An $h$-adaptive asynchronous spacetime discontinuous Galerkin method for TD analysis of complex electromagnetic media

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Outline:
1. Asynchronous Spacetime Discontinuous Galerkin method
2. Electromagnetics formulation
3. Characterization (and simulation) of dispersive media
4. Random media (elastodynamics)
1. aSDG method
Comparison of DG and CFEM methods

Consider FEs for a scalar field and polynomial order \( p = 2 \)

<table>
<thead>
<tr>
<th>( p )</th>
<th>dof</th>
<th>DG/CFEM</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>4</td>
<td>4</td>
</tr>
<tr>
<td>2</td>
<td>2.25</td>
<td>6</td>
</tr>
<tr>
<td>3</td>
<td>1.78</td>
<td>6</td>
</tr>
<tr>
<td>4</td>
<td>1.56</td>
<td>6</td>
</tr>
<tr>
<td>5</td>
<td>1.44</td>
<td>6</td>
</tr>
</tbody>
</table>

1. Balance laws at the element level
2. More flexible \( h-, hp\)-adaptivity
3. Less communication between elements
   Better parallel performance

High order polynomial \( \Rightarrow \) DG competitive
Comparison of DG and CFEM methods: Dynamic problems

1. Parabolic & Hyperbolic problems: $O(N)$ solution complexity

\[ C_{a_{n+1}} = C_{a_n} - \Delta t \left( K_{a_n} - F \right) \]

CFEM
\[ C = \frac{1}{6} \begin{bmatrix} 4 & 1 & 0 \\ 1 & 4 & 1 \\ 0 & 1 & 2 \end{bmatrix} \]

DG
\[ C = \begin{bmatrix} 1/3 & 1/3 & 0 \\ 0 & 1/3 & 1/3 \\ 0 & 0 & 1/3 \end{bmatrix} \]

$O(N^{1.5})$  $d = 2$

$O(N^2)$  $d = 3$

$O(N)$

Example:
10x finer mesh (1000x elements in 3D)

Cost:
DG: $10^3 x$
CFEM: $10^6-10^7 x$

2. Hyperbolic problems: resolving shocks / discontinuities

Discontinuities are preserved or generated from smooth initial conditions!

Burger’s equation (nonlinear)
\[ u_t + \left( \frac{1}{2} u^2 \right)_x = 0 \]

$t = 0$, smooth solution

$t > 0$, shock has formed

Global numerical oscillations

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Spacetime Discontinuous Galerkin Finite Element method:

1. Discontinuous Galerkin Method
2. Direct discretization of spacetime
3. Solution of hyperbolic PDEs
4. Use of patch-wise causal meshes

A local, O(N), asynchronous solution scheme
Direct discretization of spacetime

- Replaces a separate time integration; no global time step constraint
- Unstructured meshes in spacetime
- No tangling in moving boundaries
- Arbitrarily high and local order of accuracy in time
- Unambiguous numerical framework for boundary conditions

Shock capturing more expensive, less accurate

Shock tracking in spacetime: more accurate and efficient

Results by Scott Miller

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Spacetime Discontinuous Galerkin (SDG) Finite Element Method

DG + spacetime meshing + causal meshes for hyperbolic problems:

- Local solution property
- \( O(N) \) complexity (solution cost scales linearly vs. number of elements \( N \))
- Asynchronous patch-by-patch solver

- incoming characteristics on red boundaries
- outgoing characteristics on green boundaries
- The element can be solved as soon as inflow data on red boundary is obtained ⇒
  - partial ordering & local solution property
  - elements of the same level can be solved in parallel

Time marching

Elements labeled 1 can be solved in parallel from initial conditions; elements 2 can be solved from their inflow element 1 solutions and so forth.

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Tent Pitcher: Causal spacetime meshing

- Given a space mesh, Tent Pitcher constructs a spacetime mesh such that the slope of every facet on a sequence of advancing fronts is bounded by a causality constraint.

- Similar to CFL condition, except entirely local and not related to stability (required for scalability).
Tent Pitcher: Patch–by–patch meshing

- meshing and solution are interleaved
  - patches (‘tents’) of tetrahedra are solve immediately \( \Rightarrow O(N) \) property
  - rich parallel structure: patches can be created and solved in parallel

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A few other spacetime DG methods

- Time Discontinuous Galerkin (TDG) methods (TJR Hughes, GM Hulbert 1987)

- Elements are arranged in spacetime slabs
- Discontinuities are only between spacetime slabs
- Elements within slabs are solved simultaneously
A few other spacetime DG methods

- Spacetime discontinuous Galerkin method (JJW Van der Vegt, H Van der Ven, et al)

  - Elements are arranged in spacetime slabs
  - Discontinuities are across all element boundaries
  - Elements within slabs are solved simultaneously as this method is implicit

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A few other spacetime DG methods

A few other spacetime DG methods

- **Causal spacetime meshing** (Richter, Falk, etc.)

Similar and the predecessor to the aSDG method

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Advantages of Spacetime discontinuous Galerkin (SDG) Finite element method
1. Arbitrarily high temporal order of accuracy

- Achieving high temporal orders in semi-discrete methods (CFEMs and DGs) is very challenging as the solution is only given at discrete times.
- Perhaps the most successful method for achieving high order of accuracy in semi-discrete methods is the Taylor series of solution in time and subsequent use of Cauchy-Kovalewski or Lax-Wendroff procedure (FEM space derivatives $\Rightarrow$ time derivatives). However, this method becomes increasingly challenging particularly for nonlinear problems.
- High temporal order adversely affect stable time step size for explicit DG methods (e.g. $\frac{1}{2p+1}$ or worse for RKDG and ADER-DG methods).

Spacetime (CFEM and DG) methods, on the other hand can achieve arbitrarily high temporal order of accuracy as the solution in time is directly discretized by FEM.

$$\Delta x \quad \Delta t = C(p) \Delta x / c$$
2. Asynchronous / no global time step

- Geometry-induced stiffness results from simulating domains with drastically varying geometric features. Causes are:
  - Multiscale geometric features
  - Transition and boundary layers
  - Poor element quality (e.g. slivers)
  - Adaptive meshes driven by FEM discretization errors.

**Time-marching methods**

- Time step is limited by smallest elements for explicit methods

Explicit: Efficient / stability concerns
Implicit: Unconditionally stable

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2. Asynchronous / no global time step

- **Improvements:**
  - Implicit-Explicit (IMEX) methods increase the time step by geometry splitting (implicit method for small elements) or operator splitting.
  - Local time-stepping (LTS): subcycling for smaller elements enables using larger global time steps

- **SDGFEM**
  - Small elements locally have smaller progress in time (no global time step constrains)
  - None of the complicated “improvements” of time marching methods needed


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3. Spacetime grids and Moving interfaces

- Problems with moving interfaces:
  * Solid-fluid interaction
  * Non-linear free surface water waves
  * Helicopter rotors /forward fight
  * Flaps and slats on wings and piston engines
- Derived of a conservative scheme is very challenging:
  * Even Arbitrary Lagrangian Eulerian (ALE) methods do not automatically satisfy certain geometric conservation laws.

