Toward Extreme-Scale: High-Order Algorithms for Electromagnetic and Fluid Modeling

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ASCAC meeting , November 10, 2010

Outline

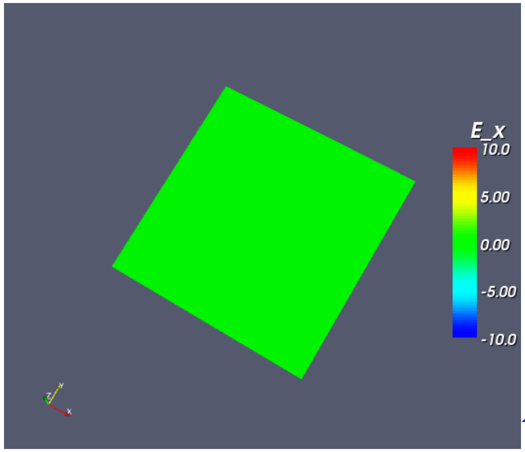
- Overview for Application Problems
- Motivation for using High-Order Methods
- Production Codes: *NekCEM* and *NekLBM*
- Efficiency and Scalability on >100K cores
- Applications: Results on Nanoscience, Accelerator, and Fluid Modeling
- Summary for Future Plans

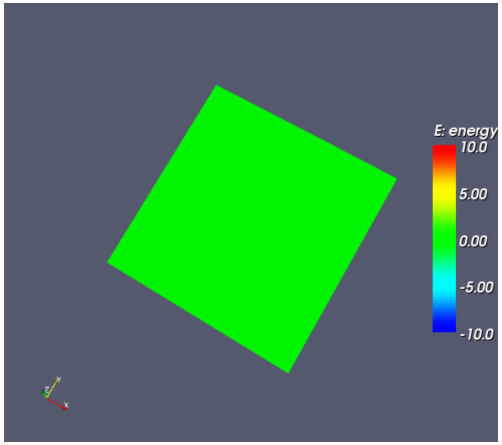
Applications

Supported by
DOE AMR Program

Nanoscience Application

Maxwell Equations + **Drude** Model



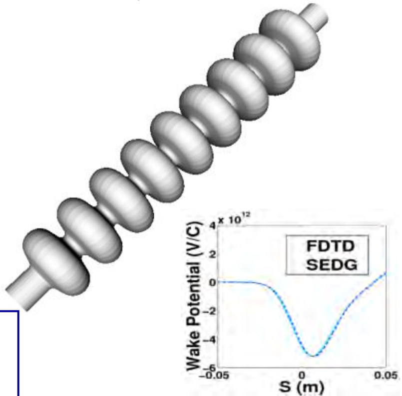


Predict Light Enhancement on the Surface of Metallic Nanodevices

High-Order Methods

Accelerator Modeling

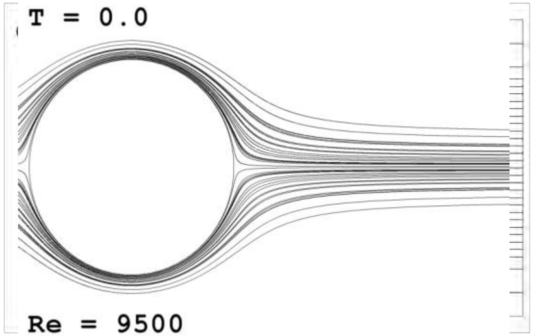
Maxwell Equations
Poisson equation



Wakefield Calculations for Accelerator Component

Fluid Simulations

Lattice Boltzmann Equations
– **Incompressible / compressible** flows at high Reynolds numbers



Motivation for High-Order Methods

- Representing geometry accurately: material discontinuities, conforming meshes

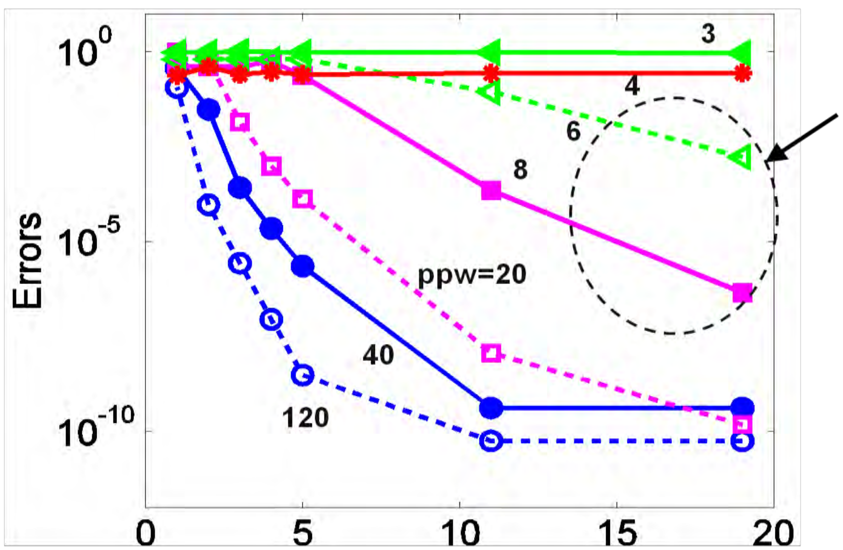
- Long time integration requires minimal numerical dispersion

- High-order methods deliver engineering accuracy with fewer points per wavelength. (min ppw = 2 by Nyquist sampling thm)

In practice, applications require:

- Efficient implementation
- Scalable parallel performance
- Flexible geometry representation

1D Maxwell, *n*=120, varying wavenumber

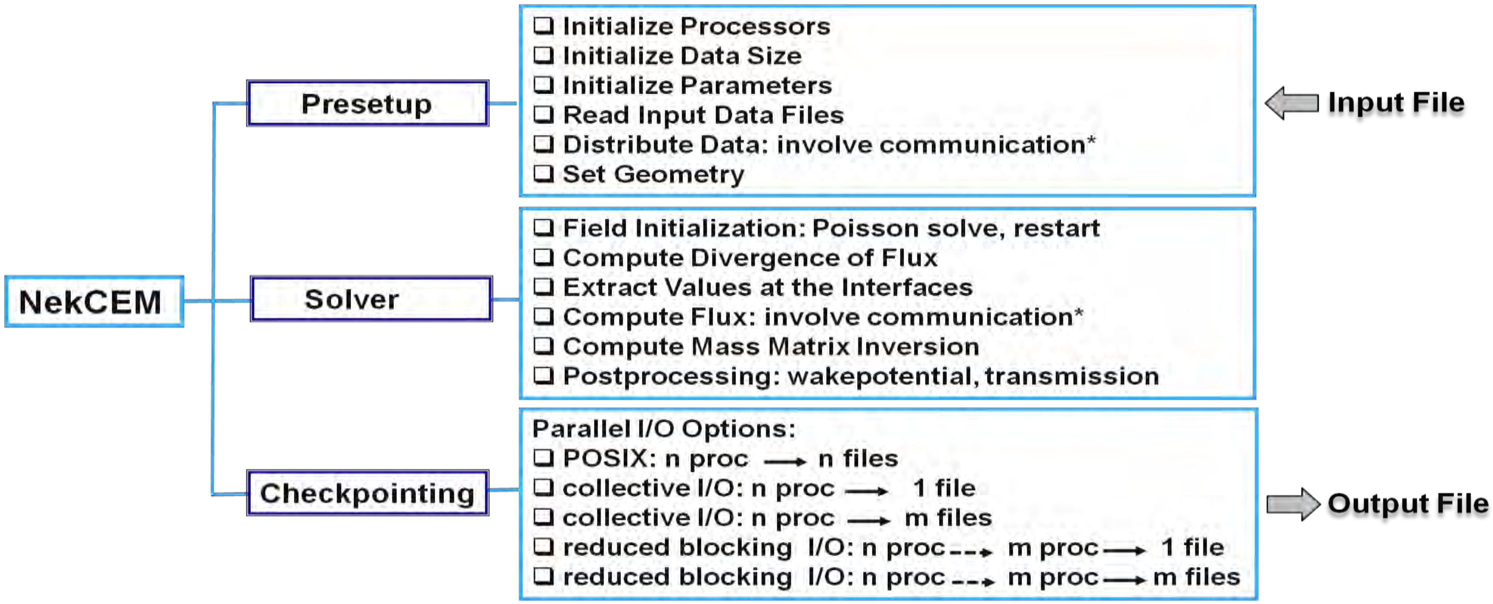


Polynomial order, N

(at fixed resolution, n=120 points)

