's equations on the Yee mesh. Second-order convergence of the error in resonant frequencies is achieved by guaranteeing first-order error on dielectric boundaries and second-order error in bulk (possibly anisotropic) regions. Convergence studies, conducted for an analytically solvable problem and for a photonic crystal of ellipsoids with anisotropic dielectric constant, both show second-order convergence in error; the convergence is sufficiently smooth such that Richardson extrapolation yields roughly third-order convergence.

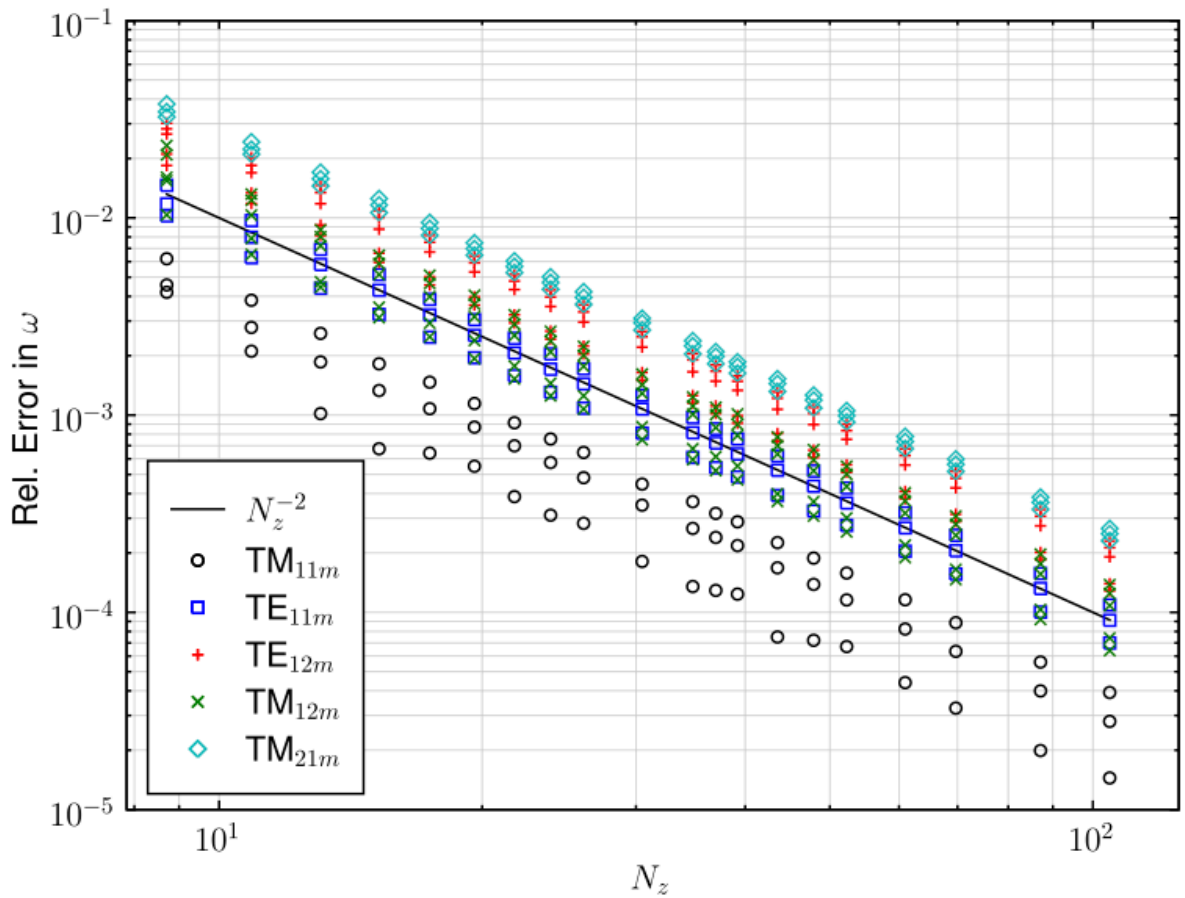
Basics of algorithm: find local, 1st-order accurate relation between E and D