- Spacetime mesh adaptive operations:
  Enable mesh smoothing and adaptive operations Without projection errors of semi-discrete methods.

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Examples from solid mechanics:
Solution dependent crack propagation

Low load

High load

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4. Adaptive mesh operations

- **Local-effect adaptivity:** no need for reanalysis of the entire domain

- **Arbitrary order and size in time:**
  
  *Example:* ADER-DG with LTS by Dumbser, Munz, Toro, Lorcher, et al.

- **Adaptive operations in spacetime:**
  
  - Front-tracking better than shock capturing
  - \(hp\)-adaptivity better than \(h\)-adaptivity

**Results**

- Shock capturing: 473K elements
- Shock tracking: 446 elements

**Sod’s shock tube problem**

Results by *Scott Miller*
4. Adaptive mesh operations highly multiscale grids in spacetime

These meshes for a crack-tip wave scattering problem are generated by adaptive operations. Refinement ratio smaller than $10^{-4}$. 

Initial crack

Time in up direction

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5. Riemann-solution free scheme

- Reimann solutions are often complicated, expensive, and even difficult to derive particularly for nonlinear and anisotropic materials. Example: Simple linear elastodynamic problem

\[
\rho^\beta c_d^\beta = \frac{w^{(1)}(1)^\alpha \rho^\beta c_d^\beta + w^{(1)}(1)^\beta \rho^\alpha c_d^\alpha}{\rho^\alpha c_d^\alpha + \rho^\beta c_d^\beta}
\]

( regions III and IV)

- Riemann solutions required for inter-element noncausal boundaries

- If interior facets are eliminated we obtain a Riemann-solver free method ⇒

- Riemann-solution free scheme can also be more efficient

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5. parallel computing (asynchronous structure)

- Outstanding base properties of serial mode
  - O(N) Complexity
  - Favors highest polynomial order
  - Favors multi-field over single-field FEMs
- Asynchronous
- Nested hierarchical structure for HPC:
  1. patches, 2. elements/cells, 3. quadrature points
  4. rows & columns of matrices
- Domain decomposition at patch level:
  - Near perfect scaling for non-adaptive case
  - 95% scaling for strong adaptive refinement
  - Diffusion-like asynchronous load balancing

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Other Applications

Fluid mechanics: Euler’s equation

Hyperbolic thermal model

Solid mechanics

Multiscale & Probabilistic Fracture
- Probabilistic crack nucleation.
- Exact tracking of crack interfaces.

Structural Health Monitoring
- Multiscale and noise free solution of scattering enables detection of defects at unprecedented resolutions.

Dynamic Contact/Fracture
- SDGFEM eliminates common artifacts at contact transitions

High resolution slip-stick-separation waves

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2. Electromagnetics
Balance laws in spacetime:
Differential forms
Balance laws for dynamic problems

For a general conservation law let:
- \( f_t \): conserved quantity = temporal flux
- \( f_x \): total outward spatial flux
- \( r \): source term

Balance law reads as

\[
\forall \omega \quad \int_{\omega} r \, dv - \int_{\partial \omega} f_x \cdot ds = \int_{\omega} r \, dv - \int_{\partial \omega} (f_x \cdot n) \, ds = \frac{d}{dt} \int_{\omega} f_t \, dv
\]
Spacetime expression of balance law: Sloppy way!

\[ F = \begin{bmatrix} f_x & f_t \end{bmatrix} \]

Spatial & temporal fluxes are Combined.

- Balance law for arbitrary \( \Omega \) in spacetime:

\[ \forall \Omega \subset \mathcal{D} : \int_{\partial \Omega} F \cdot dS - \int_{\Omega} s \ dV = \int_{\partial \Omega} (f_x n_x + f_t n_t) dS - \int_{\Omega} s \ dV = 0 \]

- Strong form:

\[ \forall x \in \mathcal{D} \setminus \Gamma : \nabla_{st} \cdot F - s = \frac{df_t}{dt} + \nabla f_x - s = 0 \quad \text{PDE} \]

\[ \forall x \in \Gamma : [F]_N = (F^* - F)_N = (f_x^* - f_x) n_x + (f_t^* - f_t) n_t = 0 \quad \text{Jump (Rankin-Hugoniot) conditions} \]
Exterior calculus: 0 to 3-forms

- $f$: 0-form \([e.g.,\text{ electric potential } f]\) \quad \Rightarrow

$$df = f_1 dx_1 + f_2 dx_2 + f_3 dx_3 = f_i dx_i = \nabla f \, dx$$

- $\mathbf{v}$: 1-form \([e.g.,\text{ electric field } \mathbf{E}]\)

$$\mathbf{v} = v^i dx_i = \mathbf{v} \, dx \quad \Rightarrow$$

$$d\mathbf{v} = (v_2^3 - v_3^2) dx_2 \wedge dx_3 + (v_1^3 - v_3^1) - dx_1 \wedge dx_3 + (v_1^2 - v_2^1) dx_1 \wedge dx_2$$

$$= \nabla \times \mathbf{v} \, *dx$$

- $\mathbf{w}$: 2-form \([e.g.,\text{ electric flux density } \mathbf{D}]\)

$$\mathbf{w} = w_i \, dx^i = \mathbf{w} \, *dx = w_1 dx_2 \wedge dx_3 - w_2 dx_1 \wedge dx_3 + w_3 dx_1 \wedge dx_2 \quad \Rightarrow$$

$$d\mathbf{w} = 3\text{-form}$$

$$d\mathbf{w} = d(w_i \, dx^i) = (w_{1,1} + w_{2,2} + w_{3,3}) \, dx_1 \wedge dx_2 \wedge dx_3 = \nabla \cdot \mathbf{w} \, \Omega$$

- 3-form: \([e.g.,\text{ electric charge density } \rho]\) \quad \Rightarrow d\rho \, \Omega = 0

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Forms in spacetime

d: spatial dimension. ★: Hodge star operator.

• 1-forms: \{dx_1, \ldots, dx_d, dt\}. Specific Definition:

\[ dx := e^i dx_i \]

• \((d + 1)\)-form: \( \Omega := dx_1 \wedge \ldots \wedge dx_d \wedge dt \).