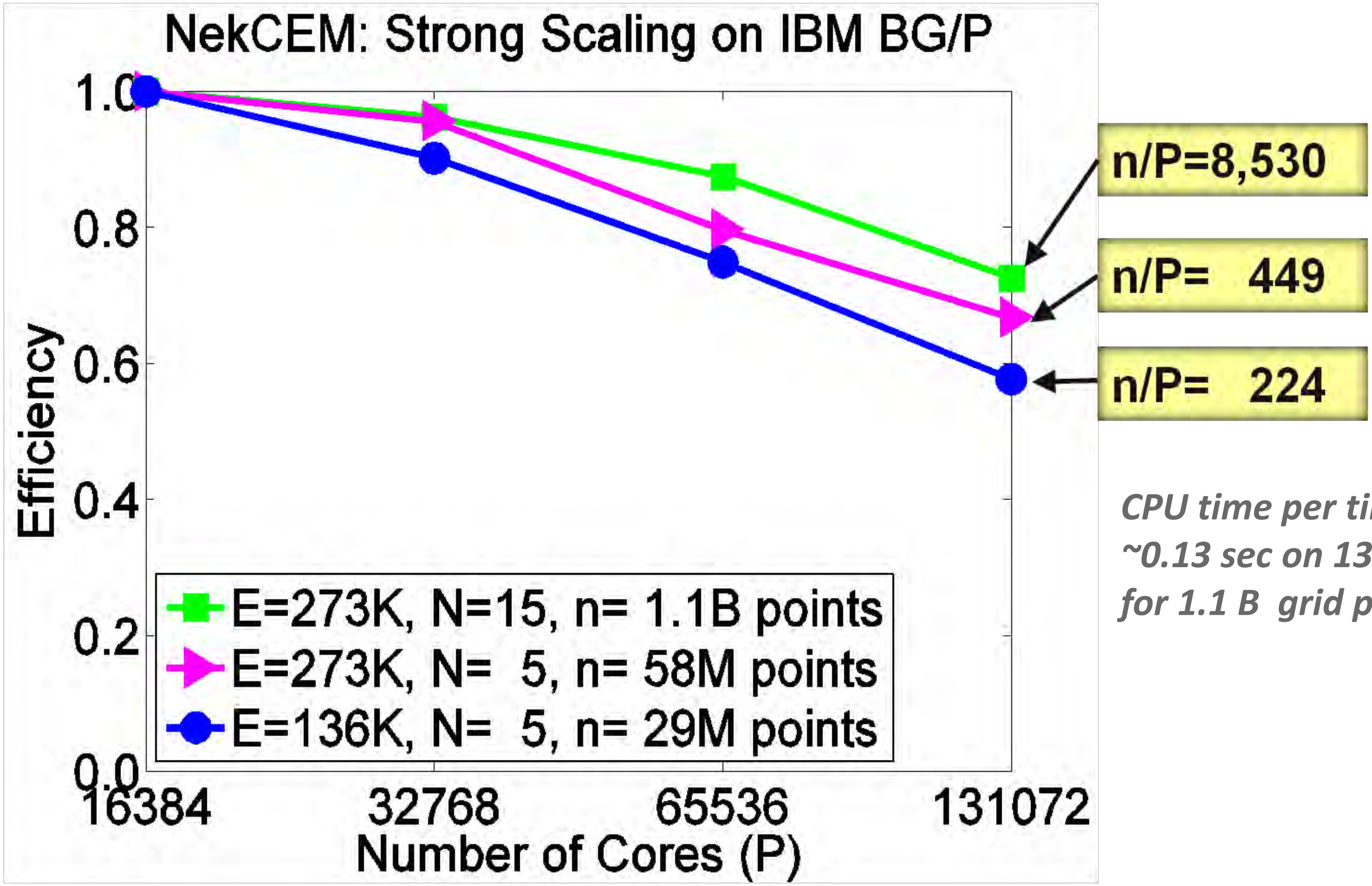
NekCEM/NekLBM

- **Spectral-Element DG Time-Domain Solvers: using core structure of *Nek5000***
  - Open source code: https://svn.mcs.anl.gov/repos/NEKCEM
  - Open source code: https://svn.mcs.anl.gov/repos/NEKLBM
  - Argonne developed (initiated) Maxwell and Boltzmann solvers in Fortran and C.
  - Currently scalable up to > 100K cores (more than 1.1 B grids points)
  - Paralle I/O: output in a single or multiple files: scalable up to 65K cores



NekCEM Runtime Tasks

Parallel Scalability



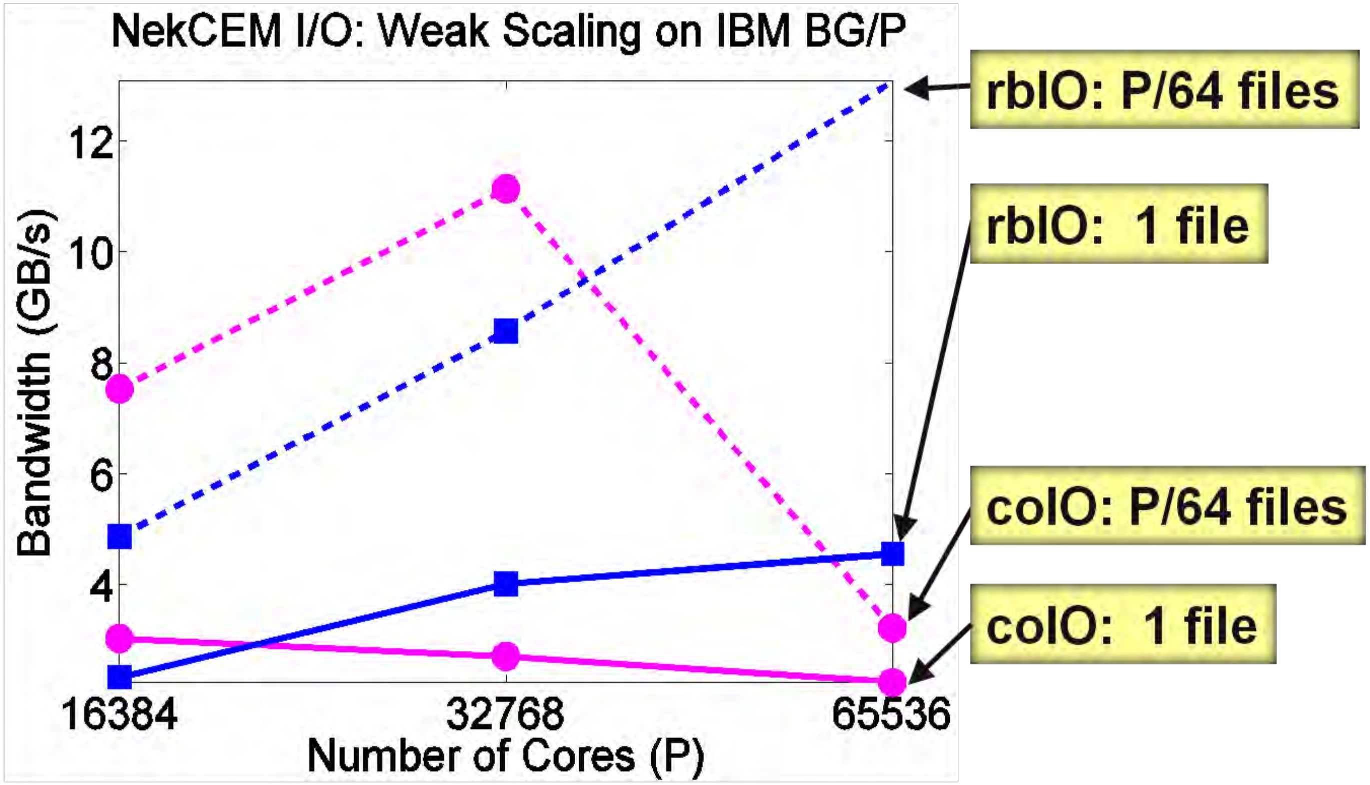
CPU time per timestep ~0.13 sec on 131K cores for 1.1 B grid points

Excellent scaling results from:

- ***DG: only six messages per element (not 26)***
- ***Vector communication (1 msg for 6 fields)***

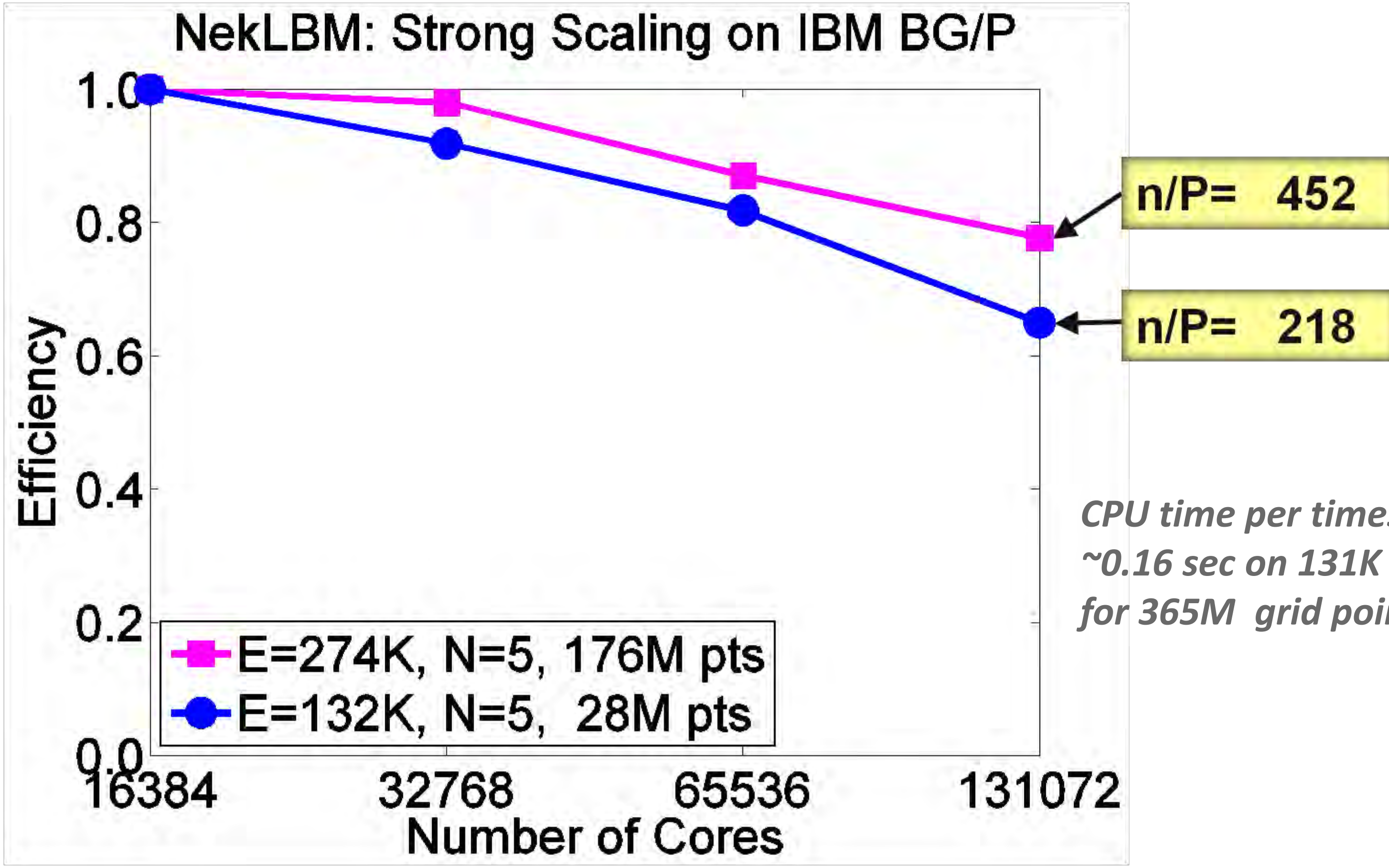
Parallel I/O Scalability

ICS 2011, Jng Fu, RPI



rbIO: reduced-blocking I/O
coIO: collective I/O

Parallel Scalability, LBM Code



CPU time per timestep ~0.16 sec on 131K cores for 365M grid points

Excellent scaling results from:

- DG: only six messages per element (not 26)

- Vector communication (1 msg for 19 fields)

Weak Formulation

- Maxwell Equation (source-free in free space) and weak form:

$$\square \frac{\partial q}{\partial t} + \nabla \bullet \mathrm{F}(q) = 0 \xrightarrow{\textit{weak form}} \left(\square \frac{\partial q}{\partial t} + \nabla \bullet \mathrm{F}(q), \phi \right)_{\Omega^e} = 0$$

$$\square = \begin{bmatrix} \mu & 0 & 0 & 0 & 0 & 0 \\ 0 & \mu & 0 & 0 & 0 & 0 \\ 0 & 0 & \mu & 0 & 0 & 0 \\ 0 & 0 & 0 & \varepsilon & 0 & 0 \\ 0 & 0 & 0 & 0 & \varepsilon & 0 \\ 0 & 0 & 0 & 0 & 0 & \varepsilon \end{bmatrix} \qquad q = \begin{bmatrix} H_x \\ H_y \\ H_z \\ E_x \\ E_y \\ E_z \end{bmatrix} \qquad \mathrm{F}(q) = -\begin{bmatrix} 0 & -E_z & E_y & 0 & H_z & -H_y \\ E_z & 0 & -E_x & -H_z & 0 & H_x \\ -E_y & E_x & 0 & H_y & -H_x & 0 \end{bmatrix}^T$$