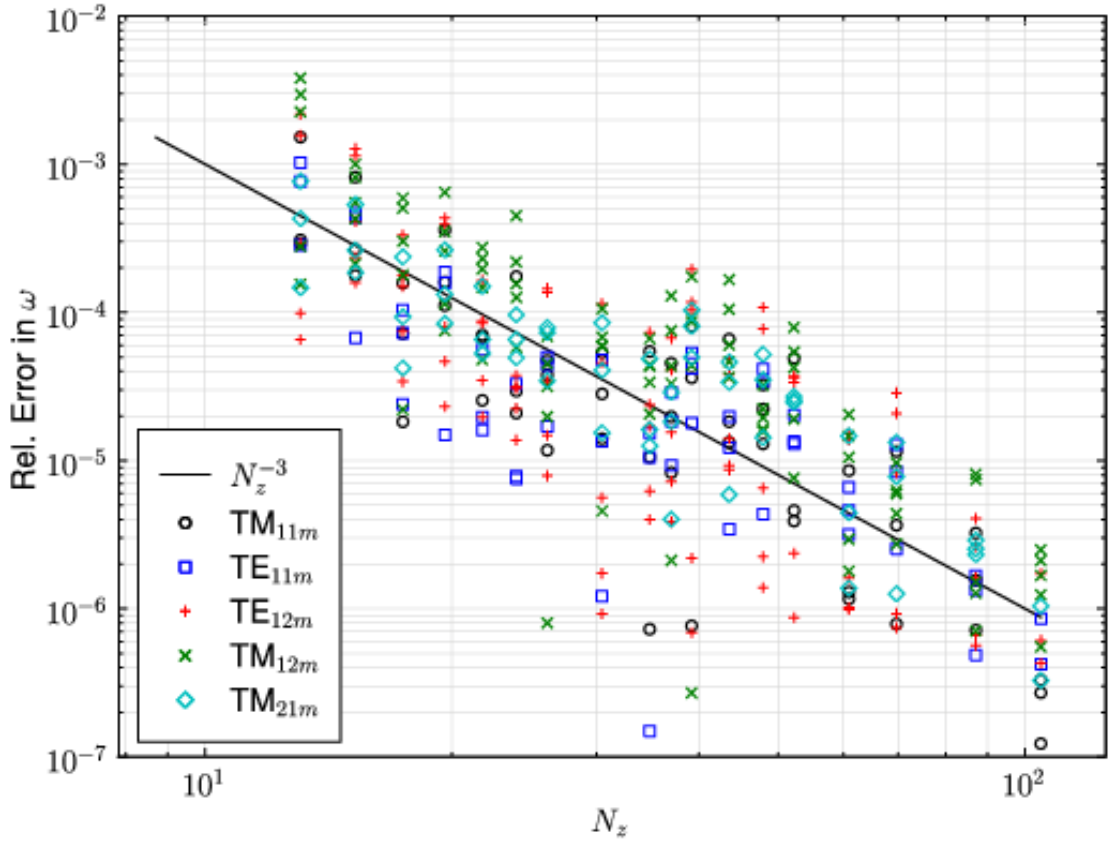
- Assume local plane having different dielectrics on each side
- Assume normal D, tangential E continuous
- Find **D**(D_n, E_t), **E**(D_n, E_t)
- Invert first to find (D_n, E_t)
- Insert these into second to get D to E transformation
- Multiple triads imply multiple methods… detail

Result: Perfect 2nd-order convergence



Dielectric sphere inside metal sphere

Frequency domain: Regular grid allows Richardson extrapolation, 3rd order for free



- Dielectric sphere inside metal sphere, Richardson

For beam simulations, need time domain

- Problem: Matrix is not symmetric
- Has numerical instability
- However, forced symmetrization gives very good answer
- GR Werner, CA Bauer, JR Cary - arXiv:1212.4857, 2012
- Accepted J. Comput. Phys., Aug 2013
- Will appear 2014

A More Accurate, Stable, FDTD Algorithm for Electromagnetics in Anisotropic Dielectrics☆

Gregory R. Werner[a,*], Carl A. Bauer[a], John R. Cary[a,b]

[a] *Center for Integrated Plasma Studies, University of Colorado, Boulder, CO 80309*
[b] *Tech-X Corporation, Boulder, CO 80303*

Abstract

A more accurate, stable, finite-difference time-domain (FDTD) algorithm is developed for simulating Maxwell's equations with isotropic or anisotropic dielectric materials. This algorithm is in many cases more accurate than previous algorithms (G. R. Werner et. al., 2007; A. F. Oskooi et. al., 2009), and it remedies a defect that causes instability with high dielectric contrast (usually for $\epsilon \gg 10$) with either isotropic or anisotropic dielectrics. Ultimately this algorithm has first-order error (in the grid cell size) when the dielectric boundaries are sharp, due to field discontinuities at the dielectric interface. Accurate treatment of the discontinuities, in the limit of infinite wavelength, leads to an asymmetric, unstable update (C. A. Bauer et. al., 2011), but the symmetrized version of the latter is stable and more accurate than other FDTD methods. The convergence of field values supports the hypothesis that global first-order error can be achieved by second-order error in bulk material with zero-order error on the surface. This latter point is extremely important for any applications measuring surface fields.