• \(d\)-forms: \{★dx^j, ★dt\}.
  Identities: \( dx_i \wedge ★dx^j = \delta^j_i \Omega \), \( dt \wedge ★dx^j = 0 \), \( dt \wedge ★dt = \Omega \) and \( dx_i \wedge ★dt = 0 \)

Example \((d = 3)\):

\[ ★dx^1 = dx_2 \wedge dx_3 \wedge dt \]
\[ ★dx^2 = dx_3 \wedge dx_1 \wedge dt \]
\[ ★dx^3 = dx_1 \wedge dx_2 \wedge dt \]

Specific Definition:

\[ ★dx := e^i ★dx^i \]
Spacetime expression of balance law: Using differential forms

- **Spacetime flux** $F$:
  - Temporal flux: $f_t = f_t \star dt$
  - Spatial flux: $f_x = f_x \star dx$

  \[
  F = f_t + f_x
  \]

- **Source term** $s = s \Omega$

- **Balance law**

  \[
  \forall \Omega \subset D : \quad \int_{\partial \Omega} F = \int_{\Omega} s
  \]

- **Strong form** (application of Stokes theorem):

  \[
  \int_{\Omega} (dF - s) = 0 \quad \Rightarrow \quad \begin{cases} 
  dF - s = (f_{t,t} + \nabla \cdot f_x - s) \Omega = 0 & \text{PDE} \\
  [F]_{\Gamma} = 0 & \text{Jump part}
  \end{cases}
  \]
Elastodynamics
Elastodynamic formulation in spacetime: Fields, fluxes and sources

- **Kinematic fields**
  \[ u = u^i e_i \quad \Rightarrow \]

  \[ \varepsilon := \dot{u} + E \text{ velocity–strain 1-form, where} \]

  \[
  \begin{aligned}
  \nu &= \mathbf{v} \cdot dt = v^i e_i dt \\
  E &= E \wedge dx = E^i_j e_i dx^j \\
  p &= p \cdot dt = p_i e^i dt \\
  s &= s \wedge *dx = s_{ij} e^i *dx_j \\
  \end{aligned}
  \]

- **Force-like fields**
  \[ M := p - s \text{ spacetime momentum flux, where} \]

- **Balance law**
  \[
  \int_{\partial Q} M - \int_Q S = 0 \quad \Rightarrow \quad \begin{cases} 
  dM - S = 0 & \text{PDE} \\
  [M] = 0 & \text{Jump conditions} 
  \end{cases}
  \]

\[ \nabla \cdot s - S = \dot{p} \]
Electromagnetics
Electromagnetics formulation in spacetime: Fields, fluxes and sources

- Electromagnetic fields

\[
U = \begin{bmatrix} E \\ H \end{bmatrix}
\]

\[
E = Edx \wedge dt = E^1 dx_1 \wedge dt + E^2 dx_2 \wedge dt + E^3 dx_3 \wedge dt
\]

\[
H = Hdx \wedge dt = H^1 dx_1 \wedge dt + H^2 dx_2 \wedge dt + H^3 dx_3 \wedge dt
\]

- Electromagnetic (total) flux densities

\[
F^t = \begin{bmatrix} D^t \\ B^t \end{bmatrix}
\]

\[
D^t = D^t \star dx \wedge dt = D_1^t dx_2 \wedge dx_3 + D_2^t dx_3 \wedge dx_1 + D_3^t dx_1 \wedge dx_2
\]

\[
B^t = B^t \star dx \wedge dt = B_1^t dx_2 \wedge dx_3 + B_2^t dx_3 \wedge dx_1 + B_3^t dx_1 \wedge dx_2
\]

- Constitutive equation

\[
\bar{F}^{t\bar{I}} = \sum_{J=1}^{2} \bar{\epsilon}^{I\bar{J}}(\omega) \star \bar{U}_J
\]

\[
\bar{F}^{t\bar{I}}(\omega) := \epsilon_\infty^{I\bar{J}} + \frac{\sigma^{I\bar{J}}}{j\omega} + \epsilon_d^{I\bar{J}}(\omega)
\]

\[
F = \begin{bmatrix} D \\ B \end{bmatrix}, \quad J = J_\sigma + J_{\epsilon_d}
\]

- Inductive

\[
D = \epsilon_\infty^{11} \star E + \epsilon_\infty^{12} \star H
\]

\[
J_{E\sigma} = \sigma^{11} E + \sigma^{12} H
\]

- Conductive

\[
B = \epsilon_\infty^{21} \star E + \epsilon_\infty^{22} \star H
\]

\[
J_{H\sigma} = \sigma^{21} E + \sigma^{22} H
\]

- Dispersive

\[
J_{\epsilon_d}^{\bar{I}} := \sum_{J=1}^{2} \{j\omega \epsilon_{_{d}^{I\bar{J}}}(\omega)\} \bar{U}_J
\]
Spacetime electromagnetic flux

Spacetime electromagnetic flux density

\[ M = F + JU. \]

\[
\begin{align*}
M^E & := D - H \\
M^H & := B + E
\end{align*}
\]

2-form fluxes in spacetime for EM problem

\[
U = \begin{bmatrix} E \\ H \end{bmatrix} = \begin{bmatrix} E^1dx_1 \wedge dt + E^2dx_2 \wedge dt + E^3dx_3 \wedge dt \\ H^1dx_1 \wedge dt + H^2dx_2 \wedge dt + H^3dx_3 \wedge dt \end{bmatrix}
\]

\[
F = \begin{bmatrix} D \\ B \end{bmatrix} = \begin{bmatrix} D_1dx_2 \wedge dx_3 + D_2dx_3 \wedge dx_1 + D_3dx_1 \wedge dx_2 \\ B_1dx_2 \wedge dx_3 + B_2dx_3 \wedge dx_1 + B_3dx_1 \wedge dx_2 \end{bmatrix}
\]

Comparison with d-form fluxes in spacetime

Acting on time-like ("vertical") boundaries

\[ \star dx := e^i \star dx^i \]

\[ = e^1dx^2 \wedge dx^3 \wedge dt + e^2dx^3 \wedge dx^1 \wedge dt + e^3dx^1 \wedge dx^2 \wedge dt \]

Acting on space-like ("horizontal") boundaries

\[ \star dt = -dx^1 \wedge dx^2 \wedge dx^3 \]
Comparison with other differential form formulation of EM problem

Fig. 2. Geometric representation of (a) a 1-form, (b) a 2-form, (c) a 3-form.