Flux

- Define numerical flux F* and integrate by parts: DG weak form

$$\left(\square \frac{\partial q^-}{\partial t}, \phi \right)_{\Omega^e} = - \; \nabla \bullet \mathrm{F}(q^-), \phi \;_{\Omega^e} + \; \vec{n} \square [\mathrm{F}(q^-) - \mathrm{F}^*(q^-, q^+)], \phi \;_{\partial\Omega^e}$$

$$n \square (\mathrm{F} - \mathrm{F}^*)(q, q^+) = \begin{Bmatrix} -Y^+ \vec{n} \times [E^+ - E] - \alpha \vec{n} \times \vec{n} \times [H^+ - H] \; /(Y + Y^+) \\ Z^+ \vec{n} \times [H^+ - H] - \alpha \vec{n} \times \vec{n} \times [E^+ - E] \; /(Z + Z^+) \end{Bmatrix}$$

SEDG Method

- Spectral element discretization: tensor product basis of 1D Lagrange interpolation polynomial based on Legendre-Gauss-Lobatto grids.

$$q_N^e(x^e) = \sum_{i=0}^{N}\sum_{j=0}^{N}\sum_{k=0}^{N} q_{ijk} l_i(\xi) l_j(\eta) l_k(\gamma)$$

- Hexahedral body-fitted mesh: Gorden-Hall mapping

$$x^e = (x, y, z) \quad \theta = (\xi, \eta, \gamma) \in [-1,1]^3$$

- 1D mass matrix is diagonal: $\hat{M}_{ij} = \sum_{k=0}^{N} w_k l_i(\xi_k) l_j(\xi_k)$

- Surface integration:

$$\oint_{\partial\Omega} \mathbf{n} \cdot (\boldsymbol{F}_\alpha - \boldsymbol{F}_\alpha^*) l_i(\xi) l_i(\eta) J \, d\xi \, d\eta$$

Semi-Discrete Formulations

$$M^{\mu}\frac{dH_x}{dt}+(D_yE_z-D_zE_y)=R(F_H)_x$$

$$M^{\mu}\frac{dH_y}{dt}+(D_zE_x-D_xE_z)=R(F_H)_y$$

$$M^{\mu}\frac{dH_z}{dt}+(D_xE_y-D_yE_x)=R(F_H)_z$$

$$M^{\varepsilon}\frac{dE_x}{dt}-(D_yH_z-D_zH_y)=R(F_E)_x$$

$$M^{\varepsilon}\frac{dE_y}{dt}-(D_zH_x-D_xH_z)=R(F_E)_y$$

$$M^{\varepsilon}\frac{dE_z}{dt}-(D_xH_y-D_yH_x)=R(F_E)$$

Mass and Stiffness matrices

$$M^{\mu}=\mu(\psi_{ijk},\psi_{\hat{i}\hat{j}\hat{k}}),M^{\varepsilon}=\varepsilon(\psi_{ijk},\psi_{\hat{i}\hat{j}\hat{k}})$$

$$D_x=\left(\frac{\partial\psi_{ijk}}{\partial x},\psi_{\hat{i}\hat{j}\hat{k}}\right),D_y=\left(\frac{\partial\psi_{ijk}}{\partial y},\psi_{\hat{i}\hat{j}\hat{k}}\right),D_z=\left(\frac{\partial\psi_{ijk}}{\partial z},\psi_{\hat{i}\hat{j}\hat{k}}\right)$$

$$(\psi_{ijk},\psi_{\hat{i}\hat{j}\hat{k}})=J(\hat{M}\otimes\hat{M}\otimes\hat{M})$$

Diagonal Mass matrix

$$\left(\frac{\partial\psi_{ijk}}{\partial x},\psi_{\hat{i}\hat{j}\hat{k}}\right)=J(G^{\xi x}D_{\xi}+G^{\eta x}D_{\eta}+G^{\gamma x}D_{\gamma}),$$

$$\left(\frac{\partial\psi_{ijk}}{\partial y},\psi_{\hat{i}\hat{j}\hat{k}}\right)=J(G^{\xi y}D_{\xi}+G^{\eta y}D_{\eta}+G^{\gamma y}D_{\gamma}),$$

$$\left(\frac{\partial\psi_{ijk}}{\partial z},\psi_{\hat{i}\hat{j}\hat{k}}\right)=J(G^{\xi z}D_{\xi}+G^{\eta z}D_{\eta}+G^{\gamma z}D_{\gamma}),$$

$$D_{\xi}=\hat{M}\otimes\hat{M}\otimes\hat{M}\hat{D},$$

$$D_{\eta}=\hat{M}\otimes\hat{M}\hat{D}\otimes\hat{M},$$

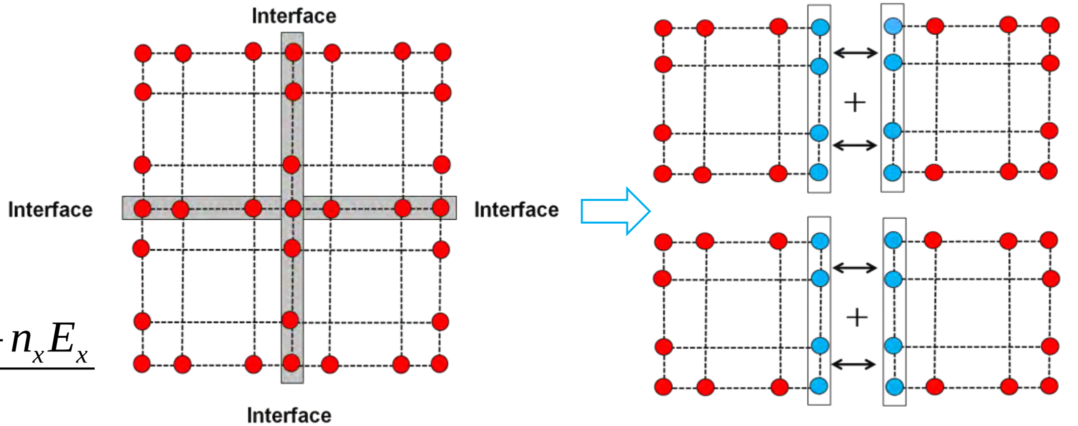
$$D_{\gamma}=\hat{M}\hat{D}\otimes\hat{M}\otimes\hat{M}$$

Tensor product of 1D differentiation matrix: ***matrix-matrix products***

Communication

- Decompose face values into local and neighboring element and assign the same form: (eg, central flux)

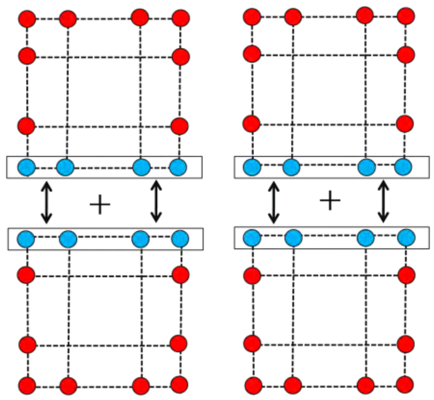
$$n_x = -n_x^+ \rightarrow n_x \frac{(E_x^+ - E_x)}{2} = \frac{-n_x^+ E_x^+ - n_x E_x}{2}$$



- Communications (upwind)

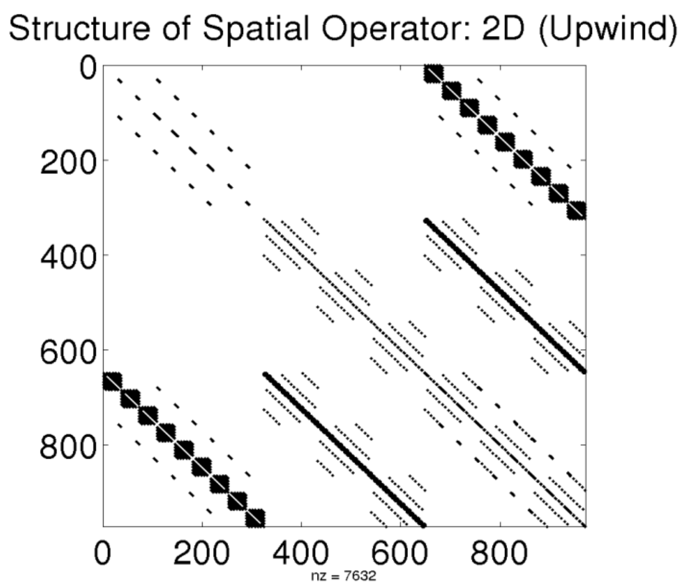
$$R(F_H) = \begin{cases} -fH_x + \alpha(n_y E_y - n_y E_z) & fH_x = n_z E_y - n_y E_z \\ -fH_y + \alpha(n_z E_x - n_x E_z) & fH_y = n_z E_x - n_x E_z \\ -fH_z + \alpha(n_x E_y - n_y E_x) & fH_z = n_x E_y - n_y E_x \end{cases}$$

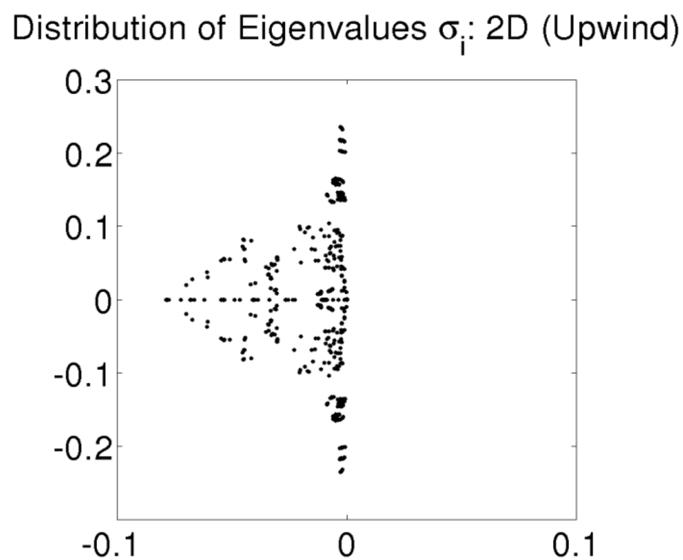
$$R(F_E) = \begin{cases} fE_x + \alpha(n_y H_y - n_y H_z) & fE_x = -(n_x H_y - n_y H_z) \\ fE_y + \alpha(n_z H_x - n_x H_z) & fE_y = -(n_z H_x - n_x H_z) \\ fE_z + \alpha(n_x H_y - n_y H_x) & fE_z = -(n_x H_y - n_y H_x) \end{cases}$$