Good results for small contrast

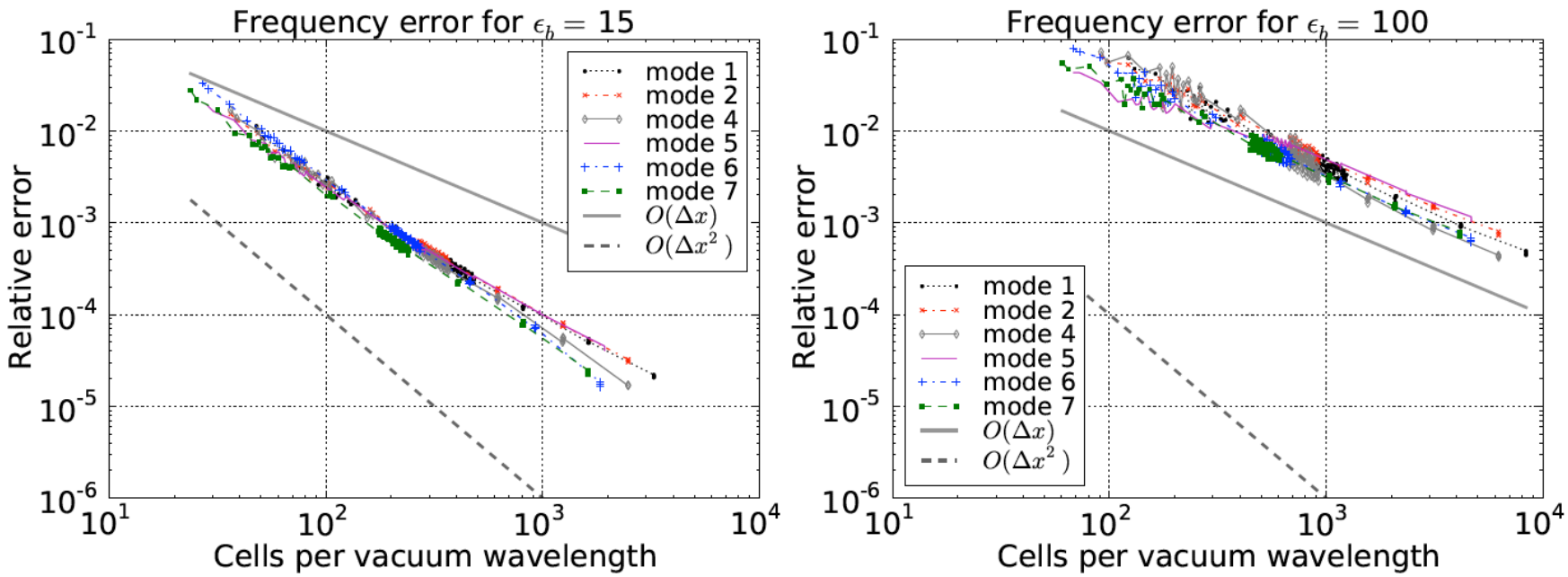


Figure 7: For the new method, 2D, isotropic: relative errors vs. resolution for mode frequencies for a 2D photonic crystal of $r/a = 0.37$ isotropic discs with dielectric contrast $\epsilon_b = 15$ (left) and $\epsilon_b = 100$ (right). Again, the error transitions from second-order to first-order. The transition point occurs at coarser resolution for higher dielectric contrast.

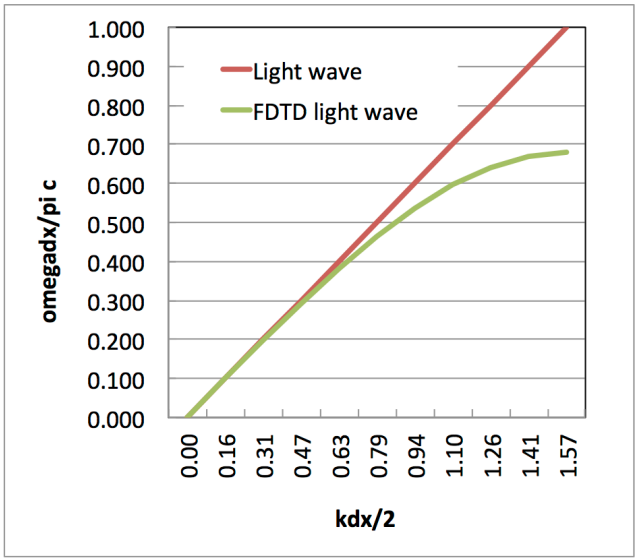
For beam problems, standard FDTD can be problematic due to dispersion

- Wavelength comparable to transverse dimension: cubic cells
- CFL implies
- At Nyquist limit
- Quite subluminal
- Choices:
  - Increase number of cells longitudinally

$$\left|\sin\left(\omega\Delta t/2\right)\right| = \left|\left(c\Delta t/\Delta x\right)\sin\left(k\Delta x/2\right)\right|$$

$$c\Delta t = \Delta x/\sqrt{3}$$

$$\frac{\omega\Delta x}{\pi c} = \frac{2\sqrt{3}}{\pi}\arcsin\left(\left(1/\sqrt{3}\right)\sin\left(k\Delta x/2\right)\right)$$



$$\left|\sin\left(v_{\varphi r}\pi/2\sqrt{3}\right)\right| = 1/\sqrt{3} \qquad \gamma_{\varphi r} = 1.36$$

$$v_{\varphi r} = 0.679$$

Controlled dispersion allows one to fix this

PHYSICAL REVIEW SPECIAL TOPICS - ACCELERATORS AND BEAMS **16**, 041303 (2013)

Generalized algorithm for control of numerical dispersion in explicit time-domain electromagnetic simulations