<table>
<thead>
<tr>
<th>$p$</th>
<th>Quantity</th>
<th>Differential Form</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>Electric Potential</td>
<td>$f(x,t)$</td>
</tr>
<tr>
<td>1</td>
<td>Electric Field</td>
<td>$\mathcal{E}(x,t) = E_x , dx + E_y , dy + E_z , dz$</td>
</tr>
<tr>
<td>1</td>
<td>Magnetic Field</td>
<td>$\mathcal{H}(x,t) = H_x , dx + H_y , dy + H_z , dz$</td>
</tr>
<tr>
<td>2</td>
<td>Electric Flux Density</td>
<td>$\mathcal{D}(x,t) = D_x , dy \wedge dz + D_y , dz \wedge dx + D_z , dx \wedge dy$</td>
</tr>
<tr>
<td>2</td>
<td>Magnetic Flux Density</td>
<td>$\mathcal{B}(x,t) = B_x , dy \wedge dz + B_y , dz \wedge dx + B_z , dx \wedge dy$</td>
</tr>
<tr>
<td>2</td>
<td>Current Density</td>
<td>$\mathcal{J}(x,t) = J_x , dy \wedge dz + J_y , dz \wedge dx + J_z , dx \wedge dy$</td>
</tr>
</tbody>
</table>


Our electromagnetic fields have an extra $dt$

$$U = \begin{bmatrix} E \\ H \end{bmatrix} = \begin{bmatrix} E^1 d x_1 \wedge dt + E^2 d x_2 \wedge dt + E^3 d x_3 \wedge dt \\ H^1 d x_1 \wedge dt + H^2 d x_2 \wedge dt + H^3 d x_3 \wedge dt \end{bmatrix}$$

$$E = \mathcal{E} \wedge dt$$

$$H = \mathcal{H} \wedge dt$$
Balance laws in spacetime

Spacetime electromagnetic flux density

\[ M = F + \mathcal{J} U, \quad \mathcal{J} := \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \]

Source terms: current and charge densities

\[ R_M := J + \rho = \begin{bmatrix} J^E_1 \star dx^1 + J^E_2 \star dx^2 + J^E_3 \star dx^3 + \rho^E \star dt \\ J^H_1 \star dx^1 + J^H_2 \star dx^2 + J^H_3 \star dx^3 + \rho^H \star dt \end{bmatrix} \]

Integral form of Maxwell equations

\[ - \int_{\partial Q} f \wedge M + \int_Q f \wedge R_M = 0 \quad (f \text{ is a 1-form}) \]

Strong form of Maxwell equations

\[ dM + R_M = 0 \quad \text{Diffuse part} \quad (\text{Provides PDEs}) \]

\[ f \wedge [M] = 0 \quad \text{Jump part} \quad (\text{Provides Boundary conditions and interface jump conditions}) \]
Strong Form to weak form and FEM formulation

a. Maxwell’s balance laws (diffuse part of the strong form)

\[
\begin{align*}
\left( \frac{\partial}{\partial t} \mathbf{D} + \mathbf{J}_E - \nabla \times \mathbf{H} \right) \times d\mathbf{x} &= 0 \quad \text{Ampère’s law} \\
\left( \frac{\partial}{\partial t} \mathbf{B} + \mathbf{J}_H + \nabla \times \mathbf{E} \right) \times d\mathbf{x} &= 0 \quad \text{Faraday law}
\end{align*}
\]

\[
\begin{align*}
(\nabla \cdot \mathbf{D} - \rho^E) \times dt &= 0 \quad \text{Gauss law for electric field} \\
(\nabla \cdot \mathbf{B} - \rho^H) \times dt &= 0 \quad \text{Gauss law for magnetic field}
\end{align*}
\]

b. Jump equations (BCs, interfaces, etc.)

\[
f \wedge [\mathbf{M}] = 0
\]

- Weighted residual statement (WRS)

\[
- \int_Q i \mathbf{\hat{U}} \wedge (d\mathbf{M}^h + R_M^h) + \int_{\partial Q} i \mathbf{\hat{U}} \wedge [\mathbf{M}]^h = 0
\]

Stokes’ theorem

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Strong Form to weak form and FEM formulation

- Weak statement (WKS)

\[
- \int_Q \left\{ di \dot{\mathbf{U}} \wedge M^h + i \dot{\mathbf{U}} \wedge R_M^h \right\} + \int_{\partial Q} i \dot{\mathbf{U}} \wedge M^* = 0
\]

\[
\int_Q \left\{ \left( -\ddot{\mathbf{E}}.D^h - \nabla \times \ddot{\mathbf{E}}.H^h + \ddot{\mathbf{E}}.J^{hE} \right) + \left( -\ddot{\mathbf{H}}.B^h + \nabla \times \ddot{\mathbf{H}}.E^h + \ddot{\mathbf{H}}.J^{hH} \right) \right\} \Omega \\
+ \int_{\partial Q} \left\{ \left( \ddot{\mathbf{E}}.D^* + \ddot{\mathbf{H}}.B^* \right) \ast dt + \left( \dddot{\mathbf{E}} \times H^* - \dddot{\mathbf{H}} \times \mathbf{E}^* \right) \ast dx \right\} = 0
\]
Time Domain Electromagnetics SDG: Balance of energy / proof of numerical stability

- Energy stability proof (dissipative method)
  \[ N := u + S \]
  \[ \Delta_D := \int_{\partial Q} N(U^*) + \int_Q R_N = \int_{\partial Q} N([U]_h) \geq 0 \]

\[ u := -\frac{1}{2} i U_I \wedge F^I = \frac{1}{2} (E.D + H.B) \star dt \]
\[ S := -i E \wedge H = E \times H \star dx \]
\[ R_N := -i U \wedge R_M = \{ E.J^E + H.J^H \} \Omega \]

- Sketch of the proof:
  - Bilinear form from the weighted residual statement:

\[ a_Q(U^h, \hat{U}) := -\int_Q i \hat{U} \wedge (dM^h + R_M^h) + \int_{\partial Q} i \hat{U} \wedge [M]_h \]
\[ = -\int_Q \left\{ di \hat{U} \wedge M^h + i \hat{U} \wedge R_M^h \right\} + \int_{\partial Q} i \hat{U} \wedge M^* \]
\[ 2a_Q(U^h, \hat{U}) = -2 \int_Q i \hat{U} \wedge R_M^h - \int_Q \left\{ i \hat{U} \wedge dM^h + di \hat{U} \wedge M^h \right\} + \int_{\partial Q} i \hat{U} \wedge \{ [M]_h + M^* \} \]

- By showing \( \hat{U}_\mathcal{I} \cdot F^\mathcal{I}^* = U_\mathcal{I}^* \cdot \hat{F}^\mathcal{I} \) and manipulation of bilinear form we can show:

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Time Domain Electromagnetics SDG: Balance of energy / proof of numerical stability

\[ 2a_Q(U^h, \hat{U}) = -2 \int_Q i \hat{U} \wedge R^h_M + \int_{\partial Q} U^*_T \cdot F^T \ast dt + 2E^* \times H^* \ast dx \]

\[ - \int_{\partial Q} \left[ U^*_T \cdot \left( F^T - \hat{F}^T \right) - \hat{U}_T \cdot \left( F^T - F^h T \right) \right] \ast dt \]

\[ - \int_{\partial Q} \left\{ \left[ (E^* - \hat{E}) \times H^* - (E^* - E^h) \times \hat{H} \right] + \left[ E^* \times (H^* - \hat{H}) - \hat{E} \times (H^* - H^h) \right] \right\} \ast dx \]

\[ + \int_Q \left\{ (\hat{H} \cdot \nabla \times E^h - H^h \cdot \nabla \times \hat{E}) - (\hat{E} \cdot \nabla \times H^h - E^h \cdot \nabla \times \hat{H}) \right\} \Omega \]

