Recent Advances in Numerical Techniques for Simulation of Transient Electromagnetic Wave Interactions

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Outline

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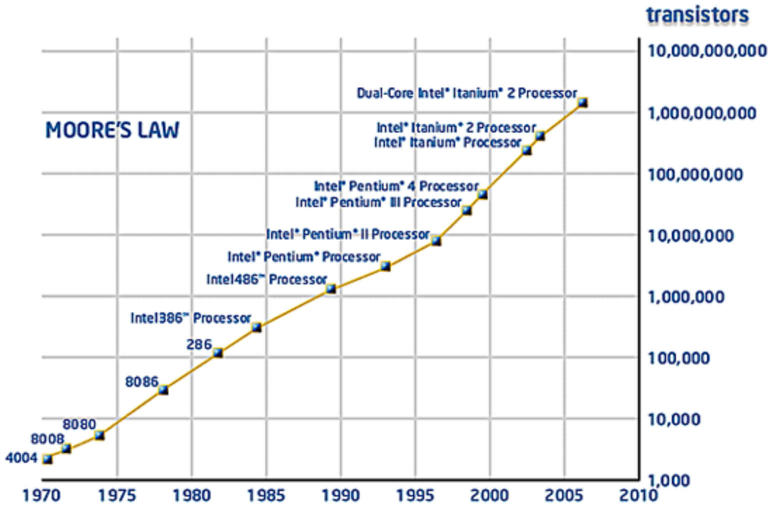
- Computational Electromagnetics (CEM)
  - Challenges and Applications
  - Frequency Domain vs. Time Domain
  - Differential Equation vs. Integral Equation Solvers
  - CEM Research Group at KAUST

- Two Recently Developed Time-Domain Solvers
  - Time Domain Discontinuous Galerkin Method with Exact Boundary Conditions
    - Introduction
    - Formulation
    - Numerical Results
    - Conclusions and Future/Ongoing Work
  - Time Domain Volume Integral Equation Solver for High Contrast Scatterers
    - Introduction
    - Formulation
    - Numerical Results
    - Conclusions and Future/Ongoing Work

- Computational Electromagnetics (CEM)
  - Challenges and Applications
  - Frequency Domain vs. Time Domain
  - Differential Equation vs. Integral Equation Solvers
  - CEM Research Group at KAUST

Simulation

- What is a “computer simulation” ?
  - It is an attempt to model a real-life or hypothetical problem on a computer so that its solution can be estimated
- Why do engineers need or prefer computer simulations ?
  - Expensive and/or impossible experiments
  - Repetitive processes, typical in design frameworks
  - Expensive human labor, cheap computing power
- Fields of electromagnetics/optics/photonics are no different. Simulation tools are needed.
  - CEM is the solution



Computational Electromagnetics (CEM)

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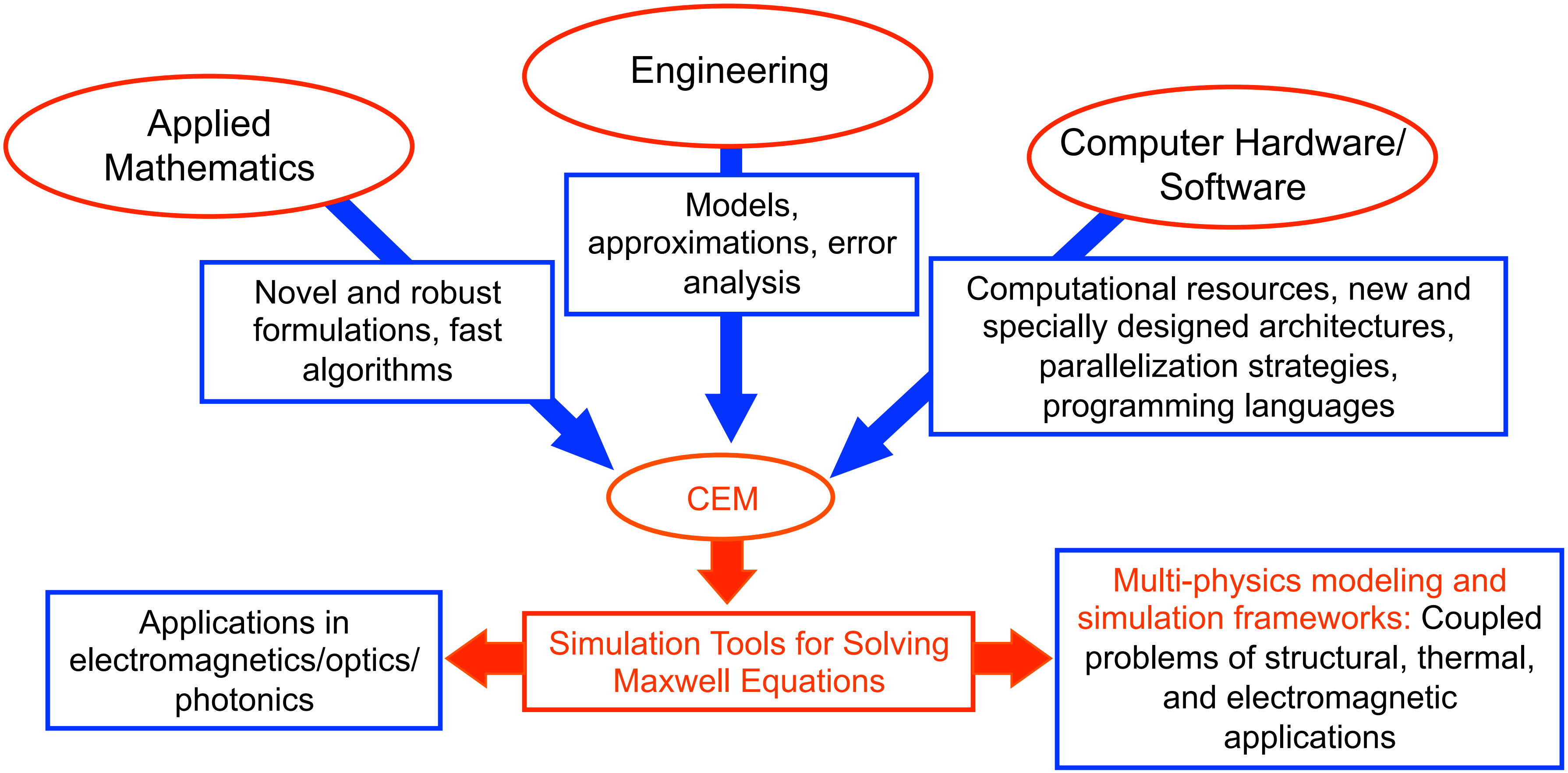

- Two Domains:
  - Frequency Domain Solvers
  - Time Domain Solvers
- Two types of Methods:
  - Differential Equation Based Solvers
  - Integral Equation Based Solvers

Frequency Domain Simulators

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Time-dependence: $e^{j\omega t}$

Time-derivative: $\dfrac{\partial}{\partial t} \to j\omega$

Time-integration: $\displaystyle\int_t dt \to \frac{1}{j\omega}$

Convolution $\to$ Multiplication

Inverse Fourier Transform to switch to time domain

Example Commercial Tools:
HFSS (FEM), Comsol (FEM), FISC (MOM), WIPL-D (MOM)

- Positives
  - Intuitively easier to understand
  - Easier to implement in general
  - Lower computational cost
  - Dispersion is easier to model

- Negatives
  - Strong nonlinearities cannot be modeled
  - Only single frequency results, no broadband data
  - Many simulations to obtain broadband results
  - Needs inverse Fourier transform as post-processors

Time Domain Simulators

Time-dependence: Arbitrary (band limited)

Fourier Transform to switch to frequency domain

Example Commercial Tools:
Many available (FDTD), No well-known commercial tools (TD-FEM, MOT-TDIE)

- Positives
  - Strong nonlinearities can be modeled
  - Provides broadband data with a single simulation
  - Transient response is easy to get
  - Provides immediately the physics, no post-processing
- Negatives
  - More difficult to implement
  - Instabilities
  - Methods to handle resonance
  - Modeling dispersion requires computation of (costly) temporal convolutions
  - Higher computational cost

Differential Equation Based Simulators

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Time-dependent:

$$\nabla \times \mathbf{E}(\mathbf{r},t) = -\mu \frac{\partial \mathbf{H}(\mathbf{r},t)}{\partial t}$$

$$\nabla \times \mathbf{H}(\mathbf{r},t) = \varepsilon \frac{\partial \mathbf{E}(\mathbf{r},t)}{\partial t} + \mathbf{J}(\mathbf{r},t)$$

$$\nabla \cdot \mathbf{E}(\mathbf{r},t) = \frac{\rho(\mathbf{r},t)}{\varepsilon}$$

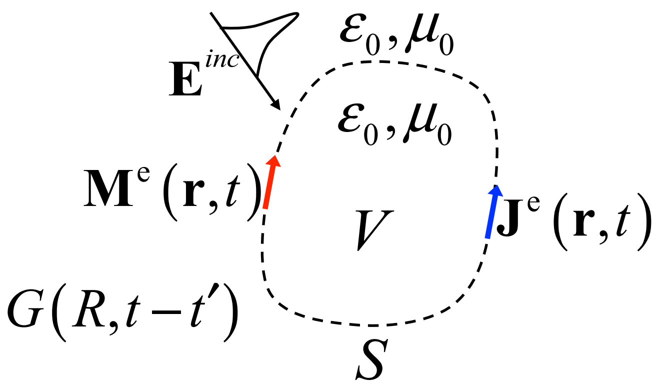
$$\nabla \cdot \mathbf{H}(\mathbf{r},t) = 0$$

Time-harmonic: $\frac{\partial}{\partial t} \rightarrow j\omega$

Example Commercial Tools:
HFSS (FEM), Comsol (FEM),
Many available (FDTD)

- Discretize differential form of Maxwell equations
- Approximate derivatives using neighboring elements (in time and space)
- Positives
  - Straightforward to implement
  - Extension to inhomogeneous media is trivial
- Negatives
  - Numerical dispersion
  - Truncation of the (open) computation domain
  - Discretization of the computation domain
  - Typically time step size is constrained by the spatial discretization
  - Inaccurate geometry representation (FDTD)

Integral Equation Based Simulators



Boundary Equation:

$$\partial_t \mathbf{E}^{\mathrm{inc}}(\mathbf{r},t)\Big|_{\tan} = \partial_t \mathbf{E}^{\mathrm{sca}}(\mathbf{r},t)\Big|_{\tan} \quad \mathbf{r} \in S$$

Time-harmonic: $\dfrac{\partial}{\partial t} \rightarrow j\omega$

Example Commercial Tools:

FISC (MOM), WPIL-D (MOM),

Not available in time domain

- Replace scatterers with equivalent surface and volume currents
- Find fields due to these currents using Green function
- Apply boundary conditions to solve for unknowns
- Positives
  - No phase dispersion
  - No grid truncation (exact radiation condition)
  - Time step size is not necessarily constrained by spatial discretization
  - Only the surface (or volume) of the object is discretized
  - Accurate representation of the geometry
- Negatives
  - More difficult to implement
  - Higher computational costs
  - Instabilities

Computational Electromagnetics (CEM)

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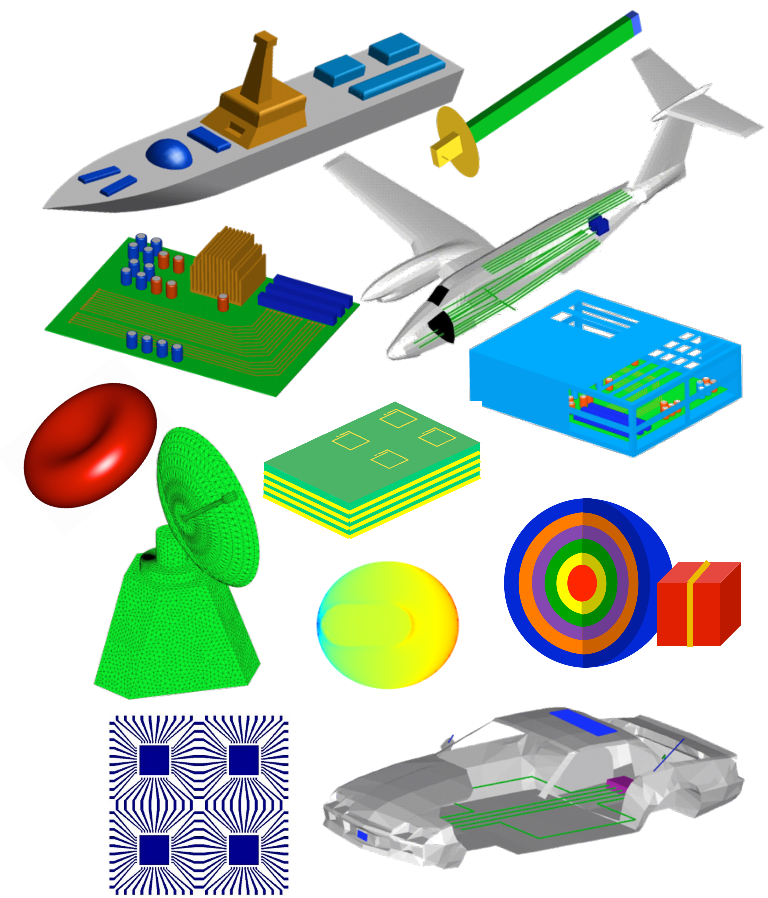
- Applications in electromagnetics/optics/photonics:
  - Radiation, radar, sensing, detection, imaging
  - EMC/EMI analysis
  - Plasmonics
  - THz wave propagation
- As a part of multi-physics modeling and simulation frameworks (coupled problems of structural, thermal, and electromagnetic applications)
  - Composite antenna design
  - Chip design and packaging
  - Vehicle (space craft, UAVs, airplanes, cars) design



