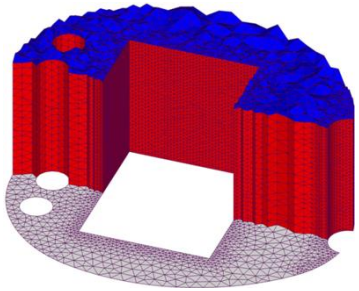

An *h*-adaptive asynchronous spacetime discontinuous Galerkin method for TD analysis of complex electromagnetic media

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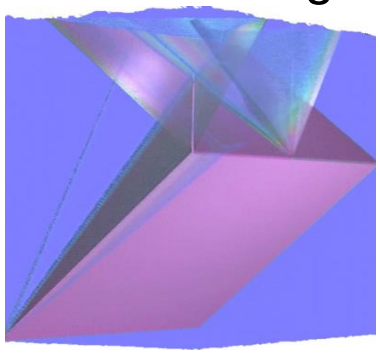
(in collaboration with) Saba Mudaliar

Wright Patterson Air Force Base, Sensor's Directorate



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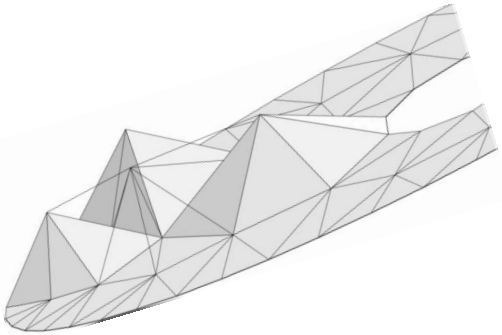


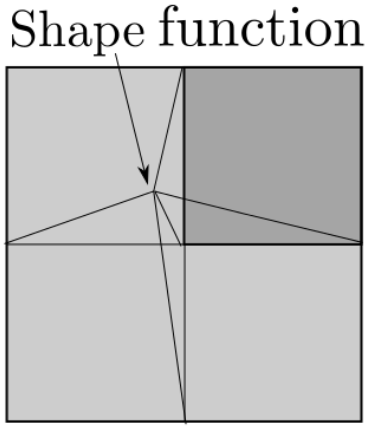
ICERM, Computational Aspects of Time Dependent Electromagnetic Wave Problems in Complex Materials, June 25-29, 2018, Providence, RI

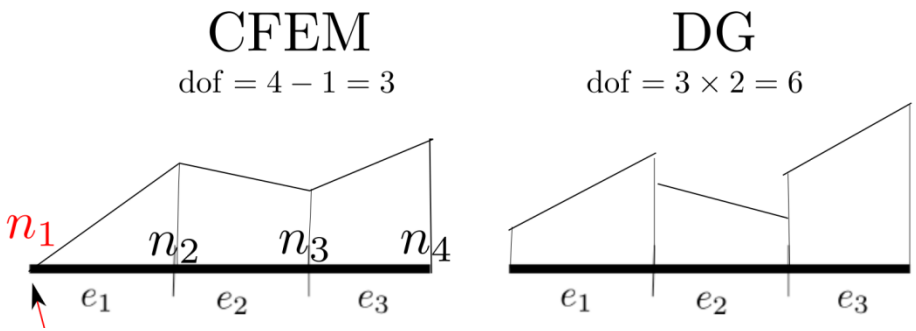
Outline:

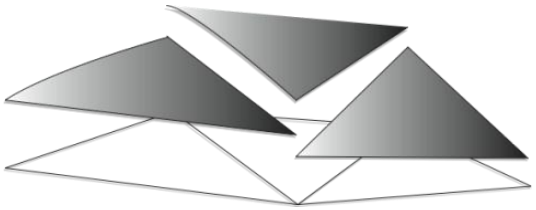
1. Asynchronous Spacetime Discontinuous Galerkin method
2. Electromagnetics formulation
3. Characterization (and simulation) of dispersive media
4. Random media (elastodynamics)

1. aSDG method

Comparison of DG and CFEM methods

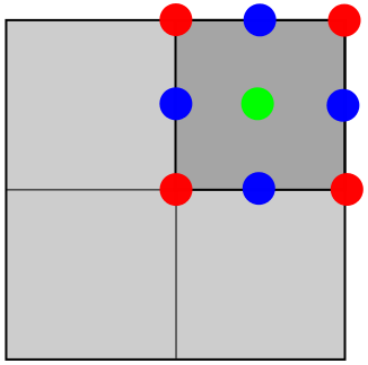


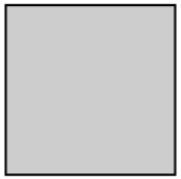




Disjoint basis

Consider FEs for a scalar field and polynomial order **p = 2**





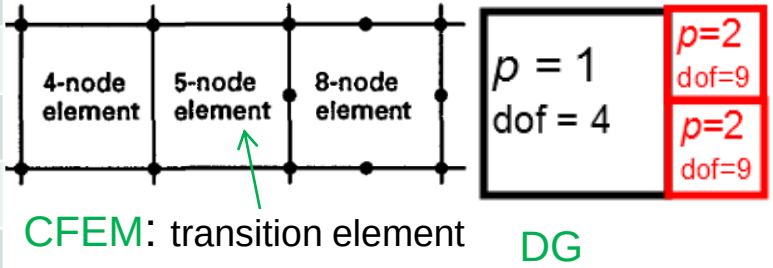
Shape (basis) functions

$$1$$
$$x \quad y$$
$$x^2 \quad xy \quad y^2$$
$$x^2y \quad xy^2$$
$$x^2y^2$$

$$\frac{\text{dof}}{\text{e}} = \frac{4}{4} + \frac{4}{2} + \frac{1}{1} = 4 \qquad \frac{\text{dof}}{\text{e}} = 9$$