Benjamin M. Cowan,* David L. Bruhwiler,† John R. Cary, and Estelle Cormier-Michel
Tech-X Corporation, Boulder, Colorado 80303, USA

Cameron G. R. Geddes
LOASIS program, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA
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We describe a modification to the finite-difference time-domain algorithm for electromagnetics on a Cartesian grid which eliminates numerical dispersion error in vacuum for waves propagating along a grid axis. We provide details of the algorithm, which generalizes previous work by allowing 3D operation with a wide choice of aspect ratio, and give conditions to eliminate dispersive errors along one or more of the coordinate axes. We discuss the algorithm in the context of laser-plasma acceleration simulation, showing significant reduction—up to a factor of 280, at a plasma density of 10^{23} m^{-3}—of the dispersion error of a linear laser pulse in a plasma channel. We then compare the new algorithm with the standard electromagnetic update for laser-plasma accelerator stage simulations, demonstrating that by controlling numerical dispersion, the new algorithm allows more accurate simulation than is otherwise obtained. We also show that the algorithm can be used to overcome the critical but difficult challenge of consistent initialization of a relativistic particle beam and its fields in an accelerator simulation.

- Gets $\omega = kc$ exactly along beam direction
- Requires propagation dx ≤ others, works for cubic cells

Controlled dispersion eliminates numerical Cerenkov, other nonphysical fields

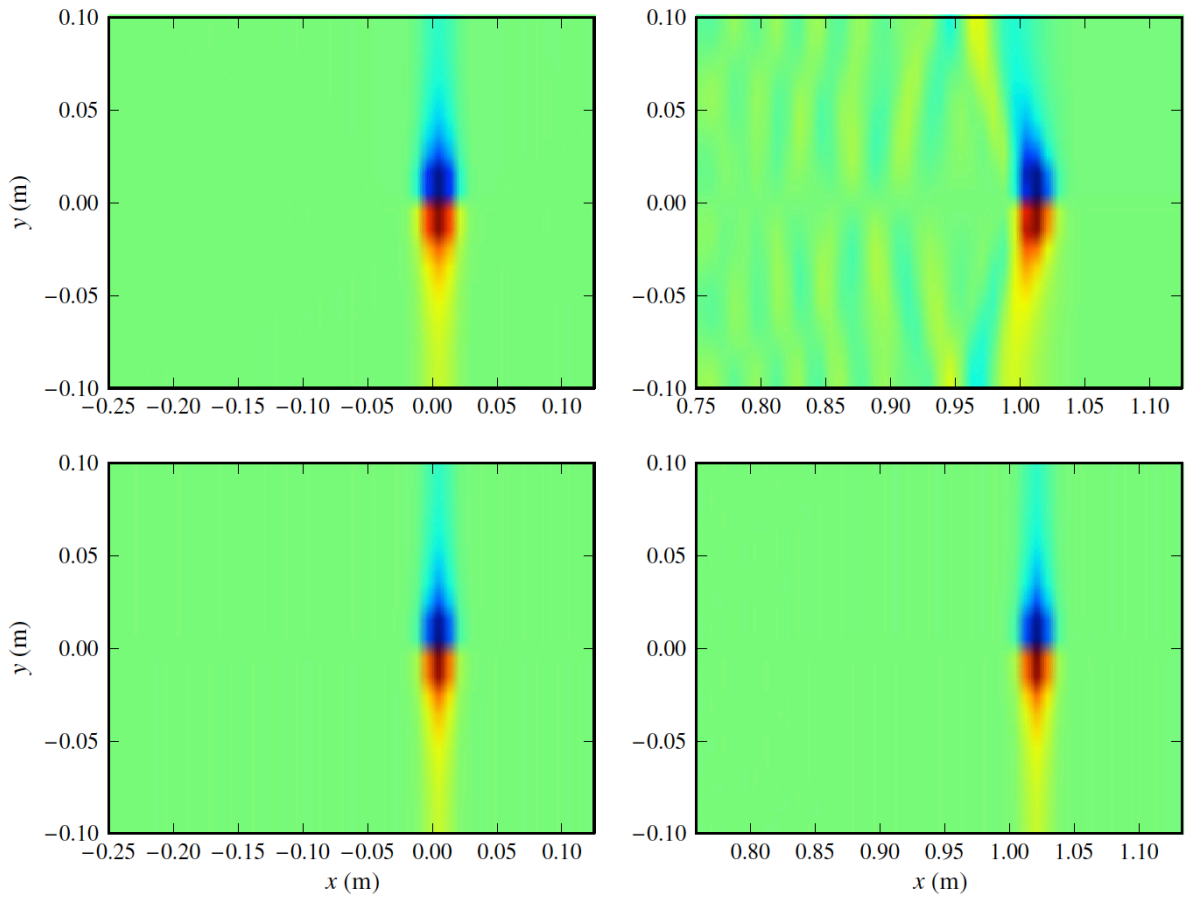


FIG. 4. Transverse field E_y at the pipe midplane in z. Top left: Initial field with the normal dispersion algorithm; bottom left: initial field with the controlled dispersion algorithm; top right: field after 1 m propagation with normal dispersion; bottom right: field after propagation with controlled dispersion.