By choosing weight functions equal to solution \( \hat{U} = U^h \) and noting \( a_Q(U^h, \hat{U}) = 0 \)

\[ \int_{\partial Q} \frac{1}{2} U^*_T \cdot F^T \ast dt + E^* \times H^* \ast dx - \int_Q i \hat{U} \wedge R^h_M = \]

\[ \int_{\partial Q} \frac{1}{2} [U^h_T]_h \cdot [F^T]_h \ast dt + [E]_h \times [H]_h \ast dx \]

That is

\[ \Delta_D := \int_{\partial Q} N(U^*) + \int_Q R_N = \int_{\partial Q} N([U]_h) \]

\[ \Delta := \int_{\partial D} N(U^*) + \int_D R_N = \sum_{Q \in P_h} \Delta_Q \geq 0 \]

But,

\[ \int_{\partial Q} N([U]_h) \begin{cases} 
= 0 \text{ outflow} \\
> 0 \text{ inflow} \\
> 0 \text{ non-causal (using Riemann values, etc.)}
\end{cases} \]

outflow

\( \Gamma_{\alpha\beta} \)

inflow

\( (q^0, t_0) \)

non-causal
Convergence studies: Energy Dissipation

Energy dissipation: Convergence rate:

\[ 2p + 1 \]
Convergence studies:
Error w.r.t. exact solution

\[ \psi := \psi_\Omega + \psi_\mathcal{F}, \text{ where} \]
\[ \psi_\Omega := \|U^h - U\|_{e,\mathcal{D}}^2 \]
\[ \psi_\mathcal{F} := \max_{1 \leq k \leq M} |U^h - U|_{e,\mathcal{F}_k}^2 \]

Convergence rate:
\[ 2p + 2 \]

Error inside elements
Error on fronts

\( d = 1 \)
\( d = 2 \)
Other types of error:
1. Divergence errors

Balance laws exactly satisfied:
\[
\begin{aligned}
&D + J^E - \nabla \times H \quad \star dx = 0 \quad \text{Ampère's law} \\
&B + J^H + \nabla \times E \quad \star dx = 0 \quad \text{Faraday law}
\end{aligned}
\]

in balance law form:
\[
- \int_Q \left\{ d\vec{U} \wedge M^h + i \vec{U} \wedge R^h_M \right\} + \int_{\partial Q} i \vec{U} \wedge M^* = 0
\]

BUT divergence laws are not even weakly enforced:
\[
\begin{aligned}
&\nabla \cdot D - \rho^E \quad \star dt = 0 \quad \text{Gauss law for electric field} \\
&\nabla \cdot B - \rho^H \quad \star dt = 0 \quad \text{Gauss law for magnetic field}
\end{aligned}
\]

Total divergence errors:
Have convergence rate of
\[
p + 1
\]
Other types of error:
2. Dispersion error

\[ p = 0 \]

\[ E = \mathcal{E} \cos(\omega t - kx) \]
\[ H = \mathcal{H} \cos(\omega t - kx) \]

\[ \Delta \omega_R := \omega_R^h - \omega_R \]
\[ \Delta \omega_I := \omega_I^h - \omega_I \]
Other types of error:

2. Dispersion error

\[ \Delta \omega_R := \omega_R^h - \omega_R \]

Dispersion error:
Convergence rate (odd \( p \)):

\[
\rho
\]

\[ \Delta \omega_I := \omega_I^h - \omega_I \]

Dissipation error:
Convergence rate (odd \( p \)):

\[
\rho + 1
\]
2D scattering problem / meshing in spacetime

Transverse Electric (TE) Initial conditions

\[
\begin{align*}
H^1(x_1, x_2) &= u(x_1 - c_1)u'(x_2 - c_2) \\
H^2(x_1, x_2) &= -u'(x_1 - c_1)u(x_2 - c_2) \\
E^3(x_1, x_2) &= 0
\end{align*}
\]

for \( u(z) = e^{-\frac{z^2}{2\sigma^2}} \)

Initial mesh

Space time meshes

R. Abedi, UTK / ICERM, June 25-29, 2018
2D scattering problem / solution visualization

(a) time $t = 0.04$

(b) time $t = 0.35$

(c) time $t = 0.45$

(d) time $t = 0.65$

(e) time $t = 1.20$

(f) time $t = 2.70$
Transverse Magnetic (TM) formulation

Initial condition:

\[ H_z = \cos\left(\frac{\pi}{2} \frac{x}{d_x}\right) \cos\left(\frac{\pi}{2} \frac{y}{d_y}\right) \]

Electric permittivity:

\[ \varepsilon_i = 1 \]
\[ \varepsilon_o = 10 \]

Magnetic permeability:

\[ \mu = 1 \]
2D scattering problem adaptive meshing
2D scattering problem adaptive meshing
Comparison of Adaptive / nonadaptive schemes

Nonadaptive

Adaptive

Initial spatial Mesh

25K elements

46 elements

R. Abedi, UTK / ICERM, June 25-29, 2018
Comparison of Adaptive / nonadaptive schemes

Nonadaptive

- 93 Hours
- Numerical dissipation $8 \times 10^{-4}$

Adaptive

- 72 Hours
- Numerical dissipation $1 \times 10^{-4}$

Even finer nonadaptive simulation

- > 500 Hours
- Numerical dissipation $2 \times 10^{-4}$
  (still larger than adaptive one)

Initial Mesh: 83K elements

R. Abedi, UTK / ICERM, June 25-29, 2018
Nontrivial target solutions are needed on interior (non-causal) facets of patches.