Computational Electromagnetics (CEM)

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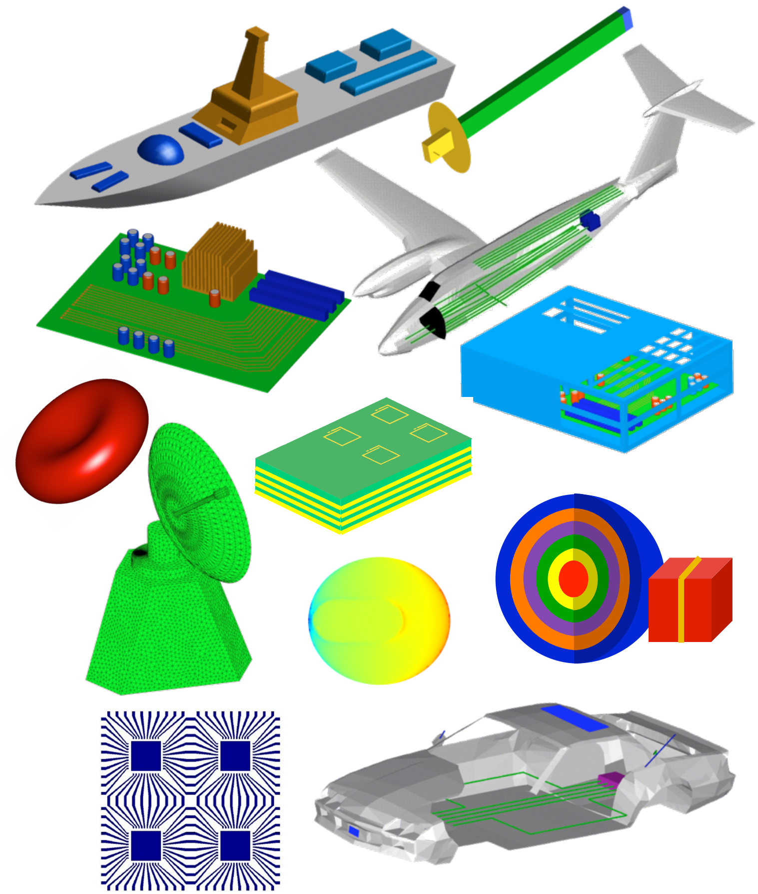
- Some of the challenges in application of CEM tools in real life scenarios
  - Large computation domains (large number of unknowns)
  - Multi-scale geometric features (large number of unknowns, poor conditioning, slow convergence rates)
  - One mesh for multi-physics simulation (multi-scale elements with high aspect ratios, large number of unknowns, poor conditioning)
  - Difficult to model highly oscillatory physical resonances in electrically large models
  - Presence of spurious modes/resonances on complex structures
  - Uncertainties in model descriptions including geometry and excitation parameters, material properties, constitutive relations
  - Loss of accuracy due to increasing complexity



CEM Research Group at KAUST – Research

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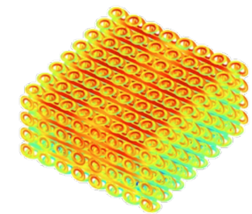
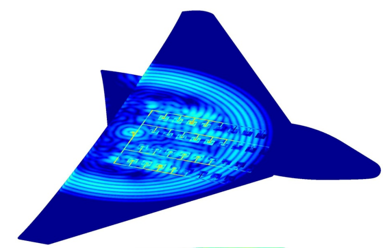
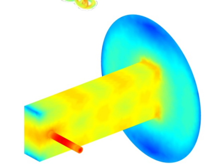
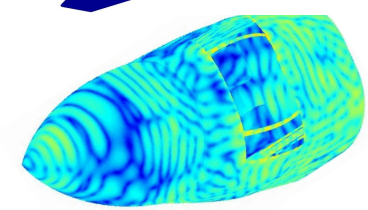
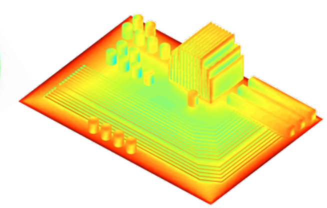
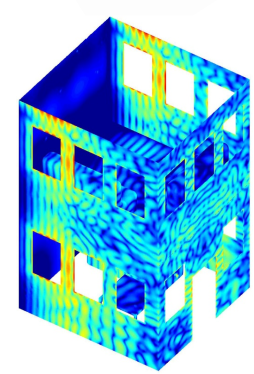
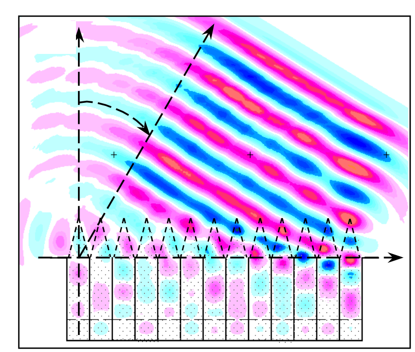
CEM research group at KAUST develops novel time domain solvers for characterizing electromagnetic wave interactions on electrically large and multi-scale structures and applies them in real-life problems of electromagnetics/optics/photonics. More specifically:

- Explicit and non-uniform, yet stable, time marching techniques for efficiently solving TDIEs (to address the increase in computation time due to matrix inversion and large number of unknowns)
- Mixed space and time discretization schemes for TDIEs (for increased accuracy)
- Exact boundary conditions in the form of TDIEs for terminating differential equation solvers (for increased accuracy)
- Blocked FFT-based schemes for accelerating the computation of space-time convolutions in TDIEs (to address the increase in computation time due to large number of unknowns)
- Calderòn- and Wavelet-based preconditioners for TDIEs (to address the ill-conditioning due to multi-scale discretizations and low-frequency excitation)
- Hybridization schemes between different-scale solvers in time domain [circuit, transmission line, and TDIE solvers] (to address the ill-conditioning due to multi-scale discretizations)

CEM Research Group at KAUST – Research

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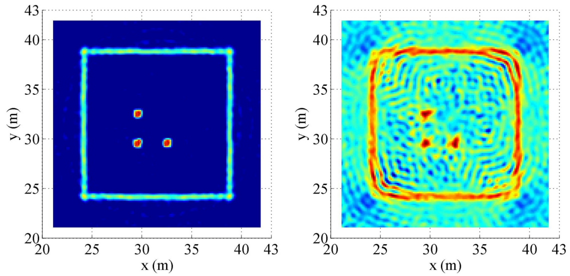
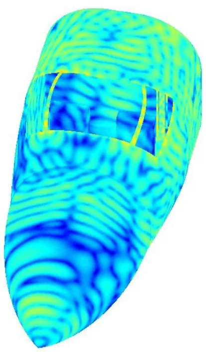
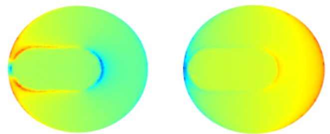
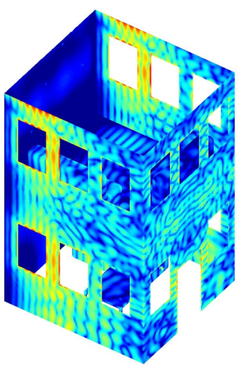
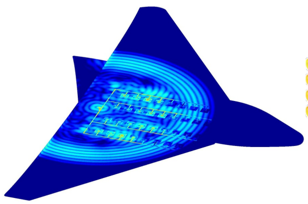
- Application of the resulting novel methods in
  - Inverse scattering problems with sparsity constraints
  - Design of plasmonic devices with applications in slow light and metamaterials
  - Uncertainty Quantification (UQ) frameworks for EMC/EMI characterization on complex electrically large platforms
  - Statistical characterization of wave propagation in harsh environments

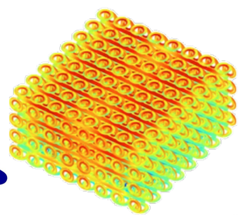


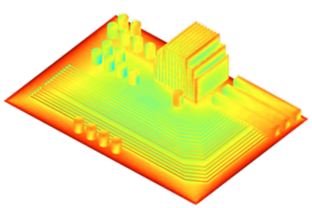


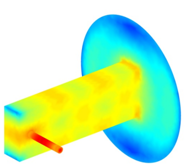


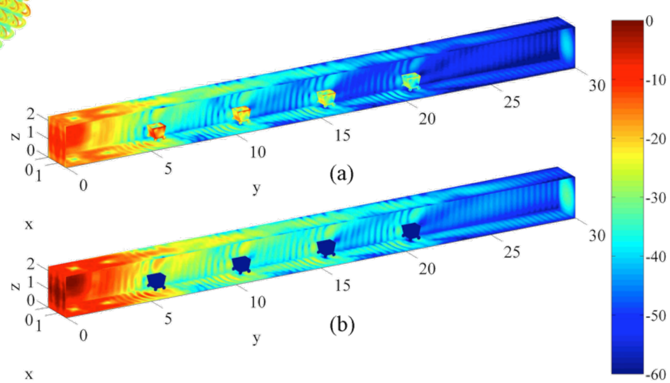


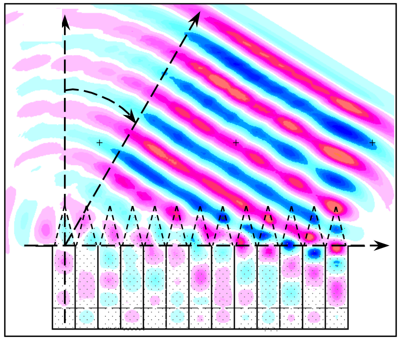












CEM Research Group at KAUST – People and Facilities

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KAUST

Work Force

PhD Students

- Muhammad Amin
- Abdulla Desmal
- Ismail Uysal
- Sadeed Sayed
- Noha Alharthi
- Ali Imran Sandhu
- Ozum Asirim

Post-Doctoral Researchers

- Kostyantyn Sirenko, PhD
- Arda Ulku, PhD
- Yifei Shi, PhD
- Mohamed Farhat, PhD

Alumni

- Mohamed Salem, PhD (Mar. 2013)
- Ahmed Al-Jarro, PhD (Nov. 2012)
- Meilin Liu, PhD (Jan. 2012)
- Umair Khalid (MS degree, Dec. 2010)
- Muhammad Furqan (Feb. 2012)
- Abdul Haseeb Muhammed (Apr. 2011)

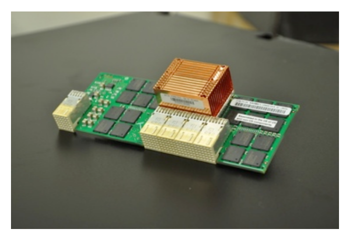
Computational Resources

Shaheen

- IBM's 16-Rack Blue Gene/P, ~65k computing cores, 222 teraflops/sec
- Expandable to petascale computing
- Supported by IBM and KAUST Supercomputing Laboratory (KSL)

Noor

- Beowulf class heterogeneous cluster
- Intel Xeon X5570, IBM Power6, ~1000 cores
- Supported by KAUST Research Computing



CEML: http://maxwell.kaust.edu.sa

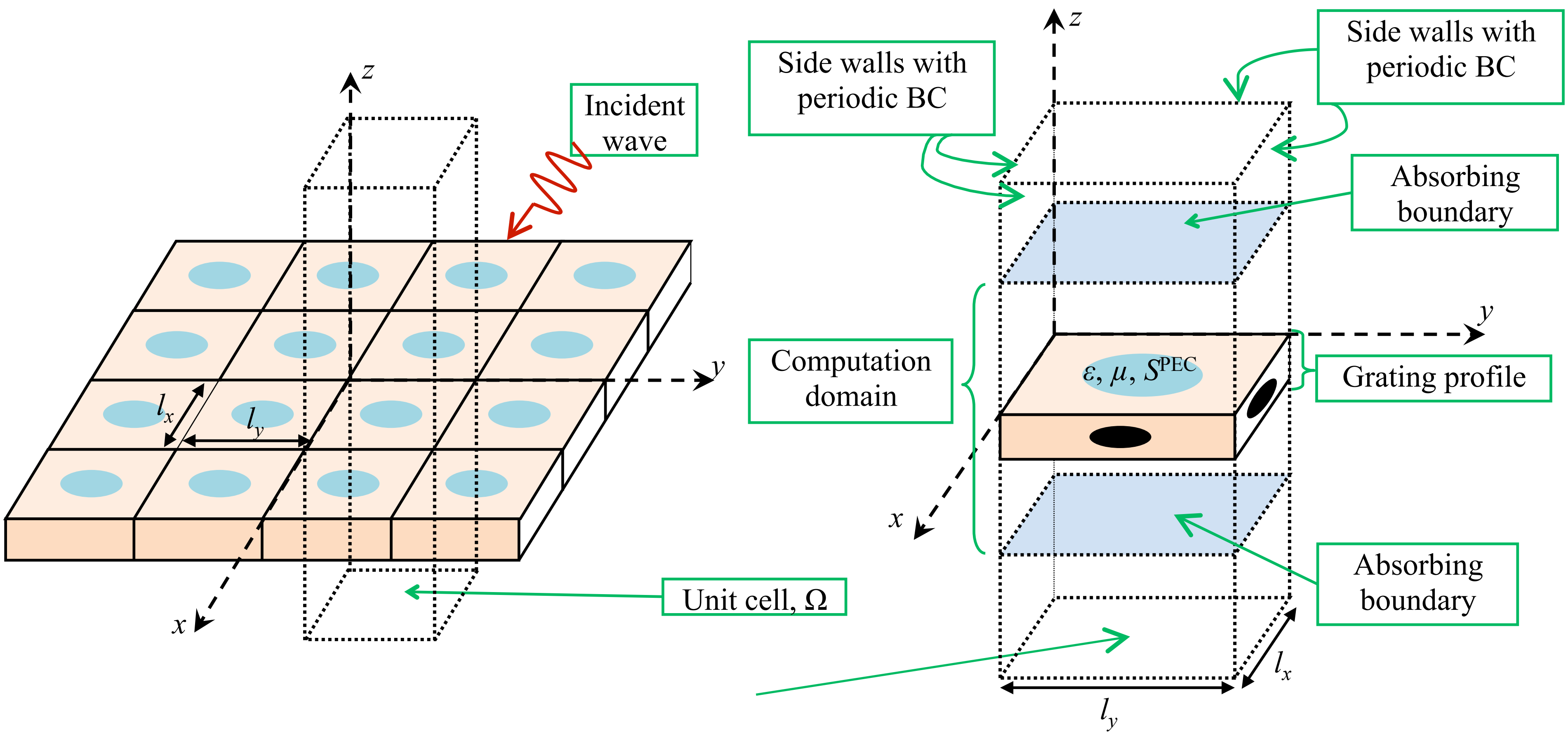
KAUST Supercomputing Laboratory: http://www.hpc.kaust.edu.sa