Controlled dispersion can give factor of 2 difference in final energy in LPA

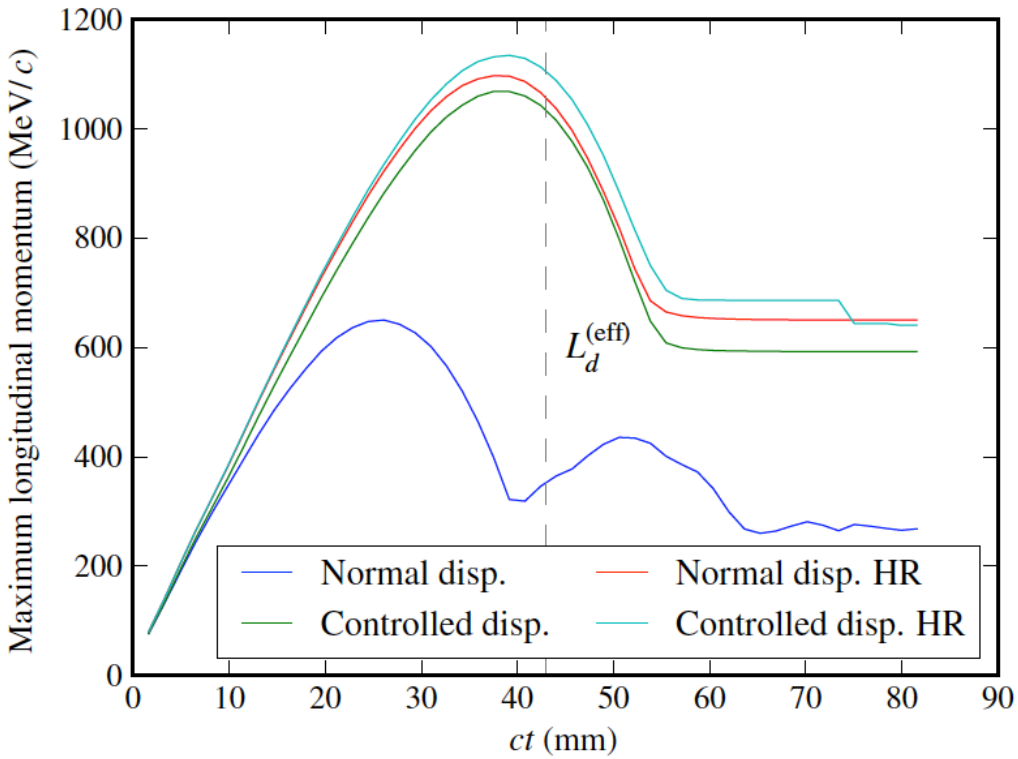
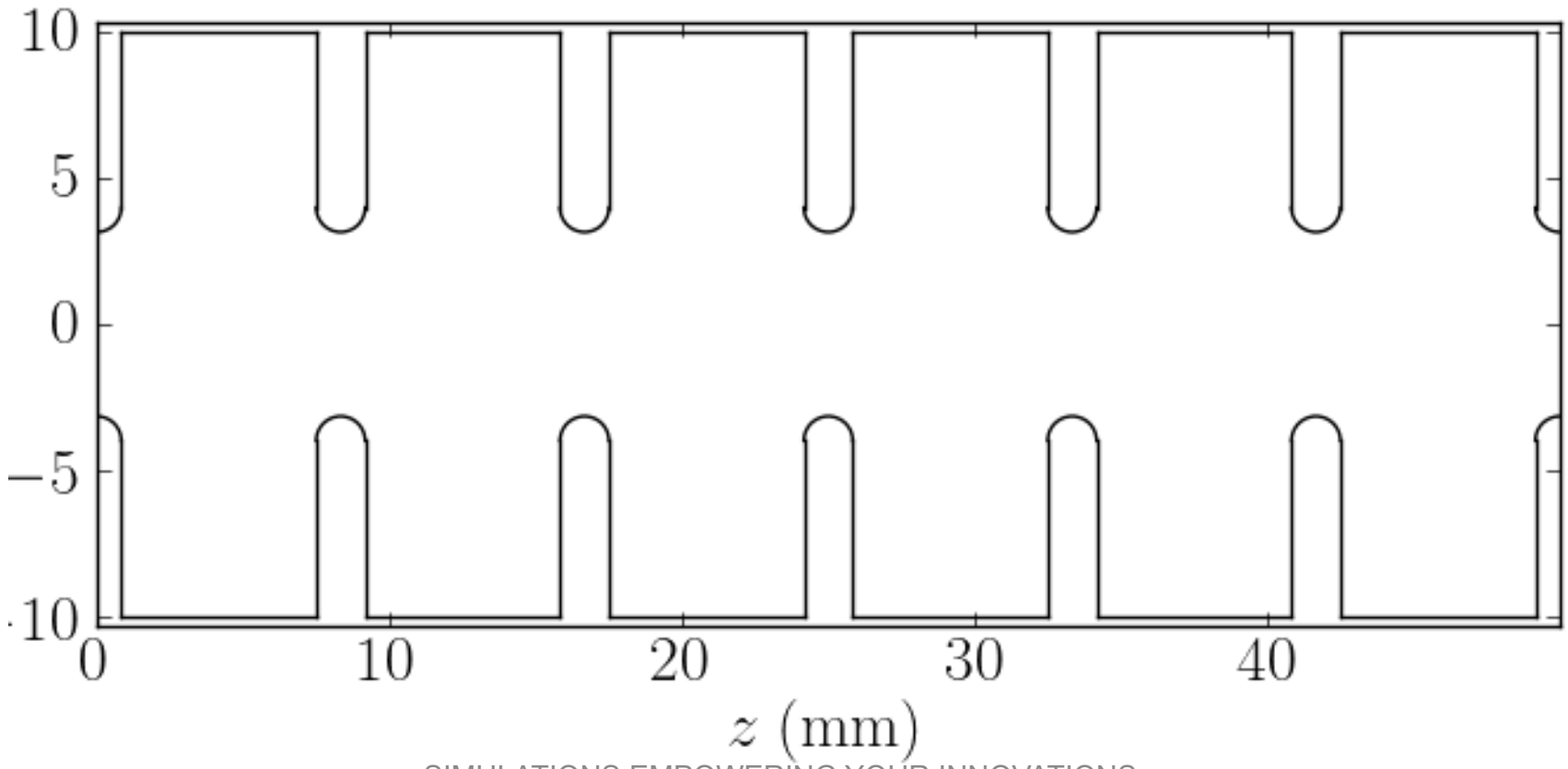