Riemann fluxes (R)

\[
E^* = \frac{(YE - n \times H)^{-} + (YE + n \times H)^{+}}{Y^{-} + Y^{+}}
\]

\[
H^* = \frac{(ZH + n \times E)^{-} + (ZH - n \times E)^{+}}{Z^{-} + Z^{+}}
\]

\[
\begin{cases}
  Z = \sqrt{\frac{n}{\epsilon}} & \text{impedance} \\
  Y = \frac{1}{Z} & \text{admittance}
\end{cases}
\]

Average fluxes (A)

\[
E^* = \frac{E^{-} + E^{+}}{2}
\]

\[
H^* = \frac{H^{-} + H^{+}}{2}
\]
Comparison of Riemann and average fluxes

Riemann solutions:
- More dispersive (especially for low $p$)
- Less oscillatory

Material 1  Material 2

Applied electric field

R. Abedi, UTK / ICERM, June 25-29, 2018
3. Dispersive media
S-parameters for a slab

Material Properties

\[(\epsilon, \mu)\]

\[
\begin{align*}
Z &= \sqrt{\frac{\mu}{\epsilon}} \quad \text{impedance} \\
\frac{1}{c} &= \frac{1}{\sqrt{\mu \epsilon}} \quad \text{wave speed}
\end{align*}
\]

Transmission / reflection coefficients

\[
\begin{align*}
\rho &= \frac{Z - Z_m}{Z + Z_m} \\
k &= \omega c \\
t(Z, c) &= \frac{T}{I} = \frac{1 - \rho^2}{(e^{jkl} - \rho^2 e^{-jkl})} \\
r(Z, c) &= \frac{R}{I} = \rho \frac{1 - e^{-2jkl}}{(1 - \rho^2 \rho e^{-2jkl})}
\end{align*}
\]

R. Abedi, UTK / ICERM, June 25-29, 2018
Unit cell to dispersive response (S-parameters) retrieval method

Inverse Problem

1. (Computationally) solve for $t, r$:

$$t(Z, c) = \frac{T}{I} = \frac{1 - \rho^2}{(e^{jkl} - \rho^2 e^{-jkl})}$$

$$r(Z, c) = \frac{R}{I} = \rho \frac{1 - e^{-2jkl}}{(1 - \rho^2 \rho e^{-2jkl})}$$

2. Inverse solution for $Z, c$ (non-uniqueness)

Elastodynamics

$$C = Zc$$

$$\rho = \frac{Z}{c}$$

Electromagnetics

$$\epsilon = \frac{1}{Zc}$$

$$\mu = \frac{Z}{c}$$

R. Abedi, UTK / ICERM, June 25-29, 2018
Time Domain vs. Frequency Domain

- Time Domain (TD) vs. Frequency Domain (FD) solvers:
  - Transient problems $\Rightarrow$ TD
  - Steady state and frequency response:
    - Small problem size $\Rightarrow$ FD
    - Large problem size $\Rightarrow$
      TD ($TDDG \approx O(N)$) FD = $O(N^\alpha)$, $\alpha \geq 1.5$
  - Material nonlinearities are better modeled in TD
  - **Entire spectrum** obtained by **one TD simulation of broadband** signal

### Table

<table>
<thead>
<tr>
<th>d</th>
<th>FD</th>
<th>TD</th>
</tr>
</thead>
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<tr>
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<td>$O(\omega^3_M)$</td>
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<tr>
<td>3</td>
<td>$O(\omega^4_M)$</td>
<td>$O(\omega^6_M)$</td>
</tr>
</tbody>
</table>

Busch:2009

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R. Abedi, UTK / ICERM, June 25-29, 2018
Time Domain vs. Frequency Domain

- Time Domain (TD) vs. Frequency Domain (FD) solvers:
  - Eigenmode analysis: Time domain
    \[ \text{TD: } O(N) \quad \text{FD: } O(N^3) \]
  - Homogenization of dispersive media:
    - Mario G. Silveirinha, PHYSICAL REVIEW B 83, 165104, Time domain homogenization of metamaterials, 2011
    - 3 to 40 times faster than FD simulations.

R. Abedi, UTK / ICERM, June 25-29, 2018
Advantages of SDG method & adaptivity in spacetime

Refinement ratio of $10^4$ increases the maximum frequency $\omega_M$ captured by 4 order of magnitudes!

R. Abedi, UTK / ICERM, June 25-29, 2018
Computation of S-parameters

Time Domain (TD)

Properties:
- Ultrashort duration pulses
  \((\sigma \to 0) \Rightarrow\)
- Broadband frequency content
  \(\omega \in [\omega_0 - \frac{1}{\sigma}, \omega_0 + \frac{1}{\sigma}]\)
- (Almost) zero solutions for initial and final times
  \(\Rightarrow\) facilitates Fourier analysis

Gaussian pulse

\[
I(x, t) = \sin(\omega_0 \tilde{t}) e^{-\frac{1}{2} \left(\frac{\tilde{t}}{\sigma}\right)^2}
\]

\[
\tilde{t} = t - \frac{x}{c} - t_0
\]

After Fourier transform

\[
\bar{r}(\omega) = \frac{\bar{R}(\omega)}{\bar{I}(\omega)}, \quad \bar{t}(\omega) = \frac{\bar{R}(\omega)}{\bar{I}(\omega)}
\]
**Inverse problem**

1. Reflection & Transmission coefficients are computed

\[ \begin{align*}
\bar{r}(\omega) &= \frac{R(\omega)}{I(\omega)}, & \bar{t}(\omega) &= \frac{R(\omega)}{I(\omega)}
\end{align*} \]

2. Inverse Problem: Given \( r \) & \( t \)

\[ \begin{align*}
    r &= \rho \frac{z^2 - 1}{z^2 - \rho^2}, &
    t &= z, \frac{1 - \rho^2}{z^2 - \rho^2}
\end{align*} \]

Find \( Z \) (Impedance) and \( k \) (wavenumber)

\[ Z = Z_0 \sqrt{\frac{(r + 1)^2 - t^2}{(r - 1)^2 - t^2}} \]

\( Z \) is uniquely determined

\[ z = e^{jkl} \]

\( z \) is uniquely determined \textbf{BUT NOT} \( k \)

\[ z = \frac{(Z + Z_0) - r(Z - Z_0)}{t(Z + Z_0)} \]

3. Once \( Z \) and \( k \) are knowns \( \Rightarrow \)

Compute effective material properties

\[ \varepsilon = \frac{k}{Z \omega}, \quad \mu = \frac{kZ}{\omega} \]
Non-uniqueness

Non-uniqueness is in the integer number of full waves in the slab.

\[ l k_R \pm = 2p\pi \]

\[ k = \frac{\phi}{l} - j \frac{\log \rho}{l}, \]

\[ \phi := \theta + 2p\pi \]

Arslanagic et al. (2013) A review scattering-parameter extraction clarification ambiguity metamaterial homogenization

R. Abedi, UTK / ICERM, June 25-29, 2018
Observation 1: Use continuity of $k$ as $\omega$ increases.

As $\omega \rightarrow 0 \Rightarrow k \rightarrow 0$

Starts from low frequency where $p = 0$ and $\omega$ increases

\[
k = \frac{\phi}{l} - j \frac{\log \rho}{l},
\]

\[
\phi := \theta + 2p\pi
\]
Test problem:
Retrieval method for solid slab

Initial space mesh

\[ \varepsilon = 1, \mu = 1 \quad \varepsilon = 0.1, \mu = 1 \quad \varepsilon = 1, \mu = 1 \]