- Time Domain Discontinuous Galerkin Method with Exact Boundary Conditions
    - Introduction
    - Formulation
    - Numerical Results
    - Conclusions and Future/Ongoing Work

- With: Ozum Asirim, Ping Li, Konstyantyn Sirenko, and Yifei Shi

Introduction

- Abstract description of structures of interest



Introduction

- Time Domain Discontinuous Galerkin Finite Element Methods (TD-DG-FEM) are an alternative to finite difference time domain (FDTD) and classical FEM schemes

  Advantages

  - Information exchange between elements using numerical flux
  - All spatial operations are localized
  - Complex/arbitrarily shaped geometries
  - Non-conformal discretization
  - Adaptive spatial meshing is easier to implement
  - Higher order expansions are easy to implement
  - (Block) diagonal mass matrix
    - Compact solvers when combined with explicit time integration schemes
  - Easier to parallelize

  Disadvantages

  - Increased number of unknowns
    - Disadvantage diminishes as expansion order increases

Introduction

- TD-DG-FEM is naturally a (spatially) high-order accuracy method
- Accuracy is often limited by
  - Computation domain truncation (PML or approximate absorbing boundary conditions) in unbounded space problems
    - Increase thickness of PML at the cost of efficiency

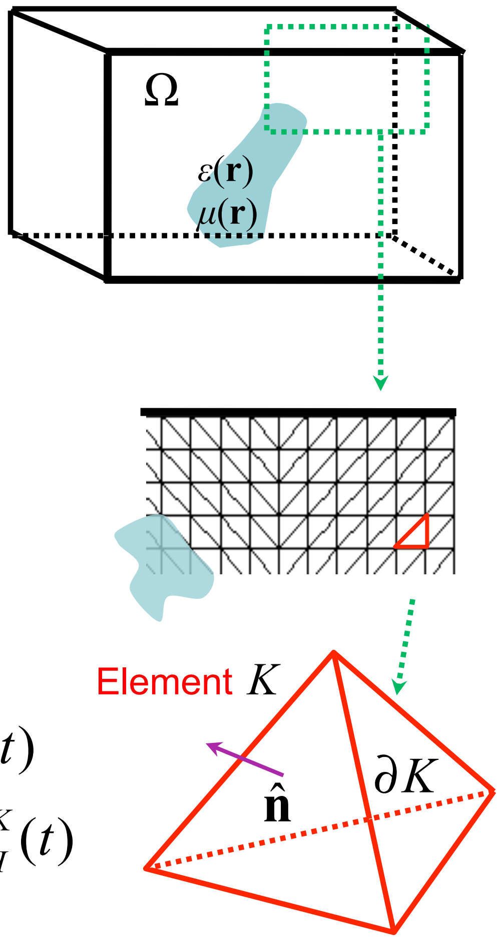
Proposed Solutions

- Exact absorbing boundary conditions with FFT acceleration

Formulation: TD-DG-FEM

- Electric field intensity $\mathbf{E}(\mathbf{r},t)$ and magnetic field intensity $\mathbf{H}(\mathbf{r},t)$ are governed by the first-order Maxwell curl equations:

$$\varepsilon(\mathbf{r})\partial_t \mathbf{E}(\mathbf{r},t) - \nabla \times \mathbf{H}(\mathbf{r},t) = 0$$
$$\mu(\mathbf{r})\partial_t \mathbf{H}(\mathbf{r},t) + \nabla \times \mathbf{E}(\mathbf{r},t) = 0$$



- Polynomial expansion:

$$\mathbf{E}(\mathbf{r},t) = \sum_{i=1}^{N_p} \left[\mathbf{E}^K(t)\right]_i \ell_i(\mathbf{r})$$
$$\mathbf{H}(\mathbf{r},t) = \sum_{i=1}^{N_p} \left[\mathbf{H}^K(t)\right]_i \ell_i(\mathbf{r})$$

- Galerkin testing:

$$\varepsilon^K \partial_t \mathbf{E}^K(t) = \mathbf{D}^K \times \mathbf{H}^K(t) + (\mathbf{M}^K)^{-1}\mathbf{L}^K\mathbf{F}_E^K(t)$$
$$\mu^K \partial_t \mathbf{H}^K(t) = -\mathbf{D}^K \times \mathbf{E}^K(t) - (\mathbf{M}^K)^{-1}\mathbf{L}^K\mathbf{F}_H^K(t)$$

J. S. Hesthaven, T. Warburton, *Nodal Discontinuous Galerkin Methods*, Springer, 2008

Formulation: TD-DG-FEM

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$$\varepsilon^K \partial_t \mathbf{E}^K(t) = \mathbf{D}^K \times \mathbf{H}^K(t) + (\mathbf{M}^K)^{-1} \mathbf{L}^K \mathbf{F}_E^K(t)$$
$$\mu^K \partial_t \mathbf{H}^K(t) = -\mathbf{D}^K \times \mathbf{E}^K(t) - (\mathbf{M}^K)^{-1} \mathbf{L}^K \mathbf{F}_H^K(t)$$

where

- Field samples to be computed: $[\mathbf{E}_v^K(t)]_i = E_{v,i}^K(t), \quad [\mathbf{H}_v^K(t)]_i = H_{v,i}^K(t), \quad v \in \{x, y, z\}$
- Differentiation matrices: $[\mathbf{D}_v^K]_{ij} = \partial_v \ell_j(\mathbf{r}_i), \; v \in \{x, y, z\}$
- Mass matrices: $[\mathbf{M}^K]_{ij} = \int_K \ell_i(\mathbf{r}) \ell_j(\mathbf{r}) \, d\mathbf{r}$
- Face/lift matrices: $[\mathbf{L}^K]_{ij} = \int_{\partial K} \ell_i(\mathbf{r}) \ell_j(\mathbf{r}) \, d\mathbf{r}, \quad j \in \{j : \mathbf{r}_j \in \partial K\}$

J. S. Hesthaven, T. Warburton, *Nodal Discontinuous Galerkin Methods*, Springer, 2008

Formulation: TD-DG-FEM

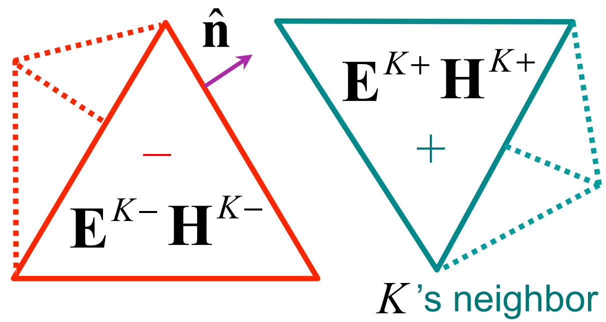
$$\varepsilon^K \partial_t \mathbf{E}^K(t) = \mathbf{D}^K \times \mathbf{H}^K(t) + (\mathbf{M}^K)^{-1} \mathbf{L}^K \mathbf{F}_E^K(t)$$

$$\mu^K \partial_t \mathbf{H}^K(t) = -\mathbf{D}^K \times \mathbf{E}^K(t) - (\mathbf{M}^K)^{-1} \mathbf{L}^K \mathbf{F}_H^K(t)$$

- Up-winding numerical flux for Maxwell equations:

$$\mathbf{F}_E^K(t) = \frac{\hat{\mathbf{n}} \times (Z^+ \Delta\mathbf{H}^K - \hat{\mathbf{n}} \times \Delta\mathbf{E}^K)}{Z^+ + Z^-}$$

$$\mathbf{F}_H^K(t) = \frac{\hat{\mathbf{n}} \times (Y^+ \Delta\mathbf{E}^K + \hat{\mathbf{n}} \times \Delta\mathbf{H}^K)}{Y^+ + Y^-}$$



- Here, $Z^{\pm} = 1/Y^{\pm} = (\mu^{\pm}/\varepsilon^{\pm})^{1/2}$, $\Delta\mathbf{E}^K = \mathbf{E}^{K+}(t) - \mathbf{E}^{K-}(t)$, $\Delta\mathbf{H}^K = \mathbf{H}^{K+}(t) - \mathbf{H}^{K-}(t)$

J. S. Hesthaven, T. Warburton, *Nodal Discontinuous Galerkin Methods*, Springer, 2008

Formulation: TD-DG-FEM

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- Numerical flux
  - Information exchange between elements
  - Stability of the whole numerical scheme
  - Impose PEC boundary conditions

$$Z^{+} = Z^{-},\ Y^{+} = Y^{-} \quad \Delta\mathbf{H}^{K} = 0,\ \Delta\mathbf{E}^{K} = -2\mathbf{E}^{K-}(t)$$

  - Impose periodic boundary conditions: "neighboring" elements are on the opposite sides of computation domain, but connected via numerical flux
  - Impose exact absorbing boundary conditions (EACs)—described next…

Formulation: EACs

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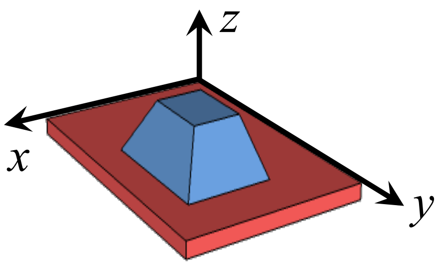
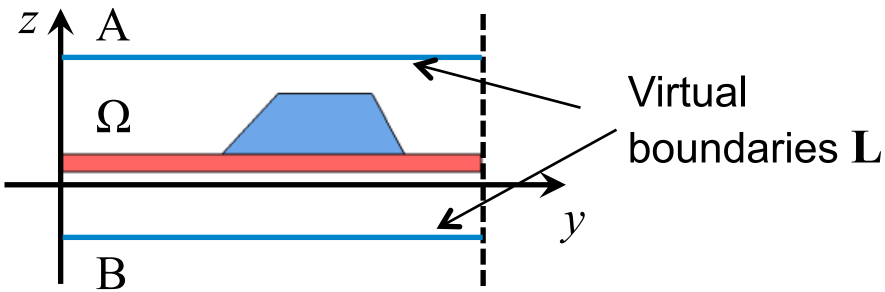


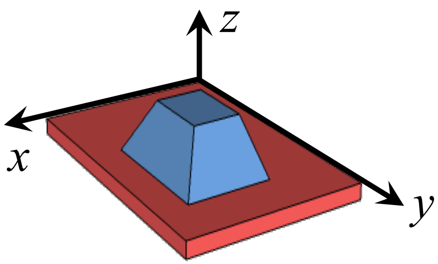


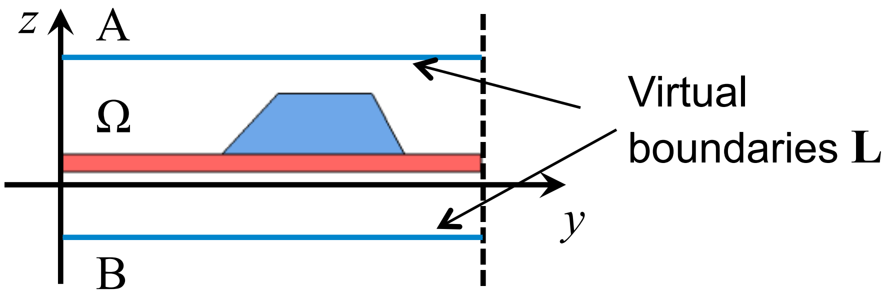
In A and B each of field comp., U, satisfies wave equation

$$\partial_t^2 U = \Delta U$$

$$U \in \{E_x, E_y, E_z, H_x, H_y, H_z\}$$

Formulation: EACs





In A and B each of field comp., U, satisfies wave equation

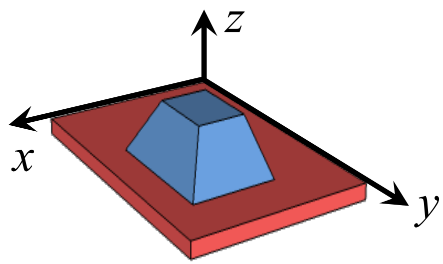
Separation of variables in **A** and **B** represents U as multiplication of known eigenfunctions $v_{m,n}$ and unknown amplitudes $u_{m,n}$