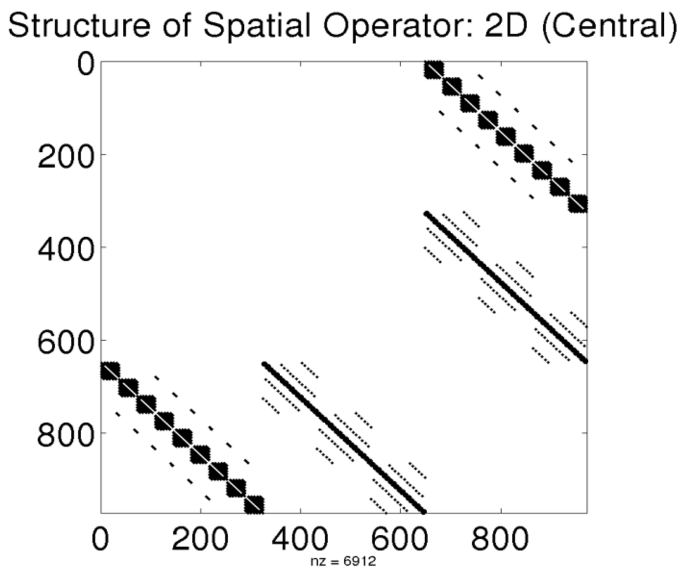


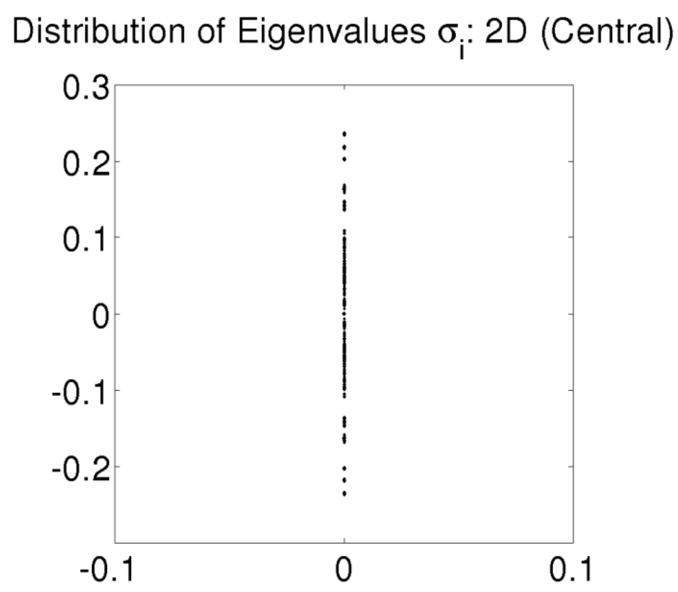
- Messages between element faces for **Ex,Ey,Ez,Hx,Hy,Hz** stored **into a single array**: ***communication latency reduction by 6x***

Spatial Operators









High-Order Time Integration

- Semidiscrete scheme::

$$\frac{dq_N}{dt} = -Aq_N,$$
$$q_N = (H_x^N, H_y^N, H_z^N, E_x^N, E_y^N, E_z^N)$$

- Exponential time integrator (Krylov subspace approximation)

$$q_N(n\Delta t + \Delta t) = e^{-\Delta t A} q_N(n\Delta t)$$

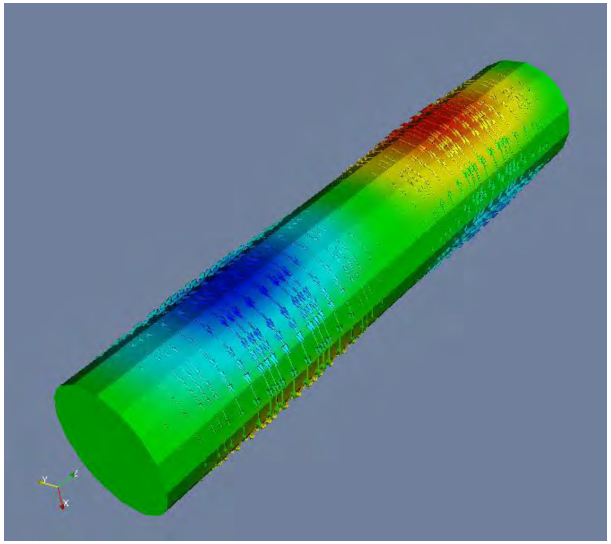
$$e^{\Delta t A} q = q + \frac{\Delta t A}{1!} q + \frac{(\Delta t A)^2}{2!} q + \cdots \approx K_m(A, q) = \text{span}\{q, Aq, A^2 q, \ldots, A^{m-1} q\}$$

$$e^{\Delta t A} q \approx V_m e^{\Delta t H} V_m^T q = V_m X e^{\Delta t \Lambda} X^{-1} V_m^T, e_{n+1} = \left\| e^{-\Delta t A} q_N^n - V_m e^{-\Delta t H_m} V_m^T q_N^n \right\| \le c_e \Delta t^m$$

$$\left\| V_m e^{-\Delta t H_m} V_m^T \right\|_2 \le \left\| e^{-\Delta t H_m} \right\|_2 \le e^{\mu(-\Delta t H_m)} \le e^{\mu(-\Delta t A)} \le 1$$

- For any real matrix A (n x n) and the Hessenberg matrix H (m x m) is ***unconditionally stable*** **if the eigenvalues of (-A) are in the negative half-plane**

3D Cylindrical Waveguide Example



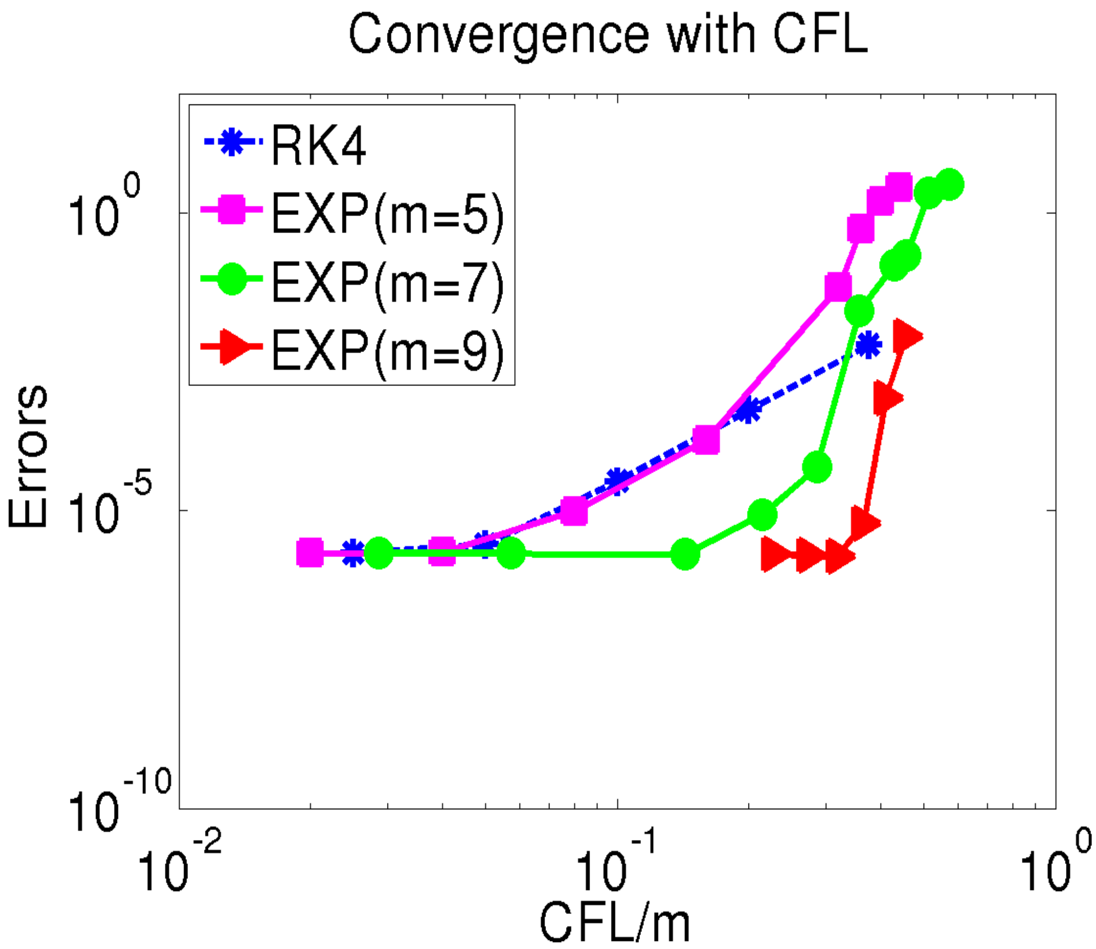
- **Analytic solutions:**

$$H_x = -k_y w \pi \gamma^{-2} \sin(k_x \pi x) \cos(k_y \pi y) \sin(\pi t - k_z z)$$
$$H_y = k_x w \pi \gamma^{-2} \cos(k_x \pi x) \sin(k_y \pi y) \sin(\pi t - k_z z)$$
$$H_z = 0$$

$$E_x = k_x k_z \pi \gamma^{-2} \cos(k_x \pi x) \sin(k_y \pi y) \sin(\pi t - k_z z)$$
$$E_y = k_y k_z \pi \gamma^{-2} \sin(k_x \pi x) \cos(k_y \pi y) \sin(\pi t - k_z z)$$
$$E_z = \sin(k_x \pi x) \sin(k_y \pi y) \cos(\pi t - k_z z)$$

Exponential Integrator: Convergence in Time

Min & Fischer

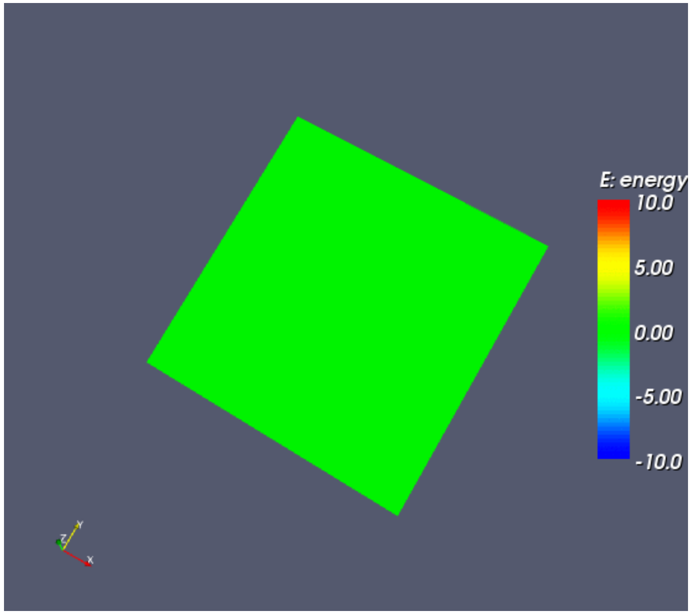


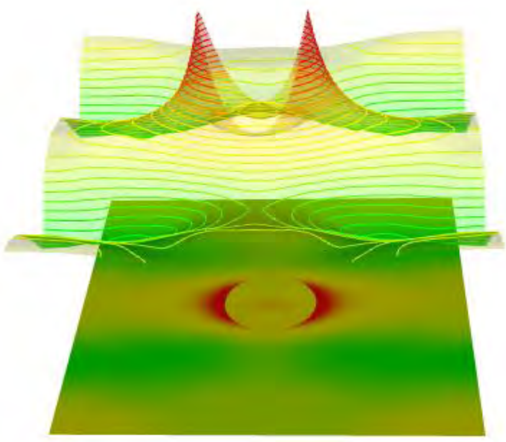
$$CFL = \max_{\Omega}\left\{\frac{\Delta t}{\text{dxmin}}\right\}$$

$$\text{dxmin} = \min_{N,E} \quad \Delta x, \Delta y, \Delta z$$

Example 1/3: Nanophotonic Devices

- Collaboration with CNM/ANL --> co-design proposal w/ MSD, CNM, MCS





Strong surface enhanced electric field (10-20 times larger) for nanoscale devices