FIG. 2. The maximum test particle momentum, as a function of normalized propagation time, which is approximately equal to propagation distance. The dashed line indicates the effective linear dephasing length, $L_d = 43.0$ mm. In the legend, "HR" refers to the high resolution simulations, with $\Delta x = \lambda_0/32$; those not labeled HR have $\Delta x = \lambda_0/16$.

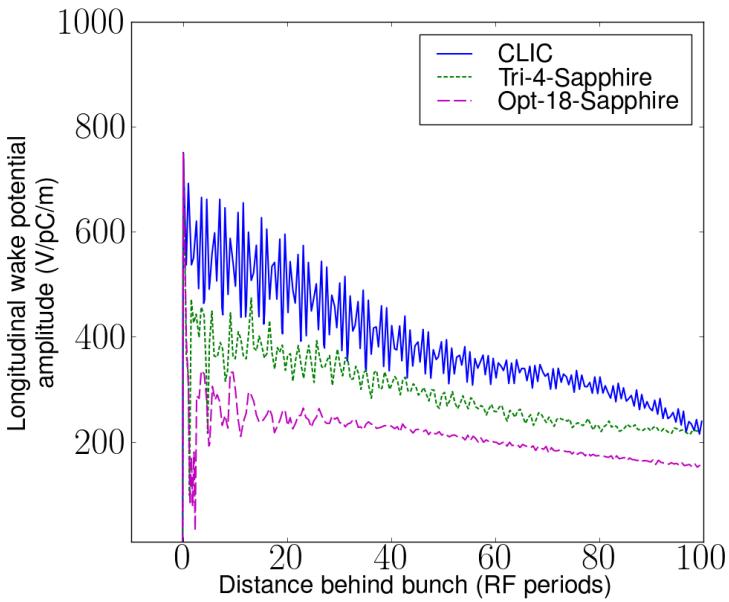
Wake fields in PhC Structures

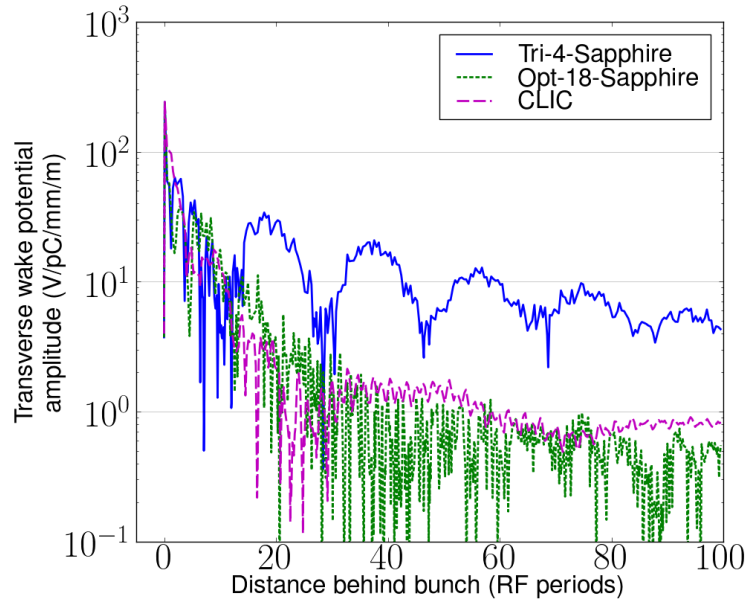
Wake potential calculations identify troubling frequencies