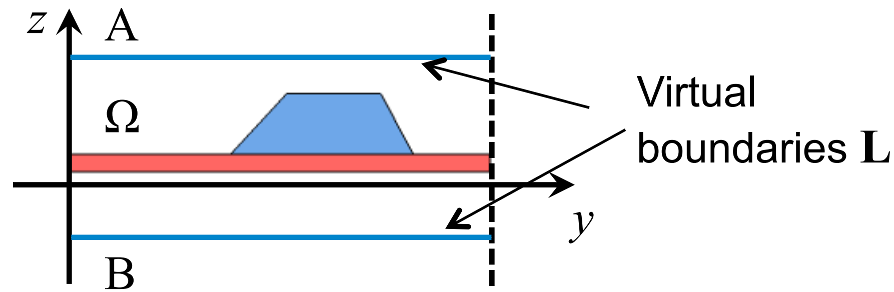
$$U(g,t) = \sum_{m,n=-\infty}^{\infty} u_{m,n}(z,t) v_{m,n}(x,y)$$

$$\partial_t^2 u_{m,n}(z,t) = \partial_z^2 u_{m,n}(z,t) - v_{m,n}^2 u_{m,n}(z,t)$$

$$u_{m,n}(z,0) = \partial_t u_{m,n}(z,t)\big|_{t=0} = 0$$

Formulation: EACs



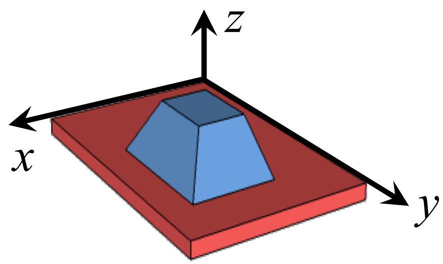


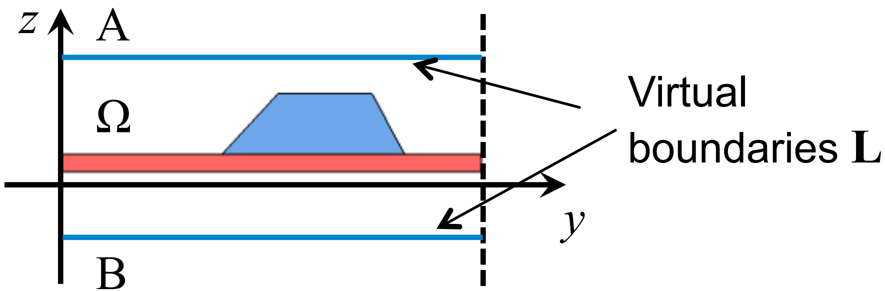
In A and B each of field comp., U, satisfies wave equation

Separation of variables in **A** and **B** represents U as multiplication of known eigenfunctions $v_{m,n}$ and unknown amplitudes $u_{m,n}$

Cosine Fourier transform with respect to z is applied to the problem for amplitudes $u_{m,n}$

Formulation: EACs





In A and B each of field comp., U, satisfies wave equation

Separation of variables in **A** and **B** represents U as multiplication of known eigenfunctions $v_{m,n}$ and unknown amplitudes $u_{m,n}$

Cosine Fourier transform with respect to z is applied to the problem for amplitudes $u_{m,n}$

Solution of the resulting generalized Cauchy problem

Formulation: EACs

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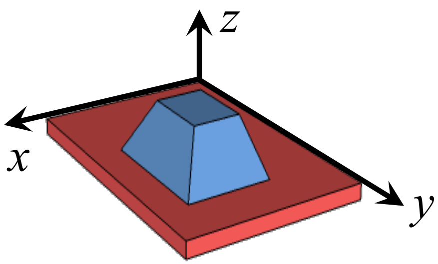
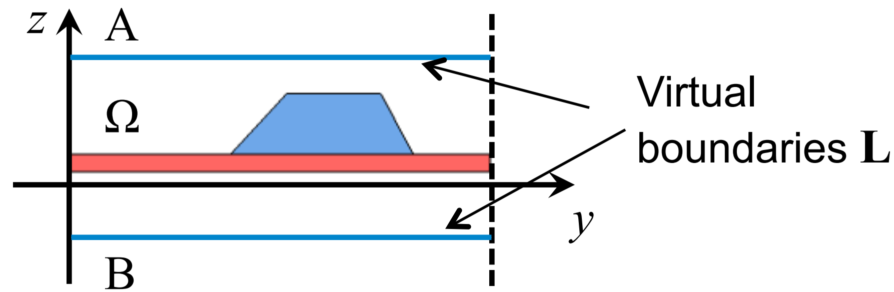


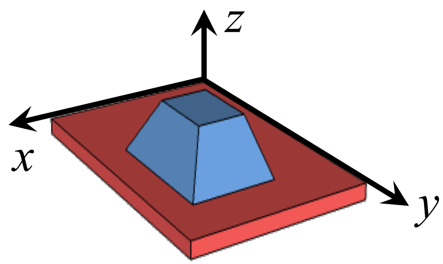


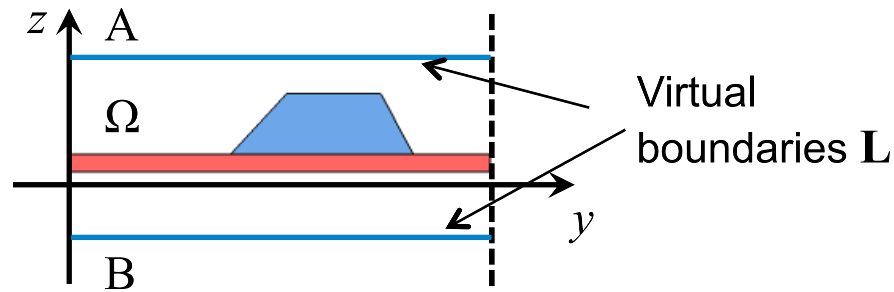
- In A and B each of field comp., U, satisfies wave equation
- Separation of variables in **A** and **B** represents U as multiplication of known eigenfunctions $\nu_{m,n}$ and unknown amplitudes $u_{m,n}$
- Cosine Fourier transform with respect to z is applied to the problem for amplitudes $u_{m,n}$
- Solution of the resulting generalized Cauchy problem
- Inverse Fourier transform is applied to the solution

$$\partial_t u_{m,n}(\mathbf{L},t) \pm \partial_z u_{m,n}(\mathbf{L},t) =$$

$$= -\lambda_{m,n} \int_0^t \frac{J_1([t-\tau]\lambda_{m,n})}{t-\tau} u_{m,n}(\mathbf{L},\tau)\, d\tau$$

Formulation: EACs





In A and B each of field comp., U, satisfies wave equation → Separation of variables in **A** and **B** represents U as multiplication of known eigenfunctions $v_{m,n}$ and unknown amplitudes $u_{m,n}$ → Cosine Fourier transform with respect to z is applied to the problem for amplitudes $u_{m,n}$ → Solution of the resulting generalized Cauchy problem → Inverse Fourier transform is applied to the solution

EM field comp., U, are reconstructed back from the amplitudes $u_{m,n}$ →

$$\boxed{\partial_t U(\mathbf{L},t) = \pm\partial_z U(\mathbf{L},t) - \sum_{m,n=-\infty}^{\infty} \left\{ \int_0^t \frac{J_1([t-\tau]\lambda_{m,n})}{t-\tau} \left[\int_{\mathbf{L}} U(\mathbf{L},\tau) v^*_{m,n}\, dS \right] d\tau \right\} \lambda_{m,n} v_{m,n}}$$

- Relates the boundary values with their normal derivative on the virtual boundaries $\mathbf{L}$, and thus could be used as a boundary condition

Formulation: EACs

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$$\partial_t U(\mathbf{L},t) = \pm\partial_z U(\mathbf{L},t) - \sum_{m,n=-\infty}^{\infty} \left\{ \int_0^t \frac{J_1([t-\tau]\lambda_{m,n})}{t-\tau} \left[\int_{\mathbf{L}} U(\mathbf{L},\tau) v_{m,n}^* dS \right] d\tau \right\} \lambda_{m,n} v_{m,n}$$

- Convenient for TD-DG-FEM framework
- EACs should be discretized with the same level of accuracy as TD-DG-FEM both in space and time
- The summations over m and n are truncated to a finite number of terms, M_h and N_h
- Field component, U, and eigenfunctions, $v_{m,n}$, are sampled at TD-DG-FEM's nodal points on the virtual boundaries, $\mathbf{L}$
- Proper (high-order) numerical quadrature rules are used for space and time integrations

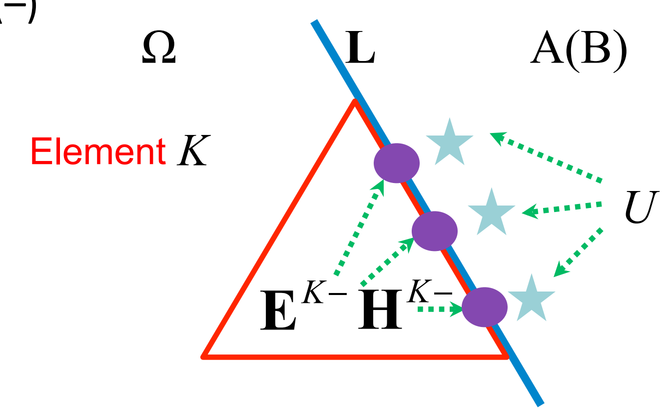
Formulation: EACs

$$\partial_t U(\mathbf{L},t) = \pm\partial_z U(\mathbf{L},t) - \sum_{m,n=-\infty}^{\infty} \left\{ \int_0^t \frac{J_1([t-\tau]\lambda_{m,n})}{t-\tau} \left[\int_{\mathbf{L}} U(\mathbf{L},\tau) v_{m,n}^* dS \right] d\tau \right\} \lambda_{m,n} v_{m,n}$$

- The derivative ∂_z is approximated from samples of U on the virtual boundaries, $\mathbf{L}$, and TD-DG-FEM samples of field components in the vicinity of $\mathbf{L}$ (within element K) using element's differentiation matrix $\mathbf{D}^K$.
- Values of EM field's components provided by EAC are used as external, '+', values in the numerical flux's $\Delta\mathbf{E}^K$ and $\Delta\mathbf{H}^K$ on the virtual boundaries $\mathbf{L}$

Element K values (–)

EAC values (+)



$$\mathbf{F}_E^K(t) = \frac{\hat{\mathbf{n}} \times (Z^+ \Delta\mathbf{H}^K - \hat{\mathbf{n}} \times \Delta\mathbf{E}^K)}{Z^+ + Z^-}$$

$$\mathbf{F}_H^K(t) = \frac{\hat{\mathbf{n}} \times (Y^+ \Delta\mathbf{E}^K + \hat{\mathbf{n}} \times \Delta\mathbf{H}^K)}{Y^+ + Y^-}$$

$$\Delta\mathbf{E}^K = \mathbf{E}^{K+}(t) - \mathbf{E}^{K-}(t)$$

$$\Delta\mathbf{H}^K = \mathbf{H}^{K+}(t) - \mathbf{H}^{K-}(t)$$

Formulation: System of Equations

- Maxwell equations and EAC are integrated in time simultaneously

$$\left.\begin{aligned}
\varepsilon^K \boxed{\partial_t} \mathbf{E}^K(t) &= \mathbf{D}^K \times \mathbf{H}^K(t) + (\mathbf{M}^K)^{-1}\mathbf{L}^K\mathbf{F}_E^K(t) \\
\mu^K \boxed{\partial_t} \mathbf{H}^K(t) &= -\mathbf{D}^K \times \mathbf{E}^K(t) - (\mathbf{M}^K)^{-1}\mathbf{L}^K\mathbf{F}_H^K(t)
\end{aligned}\right\} \text{Maxwell equations}$$

$$\left.\begin{aligned}
\boxed{\partial_t} \mathbf{U}^K(t) = \pm \mathbf{D}_z^K \mathbf{U}^K(t) \\
- \sum_{m=-M_h}^{M_h} \sum_{n=-N_h}^{N_h} \lambda_{m,n} \mathbf{v}_{m,n}^K \boxed{\int_0^t \frac{J_1[(t-t')\lambda_{m,n}]}{t-t'}} \sum_{k'} \mathbf{w}^{k'} \mathbf{U}^{k'}(t') \mathbf{v}_{m,n}^{k'}\, dt'
\end{aligned}\right\} \text{EAC}$$