Movie: Solution

R. Abedi, UTK / ICERM, June 25-29, 2018
Ambiguity in wave number in parameter retrieval method

Mid-layer is conductive

Integer \( p \) and scaled phase \( \phi/2\pi \) obtained in inverse parameter retrieval stage.
Numerical errors in computing scattering parameters

Higher errors in computing $R$ and $T$ at higher frequencies (as expected)

$\Re(T)$ vs. Frequency $\omega$

- **exact**
- $\bar{\varepsilon}_D = 10^{-10}$
- $\bar{\varepsilon}_D = 10^{-8}$
- $\bar{\varepsilon}_D = 10^{-7}$
Electromagnetics: 3 layer 1D: Stopbands, etc.

\[ \varepsilon_B = 0.1152, \quad \mu_B = 1.18 \]
\[ \varepsilon_C = 0.003125, \quad \mu_C = 7.954 \]
\[ \varepsilon_0 = 1, \quad \mu_1 = 1 \]

Electromagnetics:
3 layer 1D: Stopbands, etc.

\[ \varepsilon_B = 0.1152, \mu_B = 1.18 \]
\[ \varepsilon_C = 0.003125, \mu_C = 7.954 \]
\[ \varepsilon_0 = 1, \mu_1 = 1 \]
Example from elastodynamics: Retrieval method for 2D unit cells


Spatial mesh for the SDG method

R. Abedi, UTK / ICERM, June 25-29, 2018
Example from elastodynamics: Retrieval method for 2D unit cells
Example from elastodynamics: Retrieval method for 2D unit cells

Movie: Solution, Mesh

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Retrieval method for 2D unit cells: Transmission coefficient

\[ \text{Re}(T) \]

\[ \text{Im}(T) \]
Solution of Dispersive media in TD
Ongoing work: Elimination of convolutions in TD


Drude material

\[ \varepsilon_0 \frac{\partial E}{\partial t} = \nabla \times H - \tilde{J} + f \quad \text{in } \Omega \times (0,T), \]

\[ \mu_0 \frac{\partial H}{\partial t} = -\nabla \times E - \tilde{K} \quad \text{in } \Omega \times (0,T), \]

\[ \frac{\partial \tilde{J}}{\partial t} + \Gamma_e \tilde{J} = \varepsilon_0 \omega_{pe}^2 E \quad \text{in } \Omega \times (0,T), \]

\[ \frac{\partial \tilde{K}}{\partial t} + \Gamma_m \tilde{K} = \mu_0 \omega_{pm}^2 H \quad \text{in } \Omega \times (0,T), \]

Dispersive (metamaterial) TD PML


R. Abedi, UTK / ICERM, June 25-29, 2018
Ongoing work: Elimination of convolutions in TD

- Electromagnetic equations in FD

\[ j\omega \tilde{D}^t - \nabla \times \tilde{H} = 0 \quad : \quad \text{Ampère’s law with Maxwell addition} \]

\[ j\omega \tilde{B}^t + \nabla \times \tilde{E} = 0 \quad : \quad \text{Faraday law of induction} \]

- Frequency domain constitutive relation for an isotropic media:

\[ \tilde{D}^t(j\omega) = \tilde{\varepsilon}(j\omega) \tilde{E}(j\omega) \quad \Rightarrow \quad (j\omega) \tilde{D}^t_k(j\omega) = j\omega \tilde{\varepsilon}(j\omega) \tilde{E}^k(j\omega) \]

- Pull-back in time domain involves a convolution:

\[ \dot{D}^t_k(t) = \int_{-\infty}^{t} g(t - t') E^k(t') dt' \]

Computationally challenging to compute the convolution integral in TD!

- Solution: Elimination of convolution integral by introducing additional fields.
Elimination of convolution integral:

- Assume electrical permittivity uses a Debye dispersion model,

\[
\tilde{\varepsilon}(j\omega) = \varepsilon_\infty + \frac{\varepsilon_s - \varepsilon_\infty}{1 + (j\omega)t_0}
\]  

\[
(j\omega)D_{k}^{t}(j\omega) = (j\omega)\varepsilon_\infty \tilde{E}_k^k(j\omega) + \frac{\varepsilon_s - \varepsilon_\infty}{t_0} \tilde{E}_k^k(j\omega) + \left\{ -\frac{\varepsilon_s - \varepsilon_\infty}{t_0(1 + (j\omega)t_0)} \tilde{E}_k^k(j\omega) \right\}
\]

- By the introduction of Auxiliary Field \( P \) we get,

\[
\begin{align*}
(j\omega)\tilde{D}_{k}^{t}(j\omega) &= \varepsilon_\infty (j\omega) \tilde{E}_k^k(j\omega) + \frac{\varepsilon_s - \varepsilon_\infty}{t_0} \tilde{E}_k^k(j\omega) + \tilde{P}_{(k)}(j\omega) \\
\tilde{P}_{(k)}(j\omega) &= -\frac{\varepsilon_s - \varepsilon_\infty}{t_0(1 + (j\omega)t_0)} \tilde{E}_k^k(j\omega)
\end{align*}
\]

\[
\begin{align*}
\dot{D}_{k}^{t}(t) &= \varepsilon_\infty \dot{E}_k^k(t) + \frac{\varepsilon_s - \varepsilon_\infty}{t_0} E_k^k(t) + P_{(k)}(t) \\
t_0 \dot{P}_{(k)}(t) + P_{(k)}(t) &= -\frac{\varepsilon_s - \varepsilon_\infty}{t_0} E_k^k(t)
\end{align*}
\]

- That is convolution term is eliminated by the addition of the field \( P_{(k)} \).
Automated elimination of ADEs

• An instruction-based approach recursively derives ADEs for dispersion relations in rational function form

\[ G(j\omega) = \frac{A(j\omega)}{B(j\omega)} = \frac{A_a(j\omega)^a}{B_b(j\omega)^b} \]

• They appear in constitutive equations in the form:

Pull dispersive relation

Example:

\[ \bar{L}(j\omega) = G(j\omega)C(j\omega)\bar{X}(j\omega) \]

\[ \bar{J}_{\epsilon_d}^I := \sum_{J=1}^{2} \{ j\omega \bar{\epsilon_d}^I J(\omega) \} \bar{U}_J \]

• The pull-back to time domain is:

\[ \bar{L}(j\omega) = \bar{P}_0(j\omega) + D\bar{X}(j\omega) \Rightarrow \bar{L}(t) = P_0(t) + D\bar{X}(t) \]

time domain representation of \( L \)

\[ \dot{P}_i + R_{iP} = 0 \quad \text{for} \quad 0 \leq i \leq \text{ADEs} \]

\[ R_{iP} = \frac{B_{b-i-1}}{B_b} P_0(t) - P_{i+1}(t) + \frac{1}{B_b} \left\{ DB_{b-i-1} - \sum_{a+c=b-i-1} A_aC_c \right\} X(t) = 0, i_{\text{max}}, \text{ Source terms} \]

\[ i_{\text{max}} = \max(i_{\text{max}}^b, i_{\text{max}}^{ac}) = \max(\bar{b} - b - 1, \bar{b} - (a + c) - 1) \quad \text{and the number of ADEs} \quad n_P = i_{\text{max}} + 1 \]
Perfectly Matched Layer (PML)

- Perfectly Matched Layer (PML): Berenger, 1994
- Weng Cho Chew, H. Weedon William. A 3D perfectly matched medium from modified Maxwell’s equations with stretched coordinates, 1994

\[ s_i = 1 + \sigma_i / j\omega \]

- Complex Frequency Shifted PML (CFS-PML), Mustafa Kuzuoglu and Raj Mittra, 1996:

\[ s_i = \kappa_i + \omega_i / (\alpha_i + j\omega) \]

Attenuates evanescent waves as well.