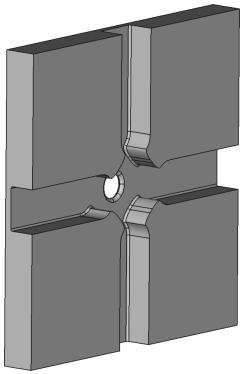
- VORPAL PIC
- 8-cell cavities; identical cells
- Bunch length σ_z = 1mm; bunch cutoff ≈ 50 GHz



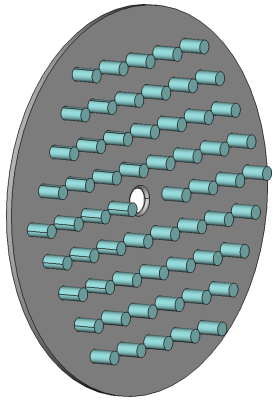
Hybrid, optimized cavities: lower longitudinal wake fields, comparable transverse



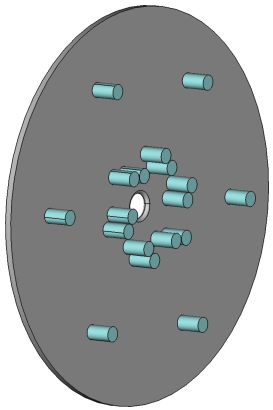




CLIC

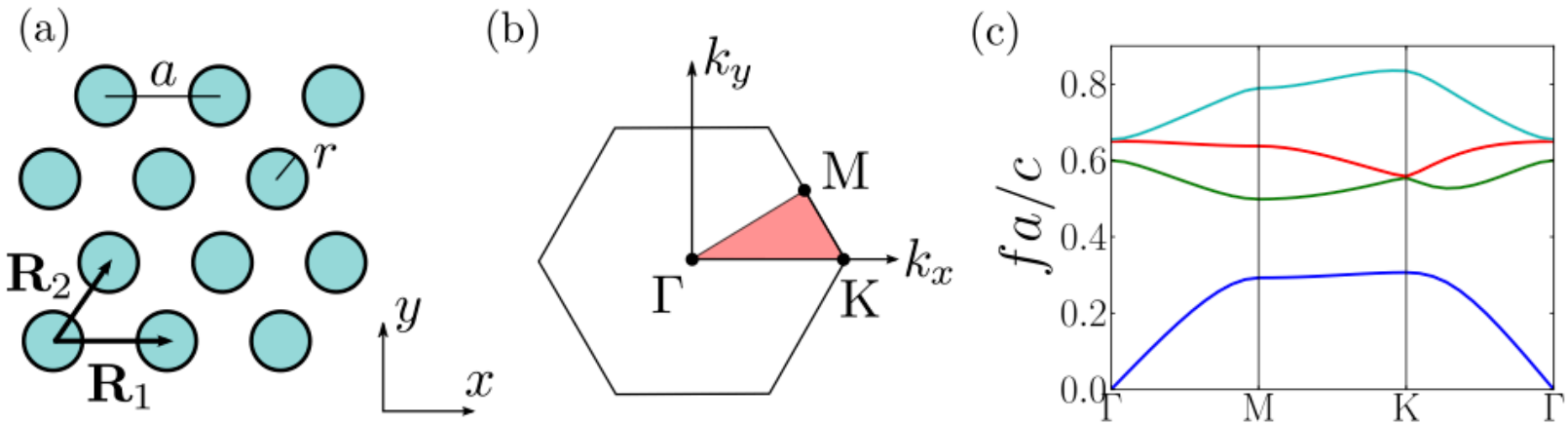


Tri-4



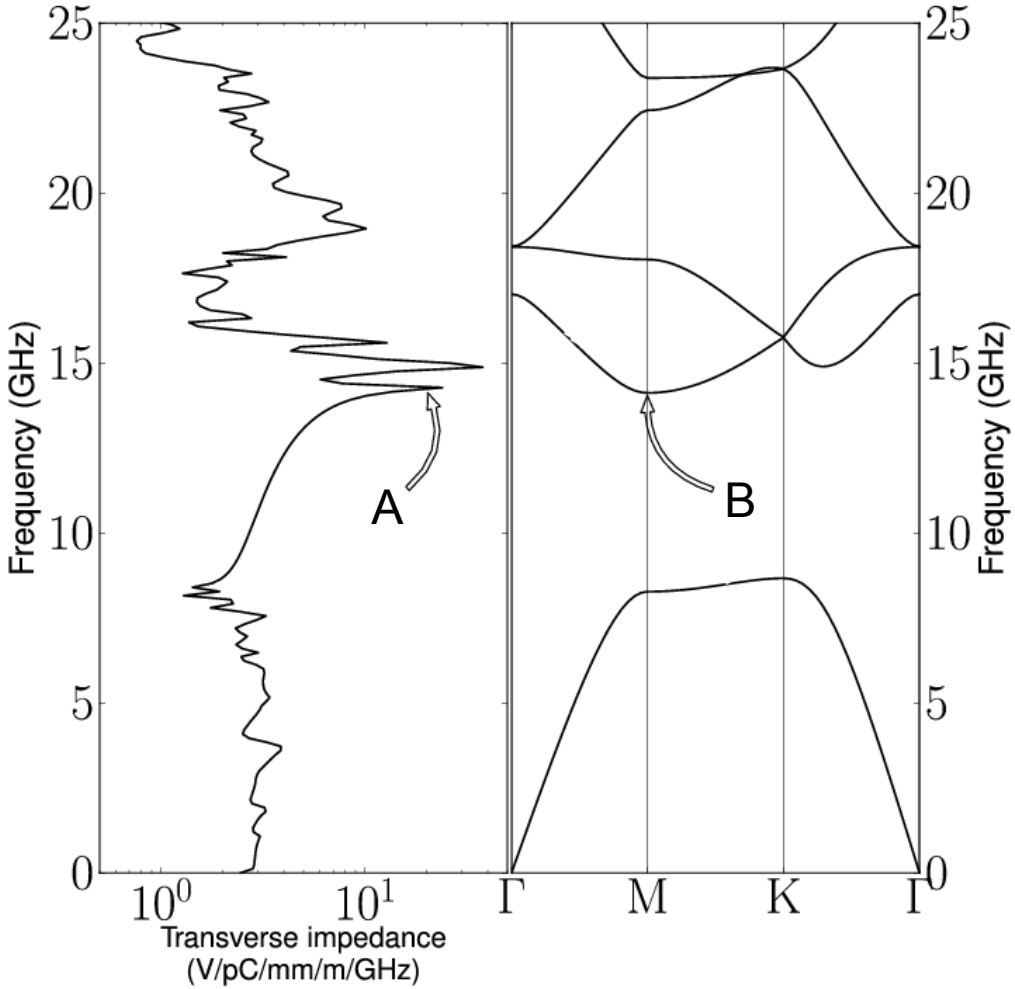
Opt-18

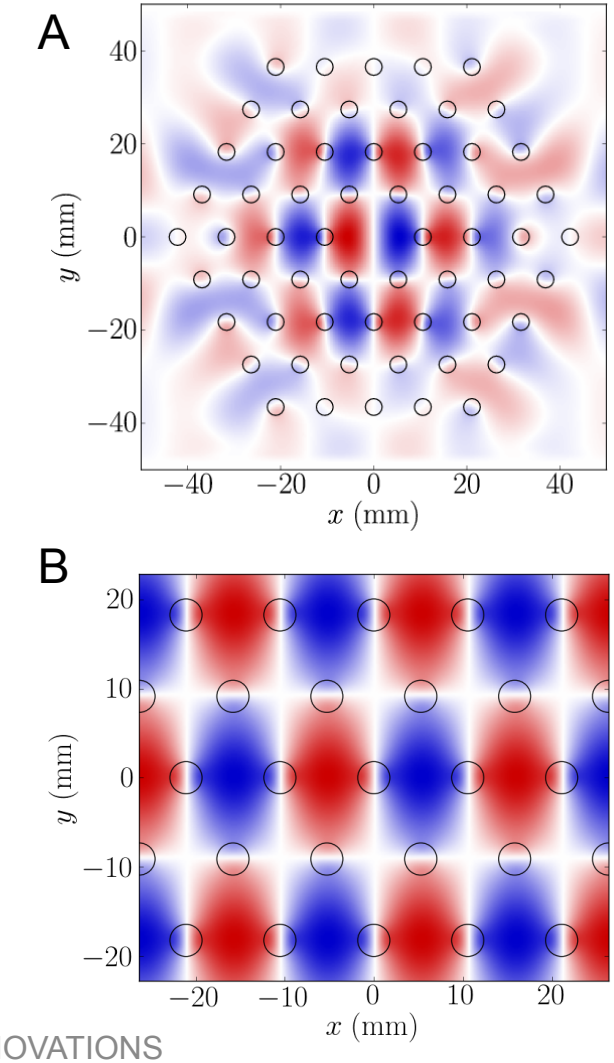
Understanding of frequency comes from computing infinite-lattice dispersion relation



Modes vary in angle
Band shown by transit in k space

Comparing transverse dipole wake impedance with PhC band diagram indicates harm from dispersion inflection points





Conclusions

- Embedded boundary algorithms can combine accuracy with data structures needed for speed
  - New frequency domain embedded boundary dielectric algorithm is second order
  - Time domain correspondent has good accuracy
  - Dispersion control removes non physical effects
- Wakefields for PhC cavities understood, modes identified

Lots of directions

- Cache aware dielectric algorithms
- Improved coupling
- Dispersive media
- Accurate surface fields (multipacting, heating, breakdown)
- Optimal implementations with advanced instructions and on accelerators
  - AVX
  - GPU
  - MIC
- Do we continue to custom code each chip? (Or move to OpenCL or OpenACC?