- Computational cost: $O(N^2 N_t^2) \Rightarrow O(N^2 N_t \log^2 N_t)$

Blocked FFTs exact, no additional numerical error

- Time Integration: Fourth order explicit Runge-Kutta method

Numerical Results: Accuracy of EACs

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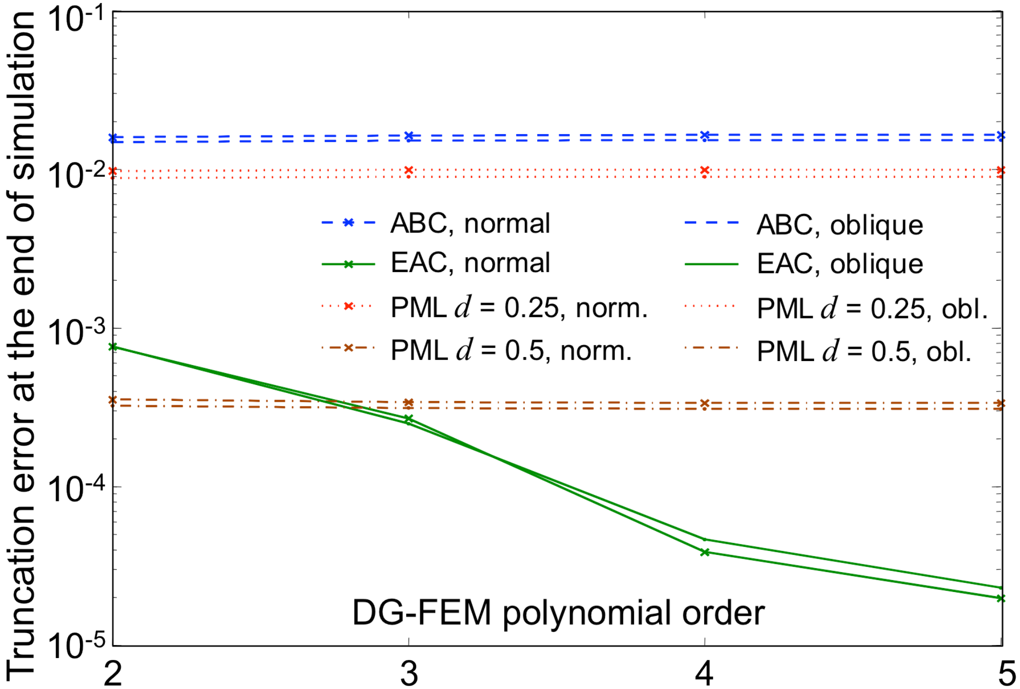
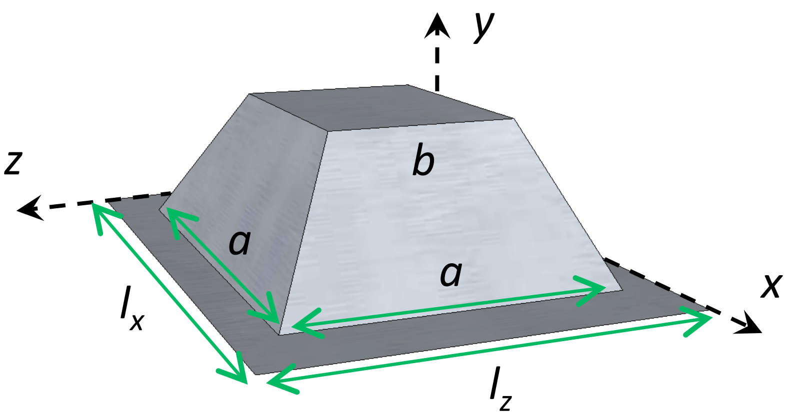
- Duration of simulation is 7.5
- Excitation signal

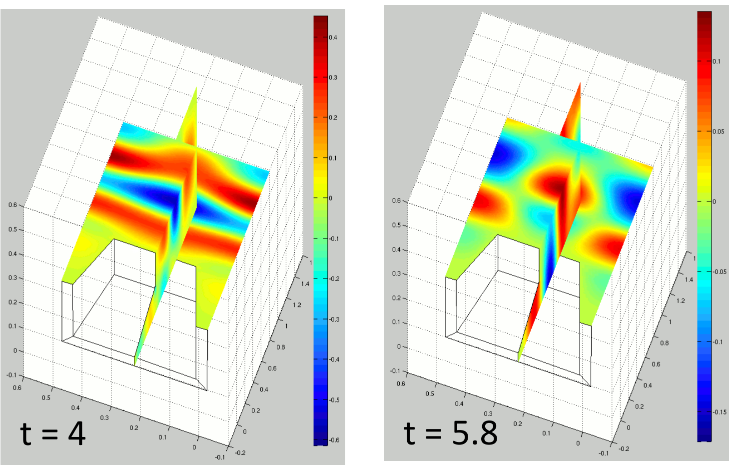
$$E_z^{\mathrm{inc}}(x,1.5,z,t) = 2e^{-(t-1.5)^2/0.13}\cos(15[t-1.5])\mu_{0,0}(x,z)$$



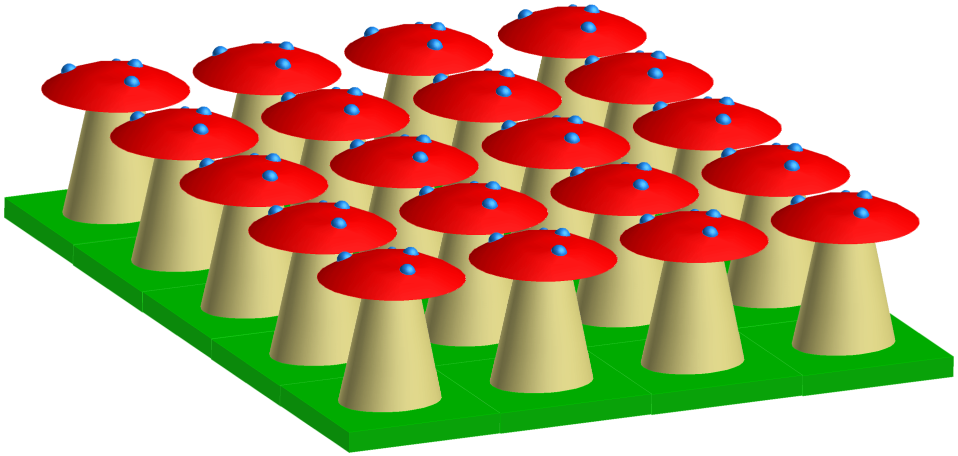


a = 0.42, b = 0.28

l_x = l_z = 0.5, h= 0.5



Numerical Results: Mushroom Gratings



- Height of the structure is 4.1 μm; diameter of PEC inclusions is 0.4 μm
- 80150 mesh elements in the computation domain. 4 809 000 unknowns
- Excitation:
- Wavelength at the center frequency is 483 nm

Numerical Results: Mushroom Gratings

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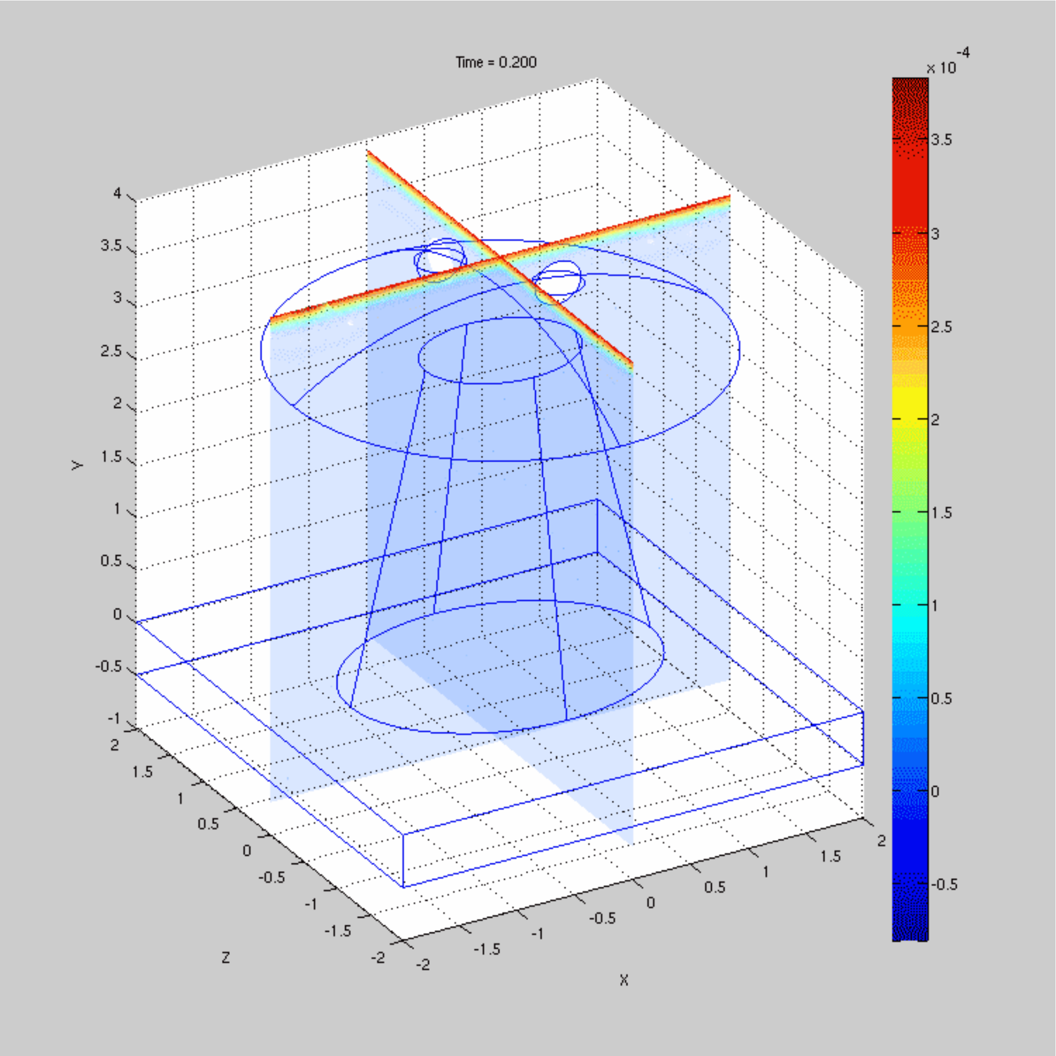

Conclusions and Future/Ongoing Work

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- Highlights:
  - Discretization and coupling of EAC equations into TD-DG-FEM discretizing Maxwell equation are described
  - Numerical results demonstrate the accuracy of EAC discretization
  - The accuracy of EAC discretization grows with the order of DG-FEM. Thus, truncation of computation domain no longer limits the overall accuracy of numerical solution

- Ongoing Work:
  - Efficient truncation methods for concave geometries
  - Incorporation of material nonlinearity

- Time Domain Integral Equation Solver for High Contrast Scatterers
    - Introduction
    - Formulation
    - Numerical Results
    - Conclusions and Future/Ongoing Work

- With: Sadeed Bin Sayed and Huseyin Arda Ulku

Introduction

- Time Domain Volume Integral Equation (TDVIE) Solvers are an alternative to finite difference time domain (FDTD) and classical FEM schemes
- TDVIEs are classically solved using Marching-on-in-time (MOT) schemes

Advantages

- No phase dispersion
- No grid truncation (exact radiation condition)
- Time step size is not necessarily constrained by spatial discretization
- Only volume of the object is discretized
- Accurate representation of the geometry

Disadvantages

- Higher computational cost
  - Addressed by PWTD and FFT based acceleration engines

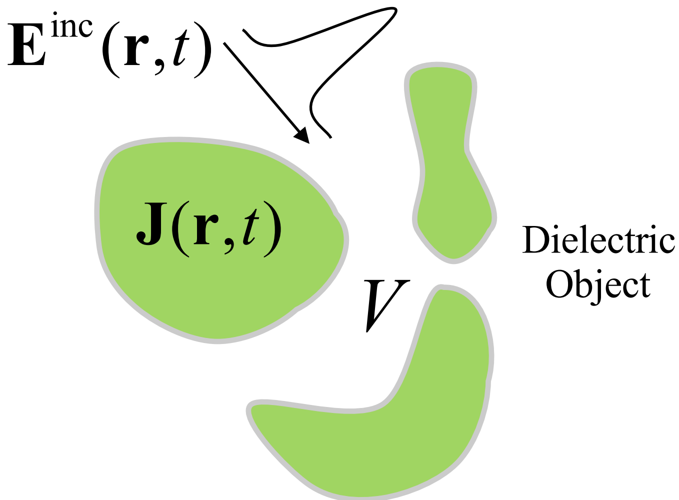
Introduction

- Instability of the MOT solution
  - Still a problem especially for high contrast scatterers

Proposed Solutions

- Band limited interpolation with short duration
- Extrapolation scheme defined on the complex frequency plane

Formulation: TDVIE



- Volumetric scatter with $\varepsilon(\mathbf{r})$ and μ_0 residing in free space with ε_0 and μ_0
- Total volume: V
- Excitation: $\mathbf{E}^{\text{inc}}(\mathbf{r},t)$ band-limited to $f_{\max}$
- Current induced in V : $\mathbf{J}(\mathbf{r},t)$

- Scattered field in terms of potentials

$$\mathbf{E}^{\text{scat}}(\mathbf{r},t) = \int_V \frac{\mu_0 \partial_t \mathbf{J}(\mathbf{r},t - R/c_0)}{4\pi R} d\mathbf{r}'$$

$$-\nabla \int_V \int_0^{t-R/c_0} \frac{\nabla' \cdot \mathbf{J}(\mathbf{r}',t')}{4\pi\varepsilon_0 R} d\mathbf{r}' \quad R = |\mathbf{r} - \mathbf{r}'|$$