Energy of the electric field |E|: Intensity is proportional to |E|^4 > 10^8

Standard FDTD does not capture correct profile on the surface (with strong oscillations):
requires very dense grid resolution in order to represent high gradient fields

Electron Movement in Metal

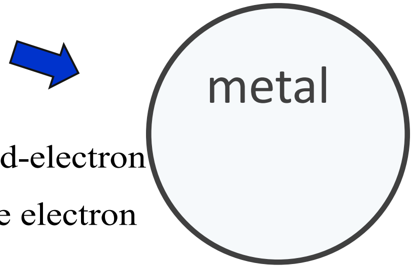
- ❑ Harmonic oscillators
- ❑ Drude model: free electrons
- ❑ Lorentzian model: bound-electrons
- ❑ Transmission calculations:

(Inside) metal

$\Gamma_j \neq 0, A_j \neq 0$

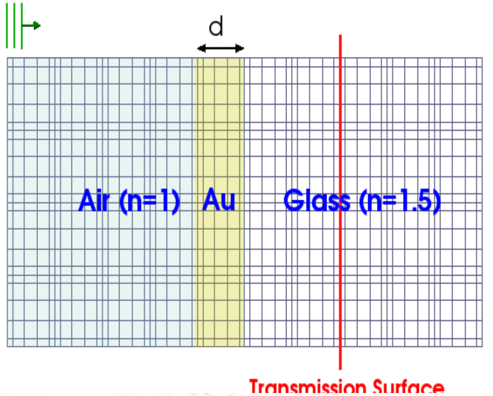
$w_j^2 \neq 0$ bound-electron

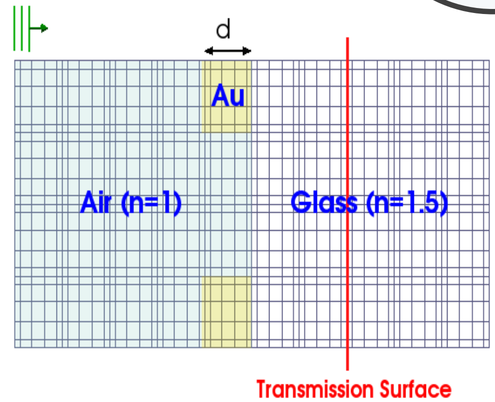
or $w_j^2 = 0$ free electron

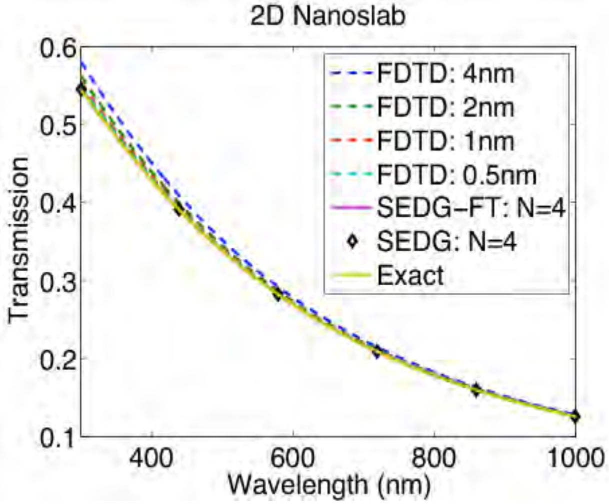


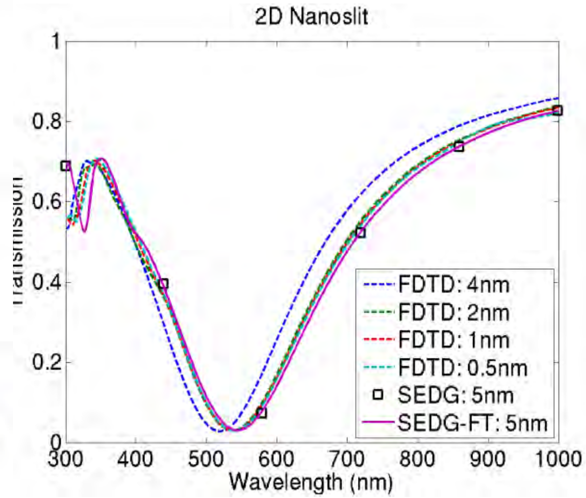
(Outside) metal

$\Gamma_j = A_j = w_j^2 = 0$





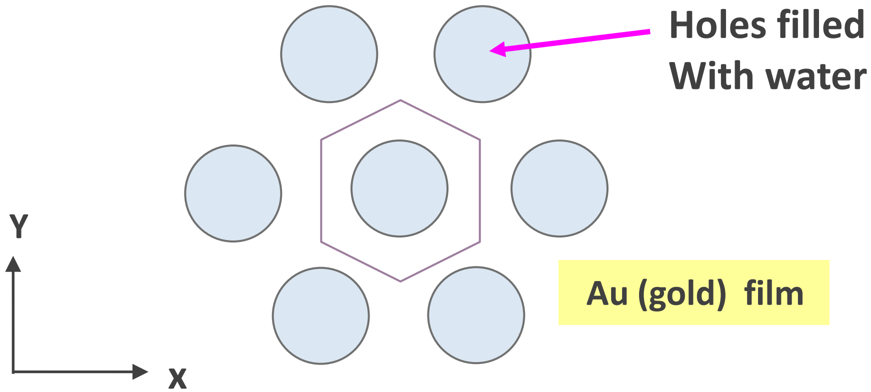




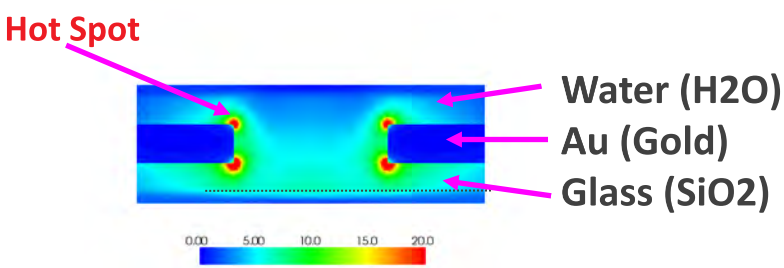
Min, Fairchild, Montgomery, Gray

Exploring a Variety of Thin Film Metal Nanoholes

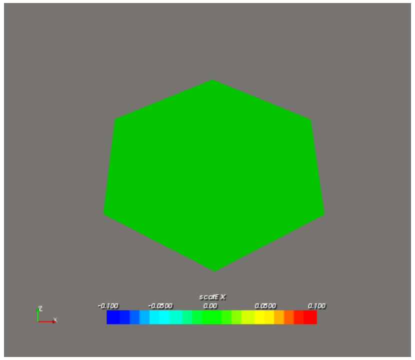
Example: Nanoholes in a *Hexagonal* Array

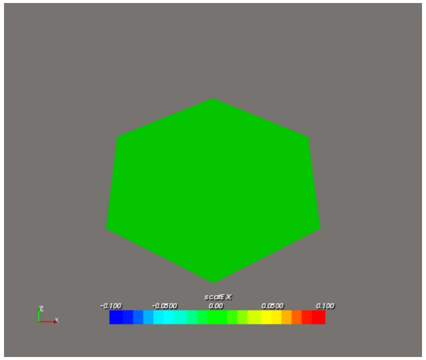


Periodic in xy and PML in z



E-field at vertical cross-section



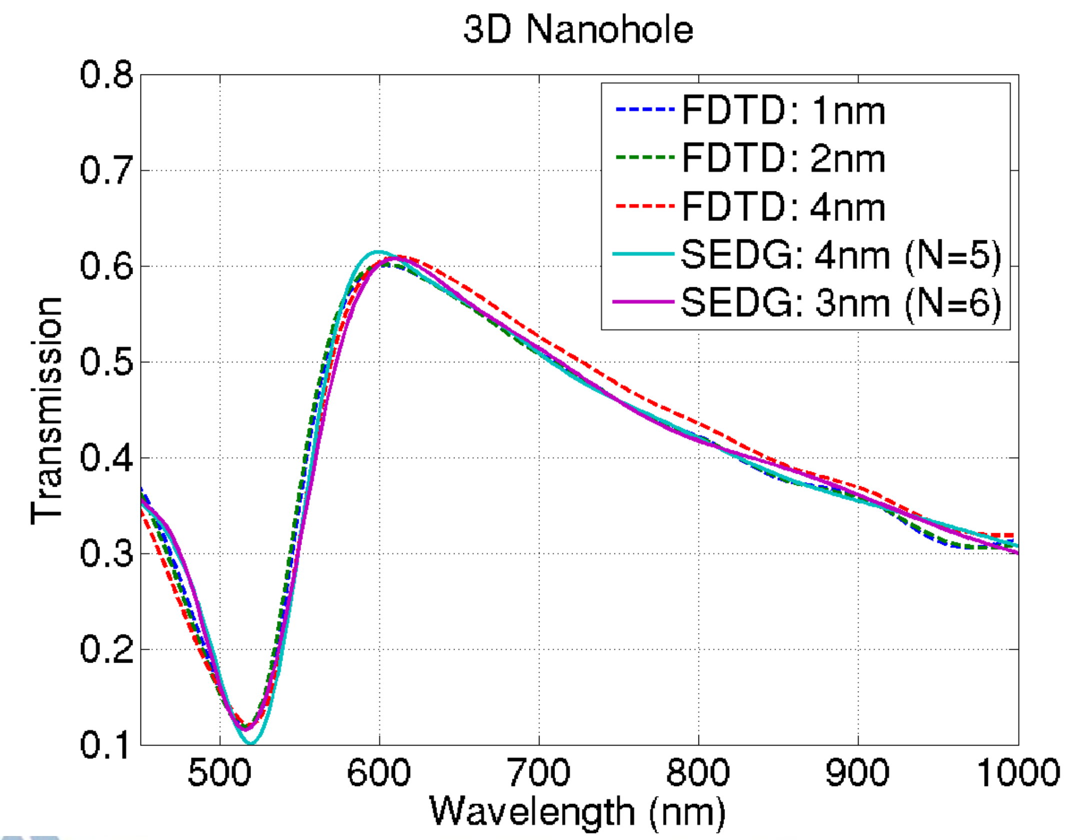


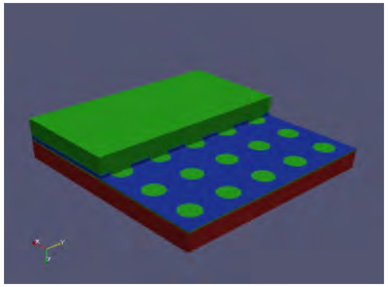
Ex field profiles with different radius:
50nm (left) and 80nm (right)