- Second order PML, Davi Correia and Jian-Ming Jin, 2005, 2006:

\[ s_i = (1 + \sigma_i / j\omega)(\kappa_i + \omega_i / (\alpha_i + j\omega)) \]

Better performance than CFS-PML at low frequencies.

- Busch, Konig 2011, etc
Time Domain Electromagnetics SDG: Formulation of PML for dispersive media

- Perfectly matched layer for bi-anisotropic dispersive media

\[
\begin{align*}
\overline{\xi}_{\text{PML}} &= (\det \overline{S})^{-1} \left[ \overline{S} \cdot \overline{\xi}(\omega) \cdot \overline{S} \right] \\
\overline{\mu}_{\text{PML}} &= (\det \overline{S})^{-1} \left[ \overline{S} \cdot \overline{\mu}(\omega) \cdot \overline{S} \right] \\
\overline{\zeta}_{\text{PML}} &= (\det \overline{S})^{-1} \left[ \overline{S} \cdot \overline{\zeta}(\omega) \cdot \overline{S} \right] \\
\overline{\lambda}_{\text{PML}} &= (\det \overline{S})^{-1} \left[ \overline{S} \cdot \overline{\lambda}(\omega) \cdot \overline{S} \right].
\end{align*}
\]

PML stretching \(\Rightarrow\) dispersive relations


<table>
<thead>
<tr>
<th>Level</th>
<th>Inductive</th>
<th>Conductive</th>
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<tr>
<td>L2</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
</tr>
</tbody>
</table>

2 Levels of ADEs needed in TD

Constitutive model

- 3 levels for linear PML (2 additional levels to the base material)
- **5 levels** for CFS-PML.
- Even more levels for second order PML.

Recursive formulation of ADEs automatically formulates PML equations.

R. Abedi, UTK / ICERM, June 25-29, 2018
Random media: Solution of stochastic PDEs
Representative Volume Elements (RVEs) versus Statistical Volume Elements (SVEs)

- RVEs are good for many elastic regime problems
- For fracture modeling (particularly quasi-brittle material):
  - Need to preserve spatial inhomogeneity
  - Randomness (sample to sample variations)

SVE sizes: Material property is probabilistic

- SVEs appropriate for fracture modeling
  (still reduce problem size by homogenization)

Ostoja-Starzewski 1998

RVE limit: $l$ is very large

PDF of a material property, e.g. stiffness

$d \ll l \ll L$
Stochastic PDEs: Elastodynamics

1. By using SVEs material inhomogeneities & sample to sample variations (randomness) are preserved.
2. Still no need to resolve all microscale details!

R. Abedi, UTK / ICERM, June 25-29, 2018
Stochastic Decomposition: Karhunen-Loeve expansion

Gaussian random field $\eta(x)$:

$$\eta(x, \omega) = \mu_\eta(x) + \sum_{i=1}^{n_{KL}} \sqrt{\lambda_i} b_i(x) Y_i(\omega)$$

$$\eta(x, \omega) \sim N(\mu_\eta, \sigma_\eta)$$

$$\eta(x) = \mu_\eta(x) + \sum_{i=1}^{n_{KL}} \sqrt{\lambda_i} b_i(x) y_i$$

Non-Gaussian random field:

$$\xi(x) = F_\xi^{-1} \left( F_\eta(\eta(x)) \right)$$

$$\eta(x) \sim N(0,1)$$

$$\tilde{s}(x) = \xi(x) = F_\xi^{-1} \left( \frac{1}{2} \left\{ 1 + Erf \left( \frac{\eta(x)}{\sqrt{2}} \right) \right\} \right)$$

(Inverse Transform Method)

Eigen-pairs $\{\lambda_i, b_i(x)\}_{i=1}^{n_{KL}}$:

$$\int_D COV_\eta(x^1, x^2) b(x^2) dx^2 = \lambda b(x^1)$$

$$COV(\tilde{s}(X), \tilde{s}(Y)) = e^{-\left( \frac{|X-Y|}{d_c} \right)^2}$$
Sample KL Random Fields

SVE1x1  SVE2x2  SVE4x4

SVE8x8  SVE16x16

R. Abedi, UTK / ICERM, June 25-29, 2018
Sample stochastic fracture results

Realizations for fracture strength based on

![SVE1x1](image1)
![SVE2x2](image2)
![SVE8x8](image3)
Uniform fracture strength

Window sizes uses for statistical volume elements

Fracture patterns under uniform load in horizontal direction

Very unrealistic fracture pattern with uniform fracture strength model

R. Abedi, UTK / ICERM, June 25-29, 2018
Effect of fracture strength randomness: e.g., SVE1x1

KL random fracture strength $\bar{s}(x)$

R. Abedi, UTK / ICERM, June 25-29, 2018
Conclusions

- Space time directly discretized ⇒ O(N) patch-by-patch scheme.
- Asynchronous solution scheme is ideal for the solution of grids with disparate length scales.
- It provides a powerful $h$-adaptive scheme in spacetime.
- Energy dissipation of all elements is non negative.
  - Convergence rate $p + 1$.
  - Used as an error indicator for adaptivity.
- Riemann vs. Average flux:
  - Average flux ⇒ less dissipative for $p = 0$.
  - Riemann flux ⇒ less oscillatory for $p \geq 0$.
- Divergence errors ⇒ $p + 1$ convergence rate.
- Von Neumann dispersion analysis ($p$ and $p + 1$ rates for odd $p$)

Nonadaptive  Adaptive

46 elements
Conclusions

- **Dispersive media:**
  - TD becomes more efficient than a FD as problem size increases.
  - Adaptivity of the aSDG method increase frequency range by 4 orders of magnitude.
  - Ambiguity on real part of wave number is resolved by continuity of wave number
  - A automated recursive method for formulation of dispersive media in TD (PML + metamaterial: in progress)

- **Random media:**
  - SVEs for characterization
  - KL method for random field realization
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