- Equivalent current in terms of electric flux density

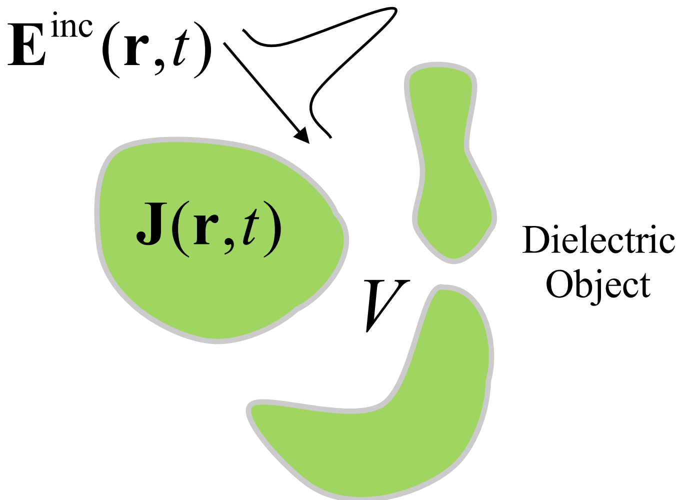
$$\mathbf{J}(\mathbf{r},t) = \kappa(\mathbf{r}) \partial_t \mathbf{D}(\mathbf{r},t)$$

$$\kappa(\mathbf{r}) = 1 - \varepsilon_0 / \varepsilon(\mathbf{r})$$

- Electric flux density in terms of electric field intensity

$$\mathbf{E}(\mathbf{r},t) = \varepsilon(\mathbf{r}) \mathbf{D}(\mathbf{r},t)$$

Formulation: TDVIE



- Volumetric scatter with $\varepsilon(\mathbf{r})$ and μ_0 residing in free space with ε_0 and μ_0
- Total volume: V
- Excitation: $\mathbf{E}^{\mathrm{inc}}(\mathbf{r},t)$ band-limited to $f_{\max}$
- Current induced in V : $\mathbf{J}(\mathbf{r},t)$

- Fields satisfy

$$\partial_t \mathbf{E}(\mathbf{r},t) = \partial_t \mathbf{E}(\mathbf{r},t) - \partial_t \mathbf{E}^{\mathrm{sca}}(\mathbf{r},t)$$

- Inserting everything above and enforcing the resulting equation at $\mathbf{r} \in V$ yields the TDIVE in $\mathbf{D}(\mathbf{r},t)$

$$\partial_t \mathbf{E}^{\mathrm{inc}}(\mathbf{r},t) = \partial_t \mathbf{D}(\mathbf{r},t) / \varepsilon(\mathbf{r})$$
$$+ \int_V \frac{\mu_0 \kappa(\mathbf{r}') \partial_t^2 \mathbf{D}(\mathbf{r}, t - R/c_0)}{4\pi R} d\mathbf{r}'$$
$$- \nabla \int_V \frac{\nabla' \cdot \left[\kappa(\mathbf{r}') \mathbf{D}(\mathbf{r}', t - R/c_0) \right]}{4\pi \varepsilon_0 R} d\mathbf{r}'$$

Formulation: MOT Solution

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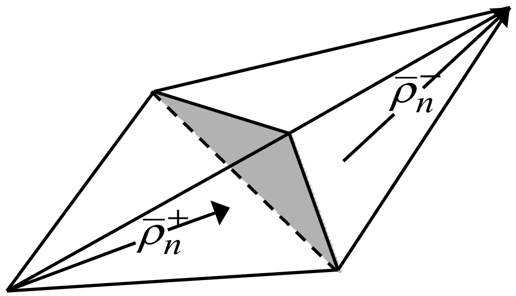
- To numerically solve the TDVIE
- Volume V is divided into tetrahedrons
- $\mathbf{D}(\mathbf{r},t)$ is expanded as

$$\mathbf{D}(\mathbf{r},t) \cong \sum_{k'=1}^{N_{\mathrm{V}}} \sum_{l'=0}^{N_{\mathrm{t}}} I_{k',l'} T_{l'}(t) \mathbf{f}_{k'}(\mathbf{r})$$

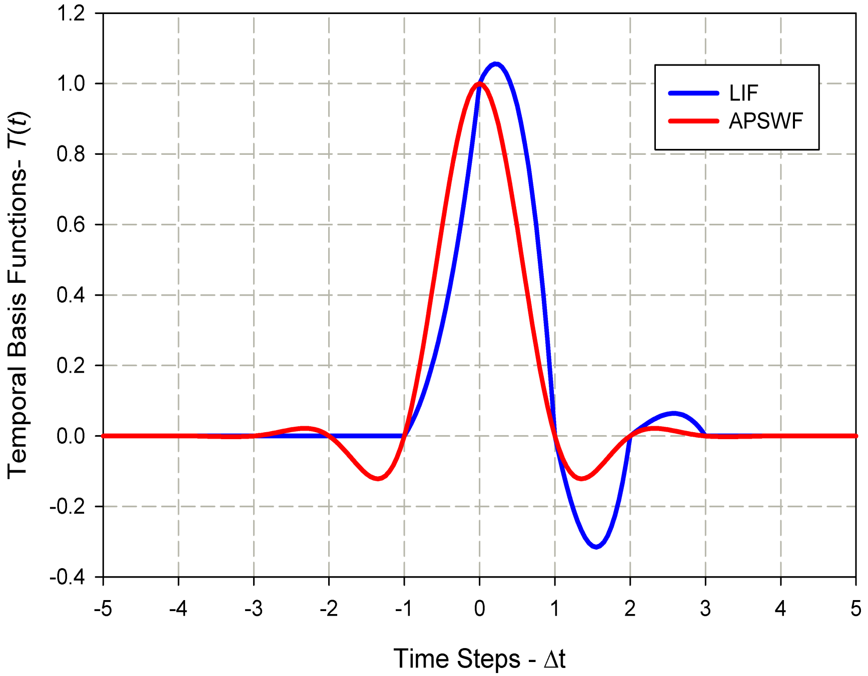
- Unknowns: $I_{k',l'}$
- Temporal basis functions: $T_{l'}(t)$
- Spatial basis functions: $\mathbf{f}_{k'}(\mathbf{r})$

$$\mathbf{f}_{k'}(\mathbf{r}) = \begin{cases} \pm \dfrac{A_k}{3V_k^{\pm}}(\mathbf{r} - \mathbf{r}_{k'}^{\pm}), & \mathbf{r} \in V_{k'}^{\pm} \\ 0 & \text{, elsewhere} \end{cases}$$



Formulation: Temporal Basis Function Selection

- Lagrange interpolation function (LIF)
  - Wide spectrum (possible source of instability)
  - Discontinuous derivatives (possible source of instability)
- Approximate prolate spheroidal wave functions (APSWF)
  - Band-limited and short temporal support
  - Have continuous derivatives
  - Non-causal
- Non-causality is fixed by temporal extrapolation !
- Future values are predicted from past values



Formulation: MOT Solution

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- Testing with $\mathbf{f}_k(\mathbf{r})$ at times $l\Delta t$ yields

$$\mathbf{Z}_0\mathbf{I}_l = \mathbf{V}_l - \sum_{l'=1}^{l-1}\mathbf{Z}_{l-l'}\mathbf{I}_{l'} \boxed{-\sum_{l'=l+1}^{l+N_{\min}^T-1}\mathbf{Z}_{l-l'}\mathbf{I}_{l'}}$$

Non-casual terms

$$\{\mathbf{Z}_{l-l'}\}_{k,k'} = \int_{V_k}\frac{1}{\varepsilon_k(\mathbf{r})}\mathbf{f}_k(\mathbf{r})\cdot\mathbf{f}_{k'}(\mathbf{r})T_{l'}(l\Delta t)\,d\mathbf{r} + \frac{\mu_0}{4\pi}\left\langle \mathbf{f}_k(\mathbf{r}),\kappa_{k'}(\mathbf{r})\mathbf{f}_{k'}(\mathbf{r}),\partial_t^2 T_{l'}(t)\right\rangle_{t=l\Delta t}$$
$$+\frac{1}{4\pi\varepsilon_0}\left\langle \nabla\cdot\mathbf{f}_k(\mathbf{r}),\nabla\cdot\left[\kappa_{k'}(\mathbf{r})\mathbf{f}_{k'}(\mathbf{r})\right],T_{l'}(t)\right\rangle_{t=l\Delta t}$$

- How is this solved ?

Solve for $\mathbf{I}_1$ $\quad \mathbf{Z}_0\mathbf{I}_1 = \mathbf{V}_1 - \mathbf{Z}_{-1}\mathbf{I}_2 + \mathbf{Z}_{-2}\mathbf{I}_3$ $\quad \hat{\mathbf{Z}}_0\mathbf{I}_1 = \mathbf{V}_1$

Solve for $\mathbf{I}_2$ $\quad \mathbf{Z}_0\mathbf{I}_2 = \mathbf{V}_2 - \mathbf{Z}_1\mathbf{I}_1 - \mathbf{Z}_{-1}\mathbf{I}_3 - \mathbf{Z}_{-2}\mathbf{I}_4$ $\quad \hat{\mathbf{Z}}_0\mathbf{I}_2 = \mathbf{V}_2 - \hat{\mathbf{Z}}_1\mathbf{I}_1$

Solve for $\mathbf{I}_3$ $\quad \mathbf{Z}_0\mathbf{I}_3 = \mathbf{V}_3 - \mathbf{Z}_1\mathbf{I}_2 - \mathbf{Z}_2\mathbf{I}_1 - \mathbf{Z}_{-1}\mathbf{I}_4 - \mathbf{Z}_{-2}\mathbf{I}_5$ $\quad \hat{\mathbf{Z}}_0\mathbf{I}_3 = \mathbf{V}_3 - \hat{\mathbf{Z}}_1\mathbf{I}_2 - \hat{\mathbf{Z}}_2\mathbf{I}_1$

....

Extrapolation

Formulation: Temporal Extrapolation

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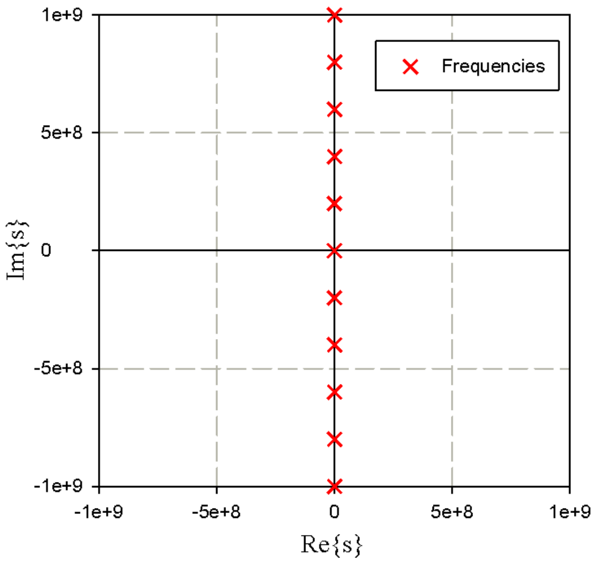
- Harmonic Based Extrapolation (HEBE)
  - Assumes that the solution can be expanded in terms of sine and cosine functions within the band of the excitation
  - Expansion coefficients (amplitude of harmonics) are found using known past samples
  - Expansion is used to predict the future samples (extrapolation)
- Known to work well and produce stable results for weak scatterers
- Unstable for strong scatters
- Strong scatterers support modes with decaying and oscillating components
- Frequency sampling cannot be accurately done on the imaginary axis (i.e., sine/cosine approximation is not accurate)



Formulation: Decaying and Oscillatory Modes

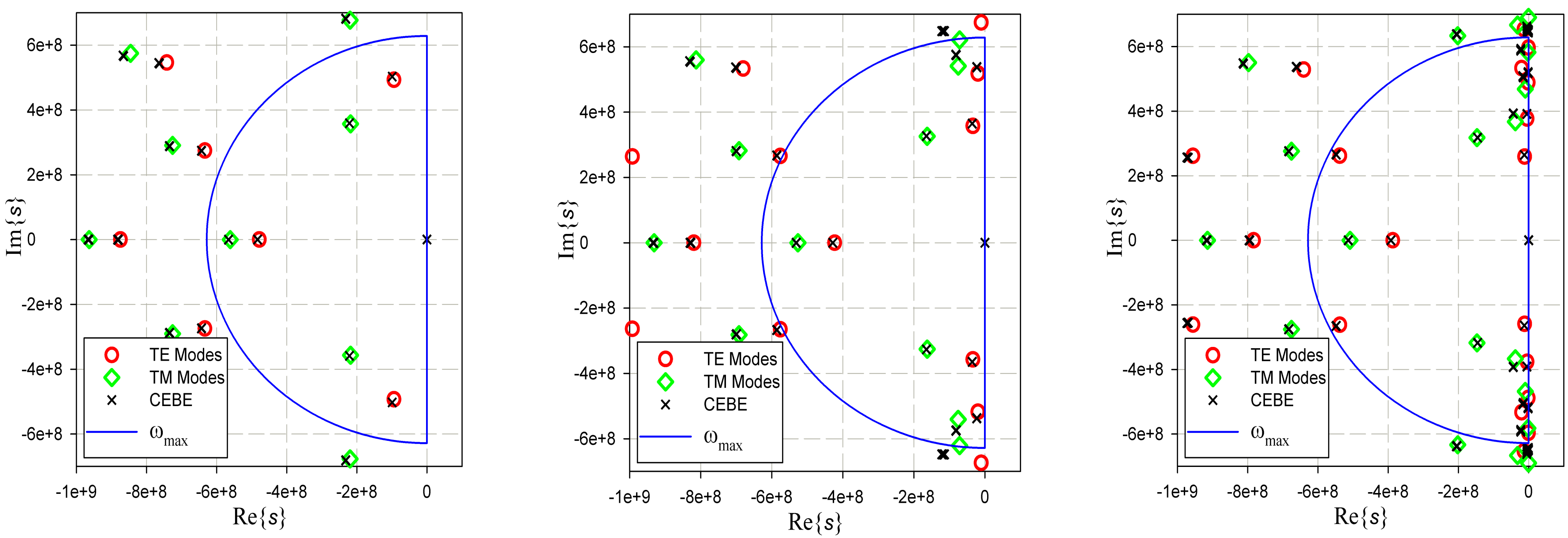
- Resonance modes of unit sphere

TE mode

$$\frac{J_{n-1/2}(\beta\rho)}{J_{n+1/2}(\beta\rho)}=\frac{H^{(2)}_{n-1/2}(\beta\rho/\sqrt{\varepsilon_r})}{H^{(2)}_{n+1/2}(\beta\rho/\sqrt{\varepsilon_r})}$$

TM mode

$$\frac{n}{\beta\rho}-\frac{J_{n-1/2}(\beta\rho)}{J_{n+1/2}(\beta\rho)}=\frac{n\varepsilon_r}{\beta\rho}+\sqrt{\varepsilon_r}\,\frac{H^{(2)}_{n-1/2}(\beta\rho/\sqrt{\varepsilon_r})}{H^{(2)}_{n+1/2}(\beta\rho/\sqrt{\varepsilon_r})}$$



$\varepsilon_r = 3$ $\varepsilon_r = 6$ $\varepsilon_r = 12$

Formulation: Temporal Extrapolation

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- Frequency sampling should be done on the complex frequency plane
- How to define a temporal extrapolation ?