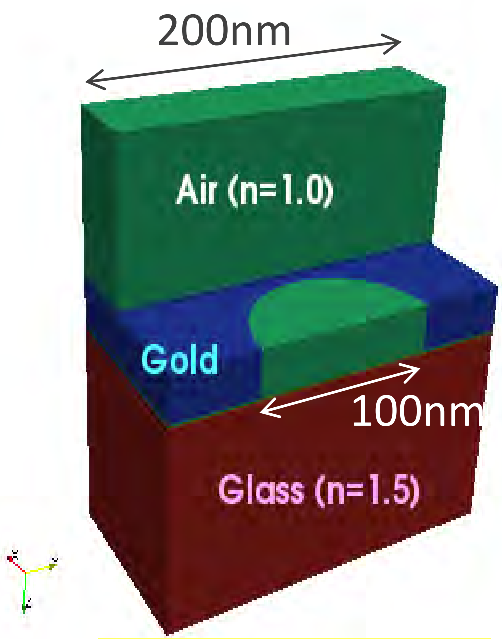
Validation for Thin Film Metallic Nano Holes

- Transmission Calculations: comparisons for Finite-Difference Time-Domain (FDTD) method and SEDG method.
- Body-fitted SEDG mesh requires **48x** fewer gridpoints.

J. Phys: 2010,
Min, Montgomery, Fischer, Gray



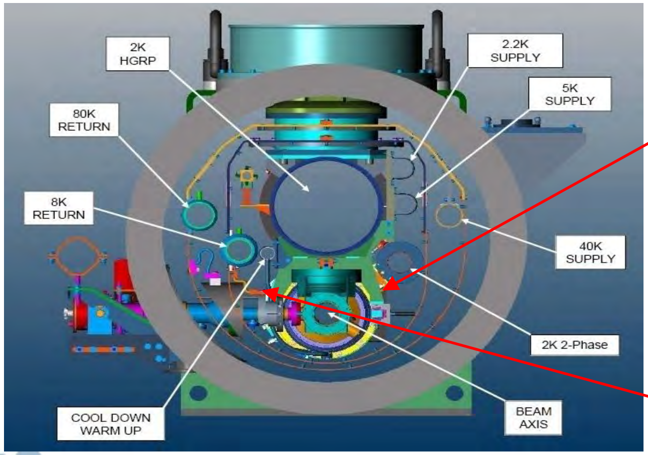




Gold film thickness = 24 nm

Accelerator Modeling

ILC cryomodule



Cavity

Coupler

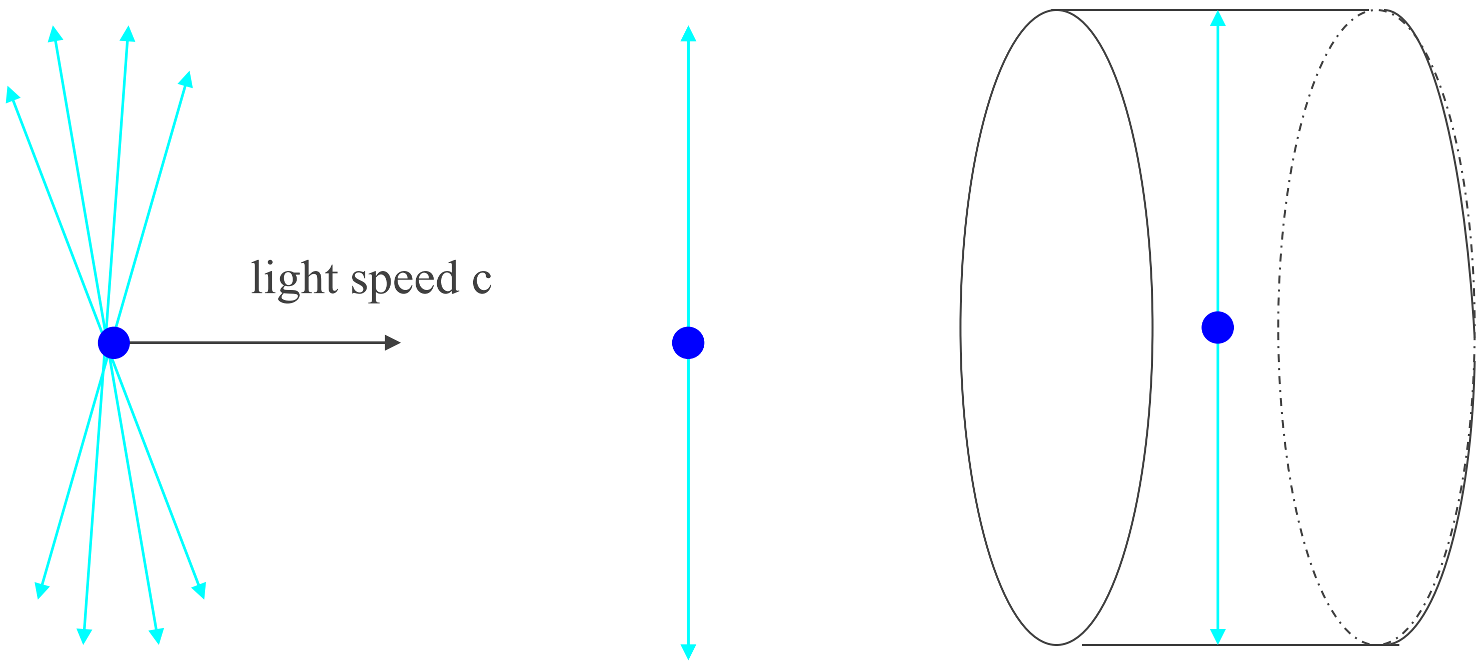
TESLA cavity

TESLA cavity: main cryomodule for future ILC

Dimension: 0.1 m x 0.1 m x 1m
Beam: 0.03mm

Beam Propagation Behaviors

- Ultra-relativistic electron beam
- Free Space and Conducting Pipe:

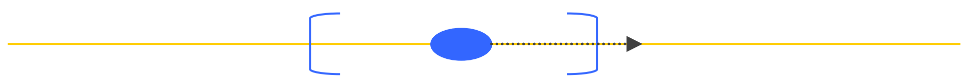


Lorentz contraction → Ez=0, Hz=0

conducting tube

Wakefield and Wakepotentials

- Longitudinal wakepotential: $W_z(r,\theta,s) = -\frac{1}{Q}\int_{-\infty}^{\infty} E_z(r,\theta,z,t(z,s))dz$
- Transverse wakepotential: $W_\perp(r,\theta,s) = \frac{1}{Q}\int_{-\infty}^{\infty} (E_\perp + c\times B)(r,\theta,z,t(z,s))dz$



$$t(z,s) = \frac{z+s}{c}$$

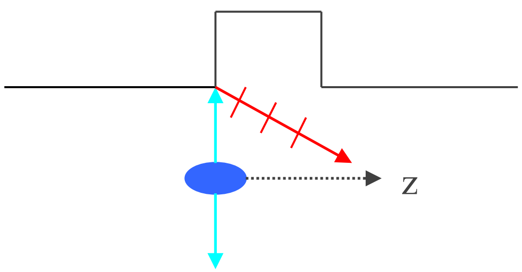
$$E = E^{freespace} + E^{radiation}$$

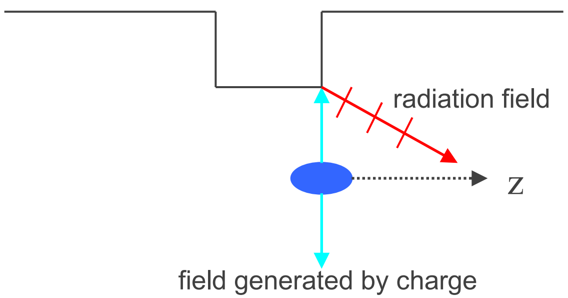
$$B = B^{freespace} + B^{radiation}$$

Generated by the Charge Distribution

+

Radiated Fields

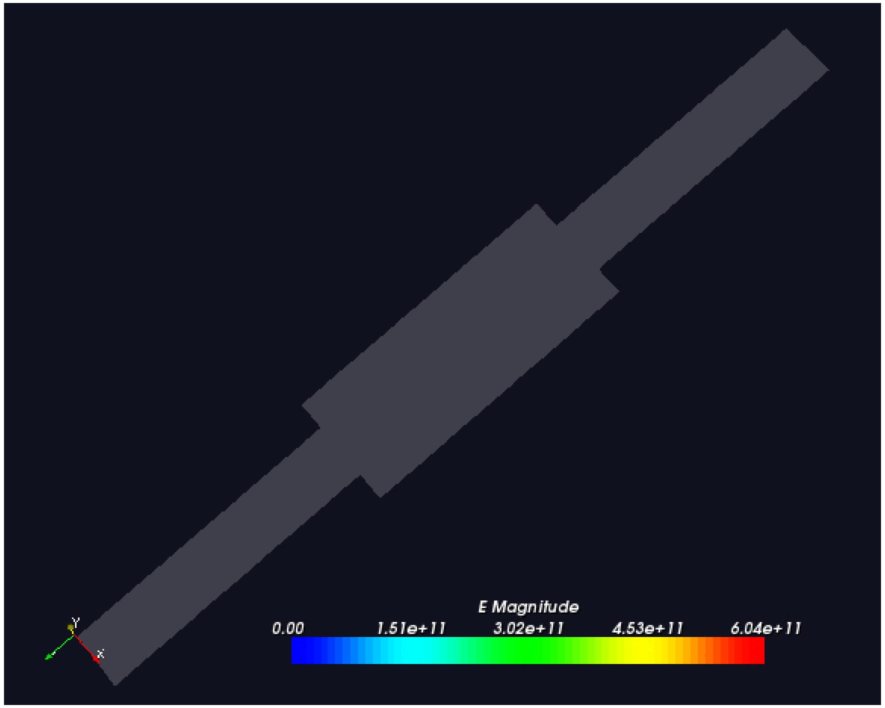




Example (2/3): Moving Electron Beam

- Collaboration with APS/ANL → ComPASS project : SLAC, Fermi,TechX.