- Solution is expanded in terms of exponentials :

$$\varphi(t) \sim \sum_{v=1}^{Nv} \alpha_v e^{\lambda_v t}$$

λ_v : complex numbers $(v = 1 \ldots N_v)$
α_v : weighting coefficients

- Suppose that λ_v are known!

- Extrapolation coefficients:

$$\varphi(t_j) = \sum_{l=1}^{k} \{\mathbf{p}\}_l \varphi(t_{j-1+l-k})$$

- Matrix relation: $\mathbf{A}_p \mathbf{p} = \mathbf{b}$

$$\{\mathbf{A}_p\}_{v,l} = e^{\lambda_v t_l}; \quad v = 1,\ldots,N_v; \quad l = 1,\ldots,k$$

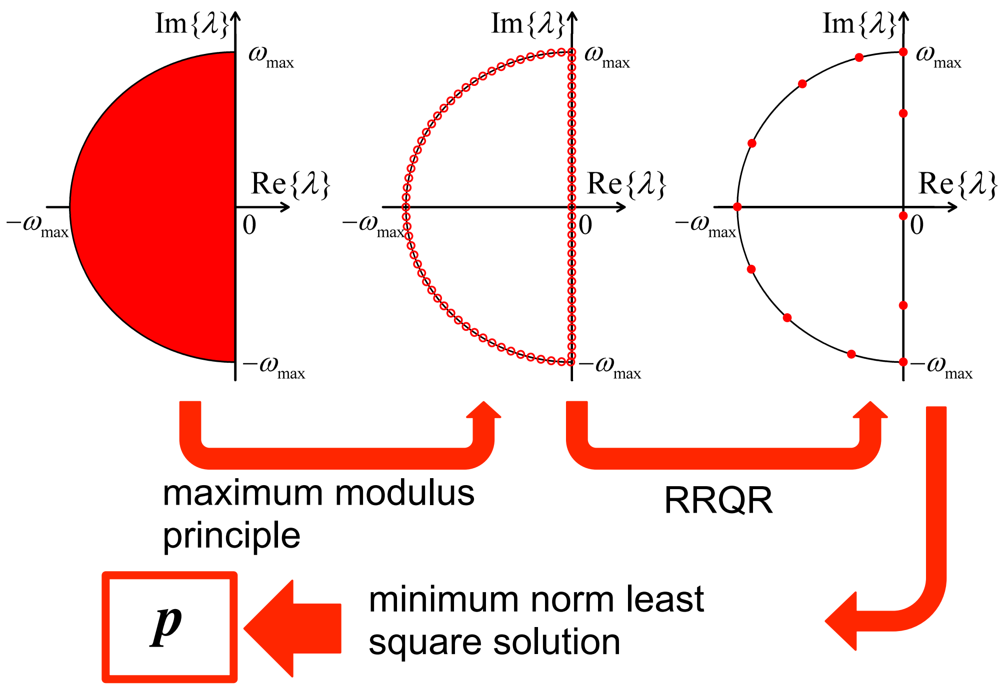
$$\{\mathbf{b}\}_v = e^{\lambda_v t_{k+1}}$$

- Solution is found by minimum norm least square solution

[1]A. Glaser and V. Rokhlin, "A new class of highly accurate solvers for ordinary differential equations," *J. of Sci. Comput.*, 38(3), pp. 368-399, March, 2009.

Formulation: Temporal Extrapolation

- How to find λ_v



$$\varphi(t) \sim \sum_{v=1}^{Nv} \alpha_v e^{\lambda_v t}$$

$$\boldsymbol{\varphi}_i = \mathbf{A}\boldsymbol{\alpha}$$

$$\{\mathbf{A}\}_{ji} = e^{\lambda_j t_i}, \; j = 1,\ldots,N, \; i = 1,\ldots,M$$

[1]A. Glaser and V. Rokhlin, "A new class of highly accurate solvers for ordinary differential equations," *J. of Sci. Comput.*, 38(3), pp. 368-399, March, 2009.

Numerical Examples: Accuracy of Extrapolation

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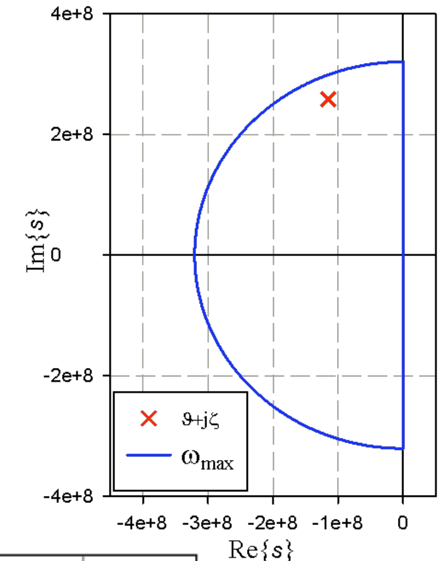
- Signal: Convolution of $r(t) = \exp(-\vartheta t)\cos(2\pi\varsigma t)$

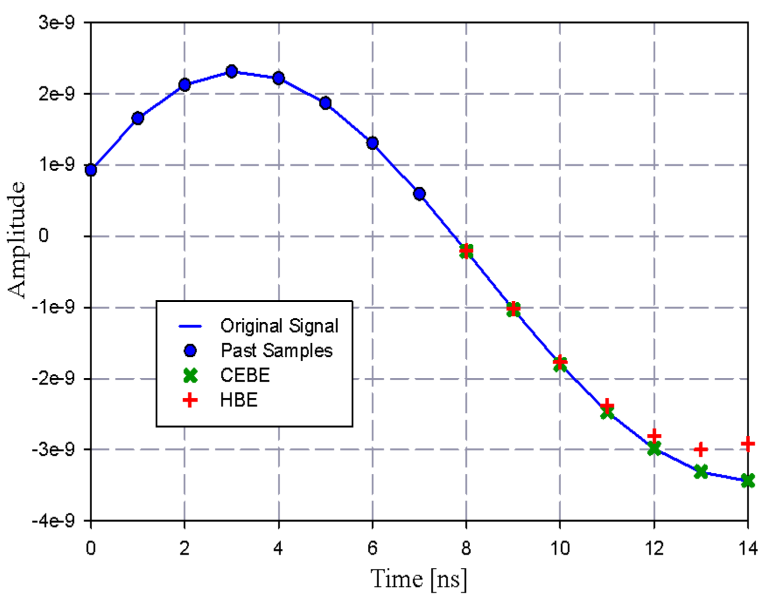
with $G(t) = \cos(2\pi f_0 t)\exp[-t^2/(2\sigma^2)]$

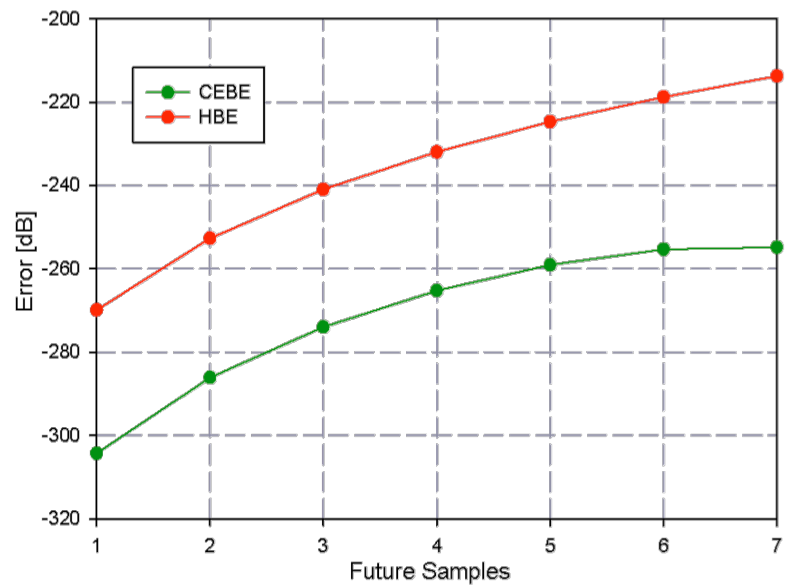
- $r(t)$ resonance mode of unit sphere with $\varepsilon_r = 12$

$$f_0 = 34 \text{ MHz}, f_{bw} = 17 \text{ MHz}, \sigma = 3/(2\pi f_{bw})$$

$$\vartheta = 11.53 \text{ Np/ns}, \; \varsigma = 41.20 \text{ MHz}$$

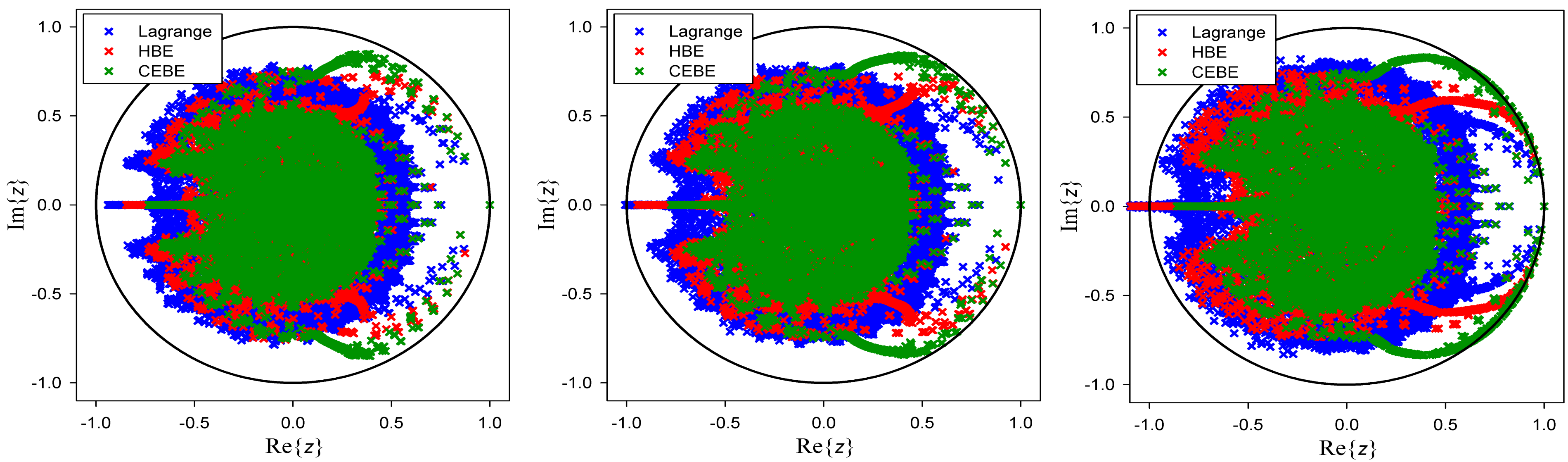






Numerical Examples: Stability of the MOT Solution

- Scatterer: Dielectric unit sphere with increasing ε_r
- Eigenvalues of the MOT matrix for different temporal basis functions are compared



$\varepsilon_r = 3$ $\varepsilon_r = 6$ $\varepsilon_r = 12$

Numerical Examples: Accuracy of the MOT Solution

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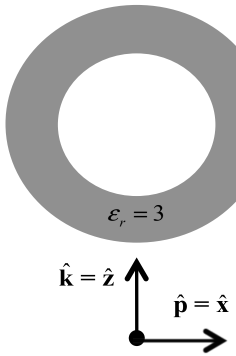
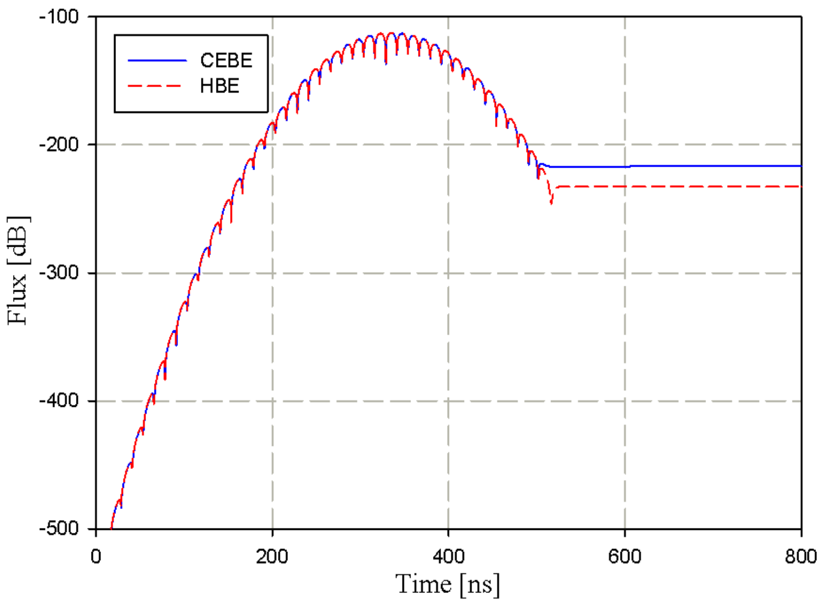
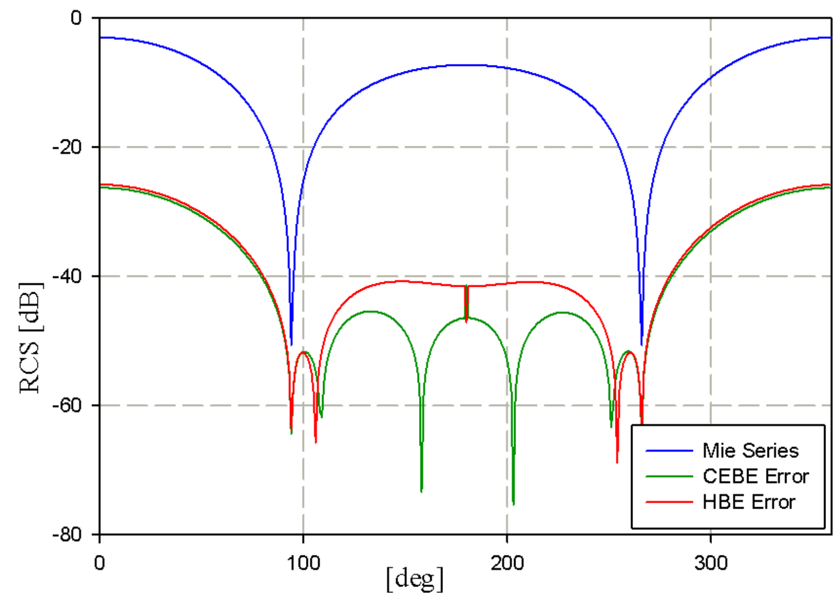
- Scatterer: Dielectric shell
- $\varepsilon_r = 3$, inner radius: 0.75m, outer radius 1m
- Excitation: $\mathbf{E}^{\text{inc}}(\mathbf{r},t) = \hat{\mathbf{p}} G(t - t_{\text{p}} - \mathbf{r}\cdot\hat{\mathbf{k}}/c)$

$$G(t) = \cos(2\pi f_0 t)\exp[-t^2/(2\sigma^2)]$$

$$f_0 = 40\text{MHz},\ f_{bw} = 20\text{MHz}, \sigma = 3/(2\pi f_{bw}),\ t_p = 14\sigma$$





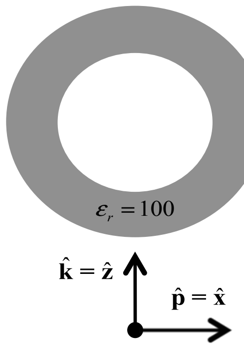


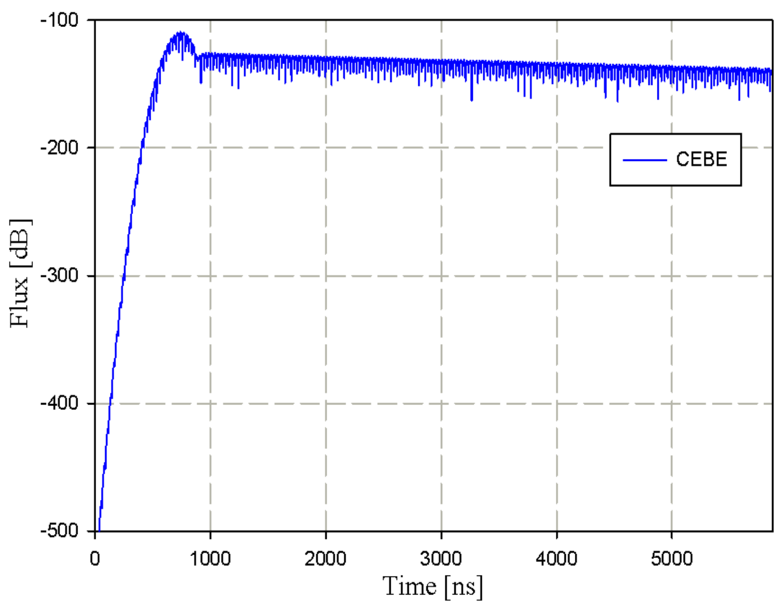
Numerical Examples: Accuracy of the MOT Solution

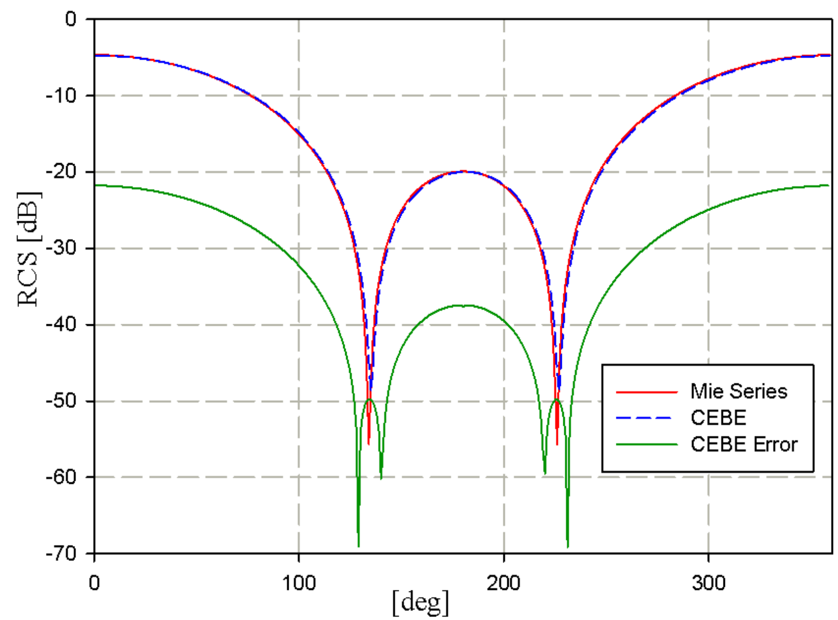
- Scatterer: Dielectric shell
- $\varepsilon_r = 100,$ inner radius: 0.75m, outer radius 1m
- Excitation: $\mathbf{E}^{\mathrm{inc}}(\mathbf{r},t) = \hat{\mathbf{p}} G(t - t_{\mathrm{p}} - \mathbf{r}\cdot\hat{\mathbf{k}}/c)$

$$G(t) = \cos(2\pi f_0 t)\exp[-t^2/(2\sigma^2)]$$

$$f_0 = 18\mathrm{MHz},\ f_{bw} = 9\mathrm{MHz},\ \sigma = 3/(2\pi f_{bw}),\ t_p = 14\sigma$$







Conclusions and Future/Ongoing Work

- Highlights:
    - A highly stable TDVIE solver is formulated and implemented
    - An extrapolation scheme defined over the complex frequency plane helps to achieve stability
    - Numerical results demonstrate the accuracy and stability of the MOT solution on high contrast scatterers

- Ongoing Work:
    - Applying the TDVIE solver on realistic structures
    - Developing an explicit MOT scheme for solving the TDVIE

CEM Research Group at KAUST – People and Facilities

King Abdullah University of Science and Technology KAUST

Work Force

PhD Students

- Muhammad Amin
- Abdulla Desmal
- Ismail Uysal
- Sadeed Sayed
- Noha Alharthi
- Ali Imran Sandhu
- Ozum Asirim

Post-Doctoral Researchers

- Kostyantyn Sirenko, PhD
- Arda Ulku, PhD
- Yifei Shi, PhD
- Mohamed Farhat, PhD

Alumni

- Mohamed Salem, PhD (Mar. 2013)
- Ahmed Al-Jarro, PhD (Nov. 2012)
- Meilin Liu, PhD (Jan. 2012)
- Umair Khalid (MS degree, Dec. 2010)
- Muhammad Furqan (Feb. 2012)
- Abdul Haseeb Muhammed (Apr. 2011)

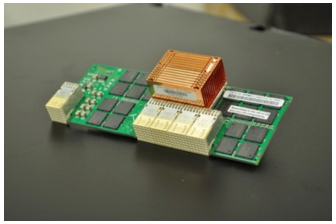
Computational Resources

Shaheen

- IBM's 16-Rack Blue Gene/P, ~65k computing cores, 222 teraflops/sec
- Expandable to petascale computing
- Supported by IBM and KAUST Supercomputing Laboratory (KSL)

Noor

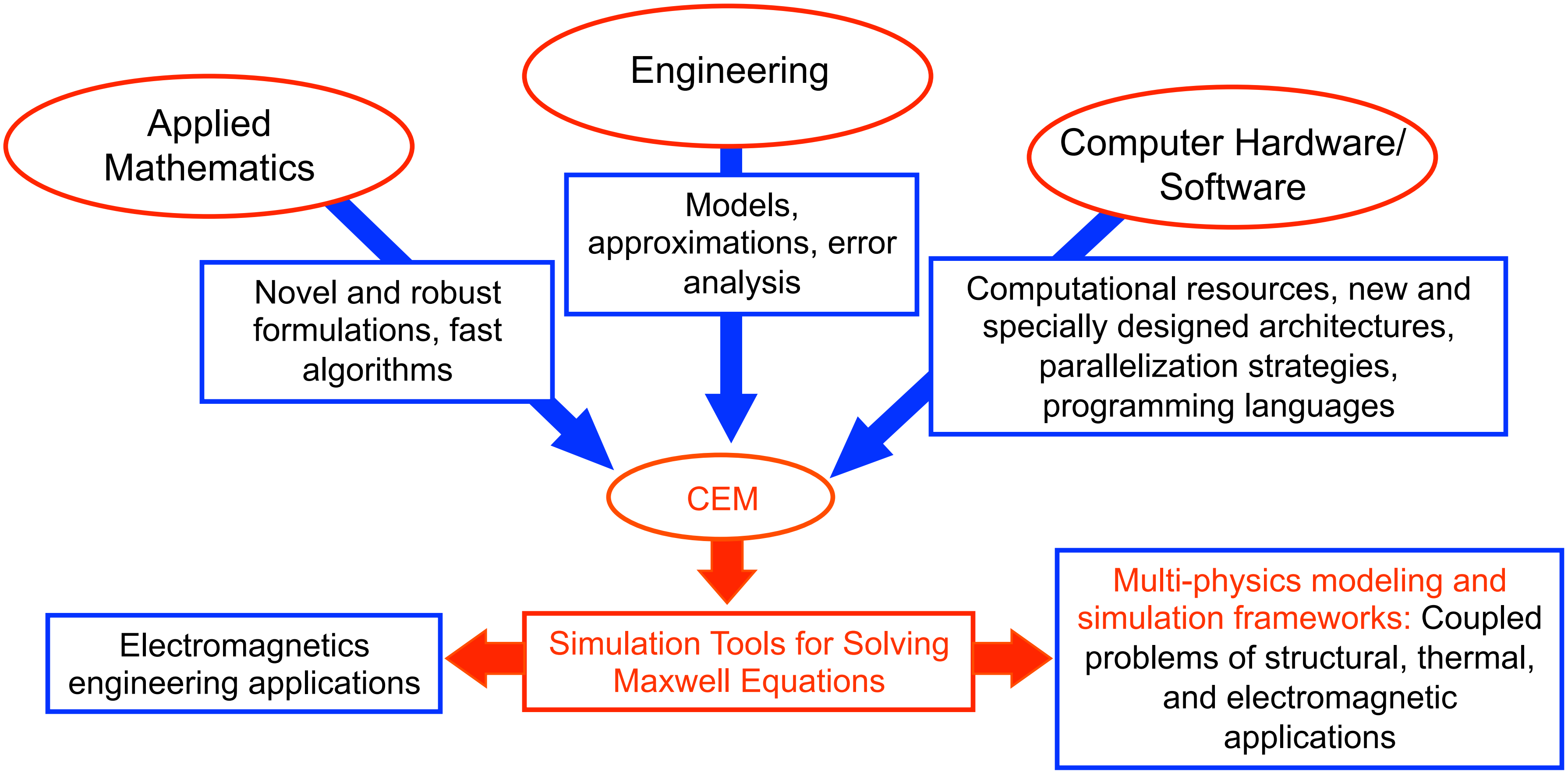
- Beowulf class heterogeneous cluster
- Intel Xeon X5570, IBM Power6, ~1000 cores
- Supported by KAUST Research Computing



CEML: http://maxwell.kaust.edu.sa

KAUST Supercomputing Laboratory: http://www.hpc.kaust.edu.sa

Computational Electromagnetics (CEM)



Main objective in CEM research: Developing efficient, rigorous, and accurate numerical methods for characterizing electromagnetic wave interactions on electrically large, multi-scale, and realistically complex structures.