3D moving beam in a pillbox cavity: wakefield simulations by SEDG+RK4
(PAC 2007, Min, Fischer, Chae)



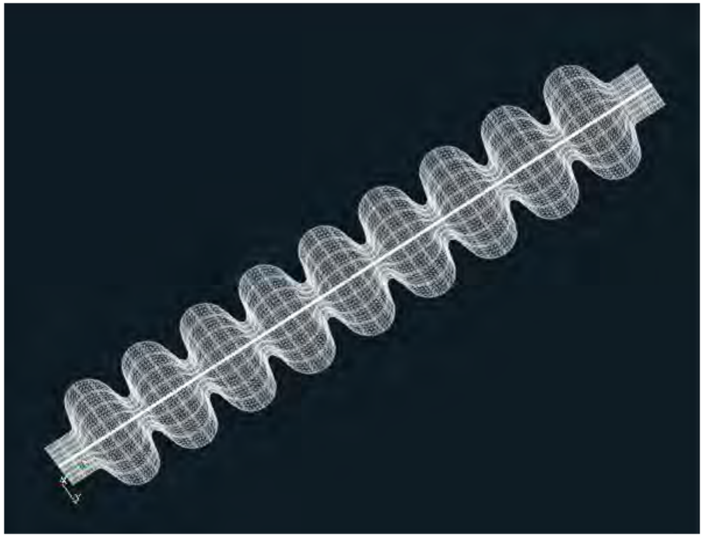
Typical dimension: 10cm x 10 cm x 1m
Beam size < 0.03 mm

There is a big scale difference between beam length and the whole device

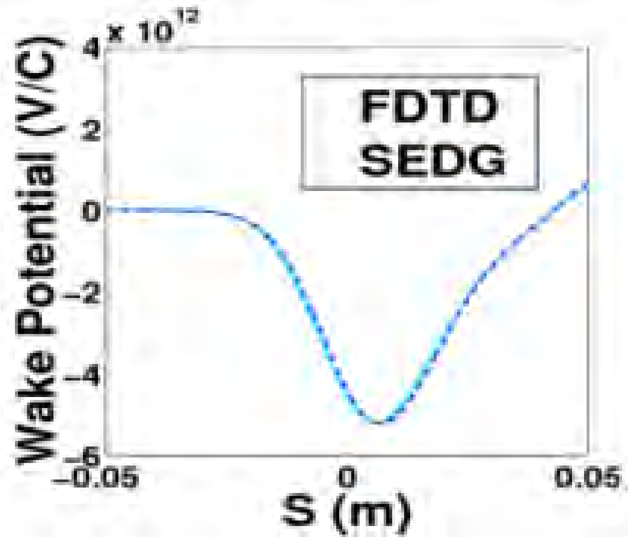
Accelerator: Code Validation

Beam dynamics Simulations: Wakefield and Wake Potential Calculations

SRF2007, Min, Fischer, & Chae



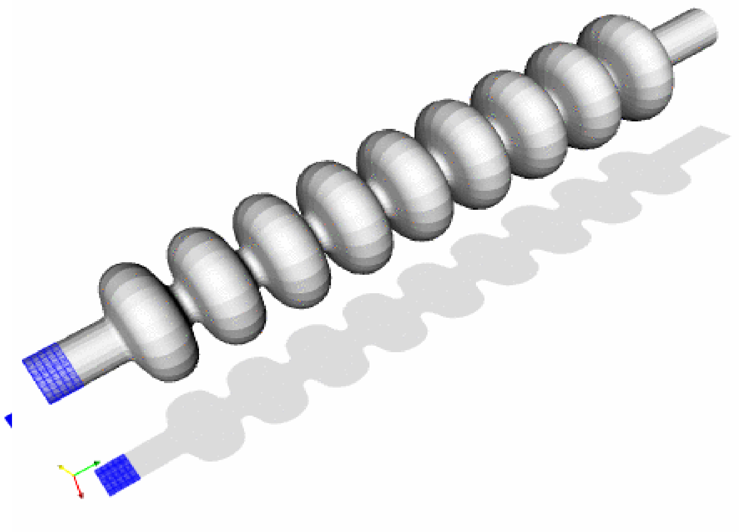
Spectral-element Mesh

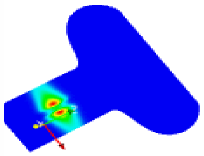


TESLA Cavity (Moving Window)

PAC 2009, Min and Fischer

- ***Speedup*** with Moving Window algorithms
  - **20x** reduction in cost over full-domain case





Boltzmann Equations

- Boltzmann equations:

$$\frac{\partial f_\alpha}{\partial t} + \mathbf{e}_\alpha \cdot \nabla f_\alpha = C$$

  Evolution of a single-particle distribution function *f* at location *x* with velocity at time *t*. Collision term *C* describes these effect of binary collisions on a single particle distribution with very complicated nonlinear integral form.

- Discrete Boltzmann equations with BGK approximation:

  simplified linearized form for the collision term

Lattice Boltzmann Method

- Lattice Boltzmann equations: restrict the particles to have 9-velocity (2D) and 19-velocity (3D) fields: $\frac{\partial f_\alpha}{\partial t} + \mathbf{e}_\alpha \cdot \nabla f_\alpha = -\frac{1}{\lambda}\left(f_\alpha - f_\alpha^{eq}\right)$

- Lattice Boltzmann Equation (T. Lee, C-L Lin, 2001):

$$f_\alpha(\mathbf{x},t) = f_\alpha(\mathbf{x}-\mathbf{e}_\alpha\Delta t, t-\Delta t) - \frac{1}{\lambda}\int_{t-\Delta t}^{t}\left(f_\alpha - f_\alpha^{eq}\right)dt'$$

$$f_\alpha(\mathbf{x},t) = f_\alpha(\mathbf{x}-e_\alpha\Delta t, t-\Delta t) - \frac{\Delta t}{2\lambda}\left(f_\alpha - f_\alpha^{eq}\right)_{\mathbf{x}-e_\alpha\Delta t,t-\Delta t} - \frac{\Delta t}{2\lambda}\left(f_\alpha - f_\alpha^{eq}\right)_{\mathbf{x},t}$$

- Modified particle distribution function:

$$\overline{f_\alpha} = f_\alpha + \frac{f_\alpha - f_\alpha^{eq}}{2\tau}, \quad \overline{f_\alpha^{eq}} = f_\alpha^{eq}; \quad \rho = \sum_{\alpha=0}^{8}\overline{f_\alpha^{eq}} = \sum_{\alpha=0}^{8}\overline{f_\alpha}, \quad \rho u = \sum_{\alpha=0}^{8} e_\alpha \overline{f_\alpha^{eq}} = \sum_{\alpha=0}^{8} e_\alpha \overline{f_\alpha}$$

$$\overline{f_\alpha}(\mathbf{x},t) - \overline{f_\alpha}(\mathbf{x}-\mathbf{e}_\alpha\Delta t, t-\Delta t) = -\frac{1}{\tau+0.5}\left(\overline{f_\alpha} - \overline{f_\alpha^{eq}}\right)(\mathbf{x}-\mathbf{e}_\alpha\Delta t, t-\Delta t)$$

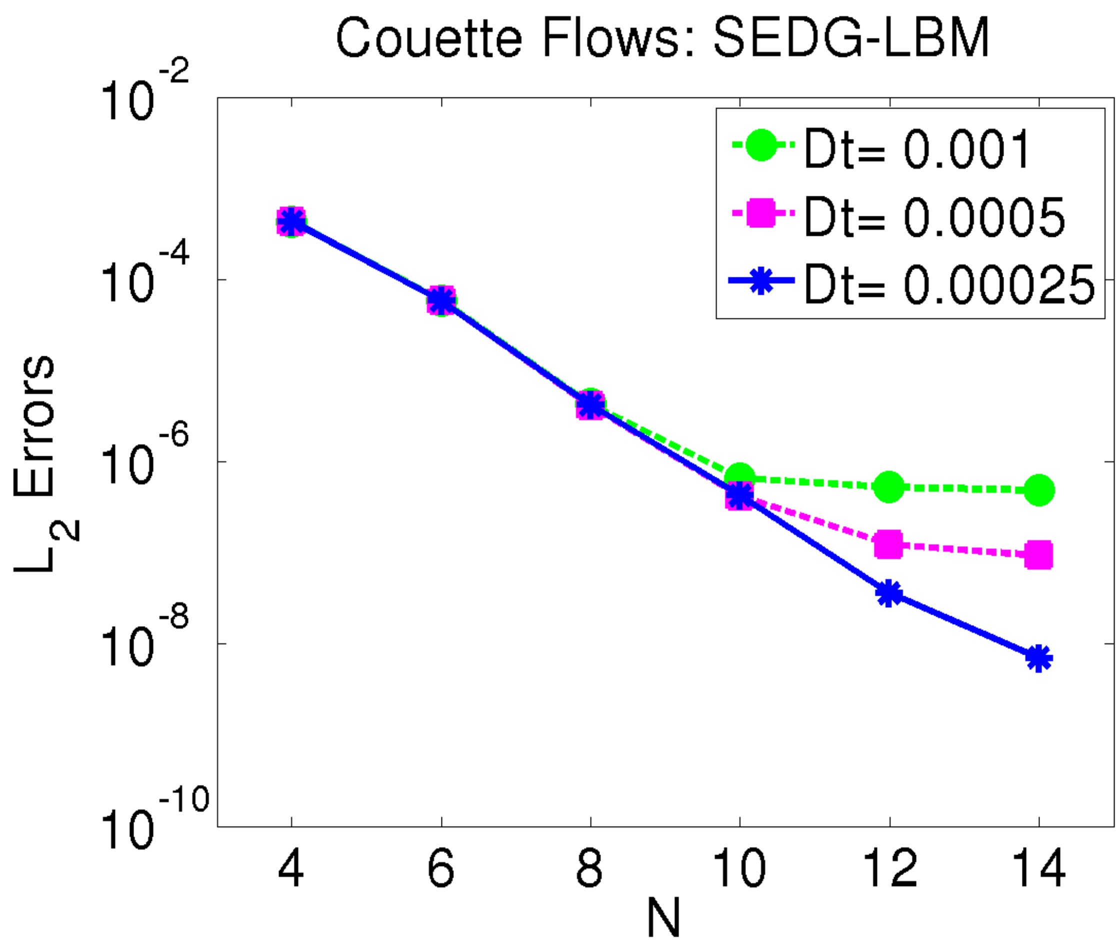
$$q_\alpha(\mathbf{x},t) = \overline{f_\alpha}(\mathbf{x},t) - \frac{1}{\tau+0.5}\left(\overline{f_\alpha} - \overline{f_\alpha^{eq}}\right)(\mathbf{x},t)$$

- **Collision step**: $q_\alpha(\mathbf{x},t) = \overline{f_\alpha}(\mathbf{x},t) - \frac{1}{\tau+0.5}\left(\overline{f_\alpha} - \overline{f_\alpha^{eq}}\right)(\mathbf{x},t)$

- **Advection step**: $\frac{\partial q_\alpha}{\partial t} + e_\alpha \cdot \nabla q_\alpha = 0$

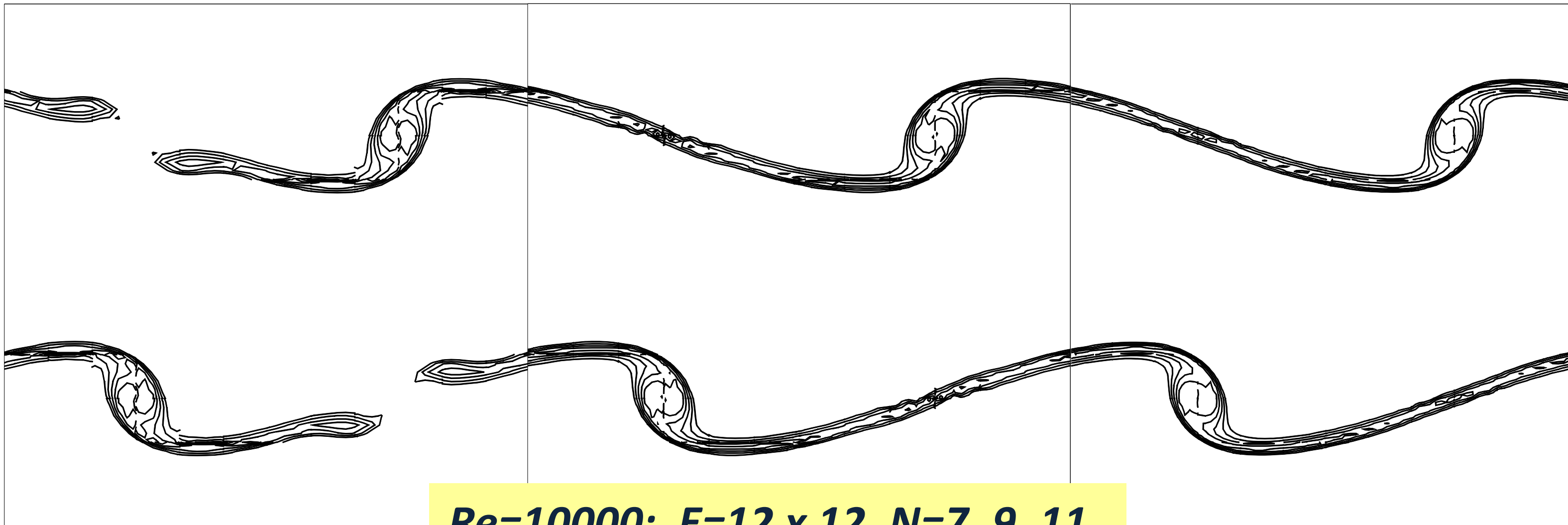
Convergence: Couette Flows (SEDG-LBM)

Min & Lee

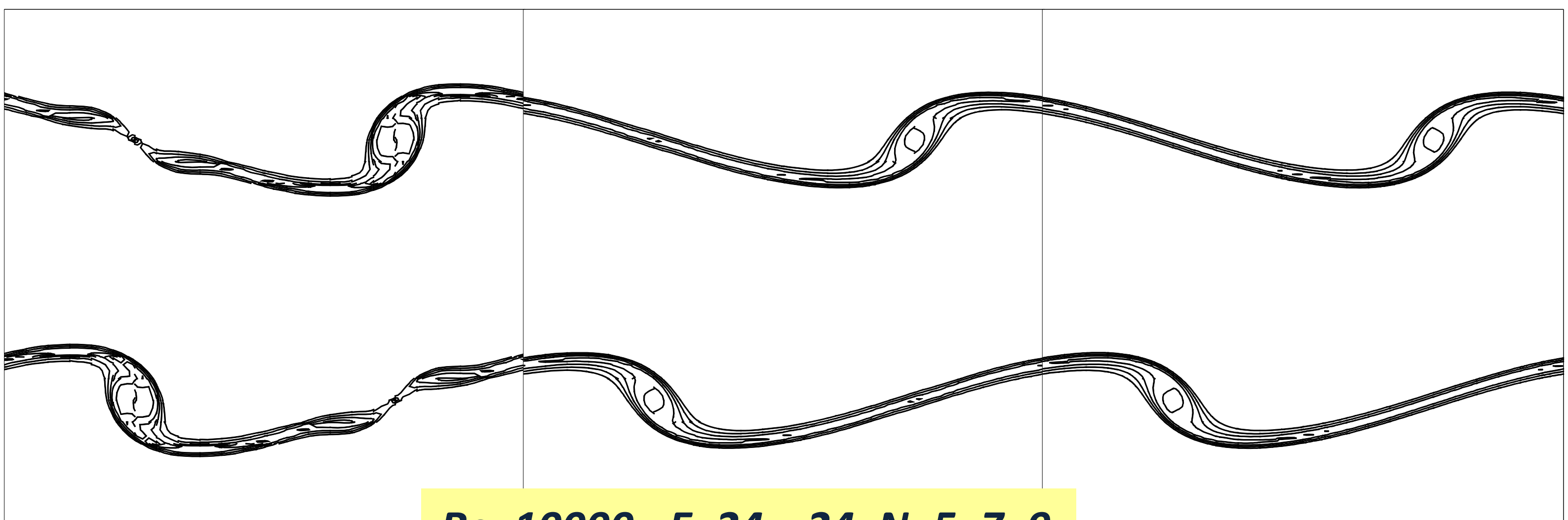


Re=2000; E=3 x 3

Convergence for a Vortex Roll-Up Problem



Re=10000; E=12 x 12, N=7, 9, 11



Re=10000; E=24 x 24, N=5, 7, 9

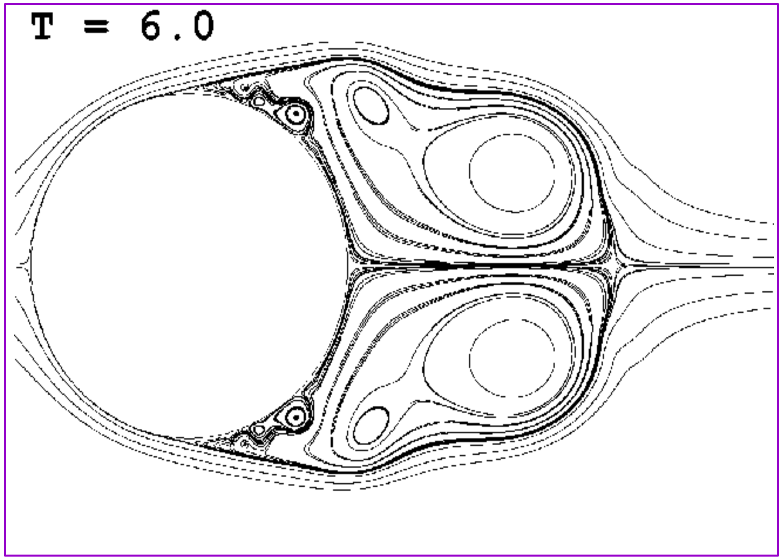
Min & Lee

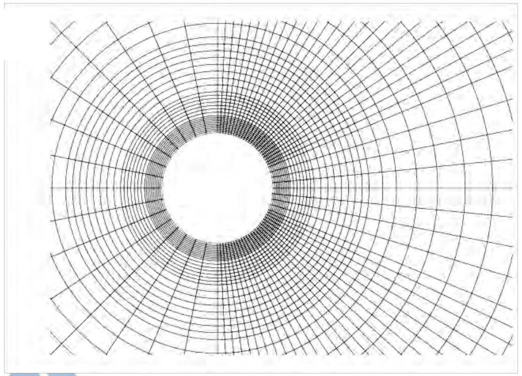
Spectral Element DG-LBM Method

Flows Past a Cylinder

JCP 11, Min & Lee

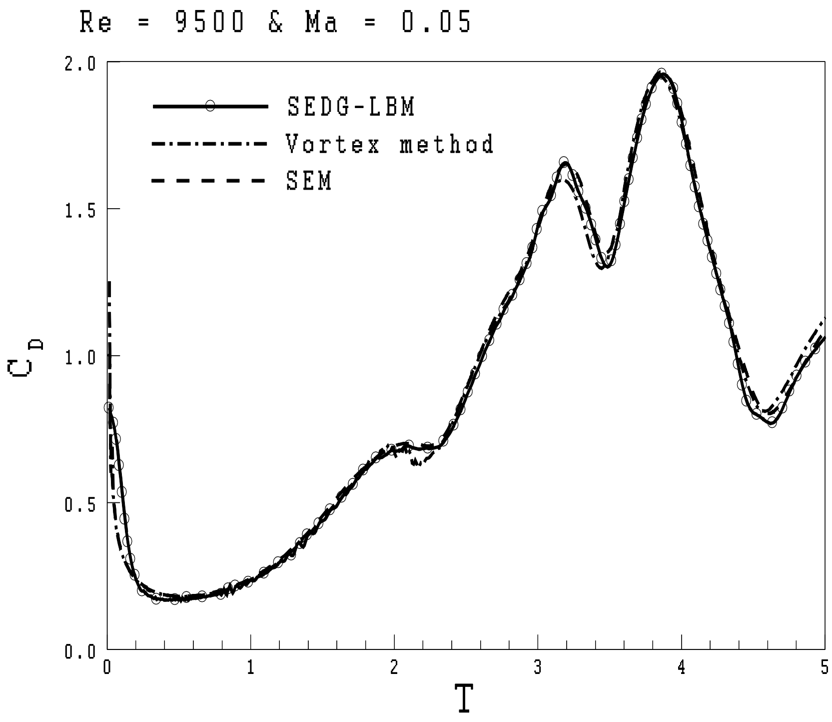
Streamline for Re= 9500





E=3,758, N=5,
Total Grid Points =135,288.

Code Validation: Drag Coefficient



- **Vortex Method** :
  P. Koumoutsakos, J. Fluid Mech., 1995
- **Spectral-Element Method** (SEM):
  P. Fischer, J. Comp. Phys., 1997

Summary (Future Plan)

- **Expansion in Applications and Collaborations:**
  - Accelerator modeling: possible participation for SciDAC ComPASS project
  - Nanomaterial applications: co-design proposal on design/optimization
  - Lattice Boltzmann modeling for compressible flows: with CUNY

- **Expansion to Nano Solar Cell Applications**
  - time-dependent Schrödinger-Poisson solver

- **Enhance Geometric Flexibility: hybrid element meshes**
- **Efficient Timestepping Methods (e.g., SSP, exponential integrators)**
- **Alternative Programming Models for Extreme Scale**

Thank You!