p	dof DG/CFEM
1	4
2	2.25
3	1.78
4	1.56
5	1.44

1. Balance laws at the element level
2. More flexible *h*-, *hp*-adaptivity



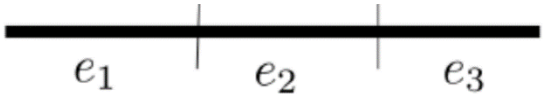
3. Less communication between elements ⇨ Better parallel performance

High order polynomial ⇨ **DG competitive**

Comparison of DG and CFEM methods: Dynamic problems

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

$$\mathbf{C}\mathbf{a}_{n+1} = \mathbf{C}\mathbf{a}_n - \Delta t\left(\mathbf{K}\mathbf{a}_n - \mathbf{F}\right)$$ Explicit solver



CFEM

$$\mathbf{C} = \frac{1}{6}\begin{bmatrix} 4 & 1 & 0 \\ 1 & 4 & 1 \\ 0 & 1 & 2 \end{bmatrix}$$

DG

$$\mathbf{C} = \begin{bmatrix} 1 & \frac{1}{2} & 0 & 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{3} & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & \frac{1}{2} & \frac{1}{3} & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & \frac{1}{2} \\ 0 & 0 & 0 & 0 & \frac{1}{2} & \frac{1}{3} \end{bmatrix}$$

e_1 e_2 e_3

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

$O(N^2)$ d = 3

O(N)

Example:

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

Cost:

DG: 10^3x

CFEM: 10^6-10^7x

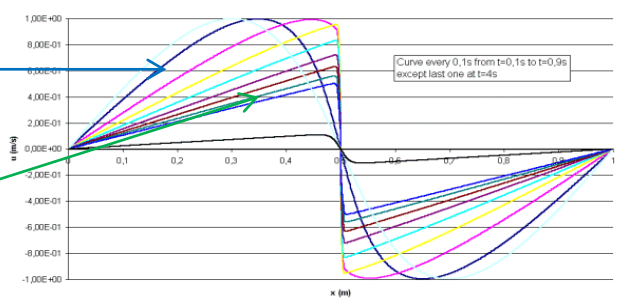
2. Hyperbolic problems: resolving shocks / discontinuities

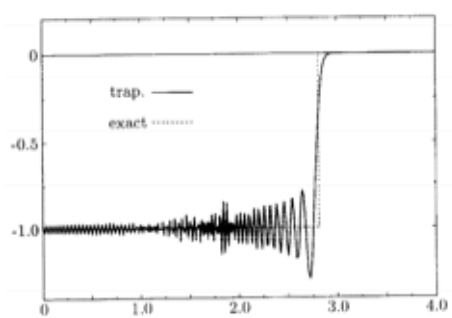
Discontinuities are preserved or generated from smooth initial conditions!

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

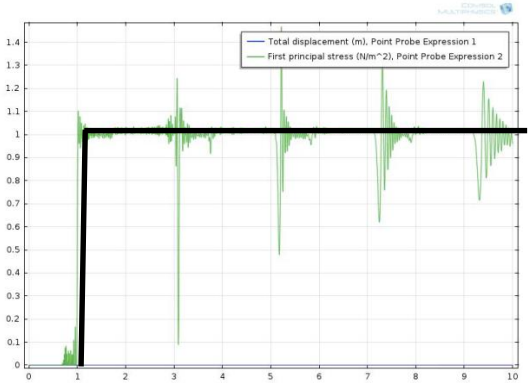
t = 0, smooth solution

t > 0, shock has formed





Global numerical oscillations



COMSOL

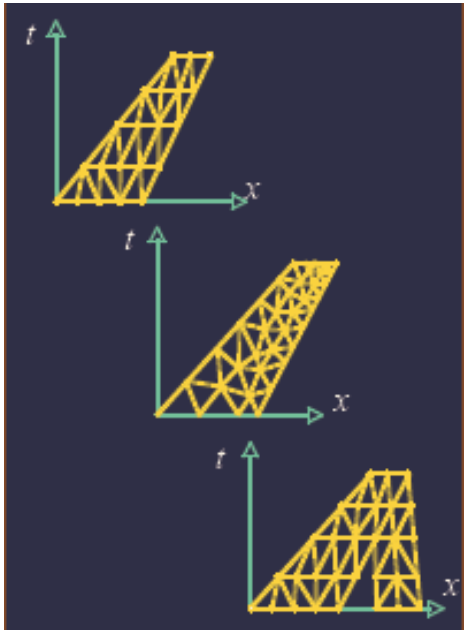
Spacetime Discontinuous Galerkin Finite Element method:

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

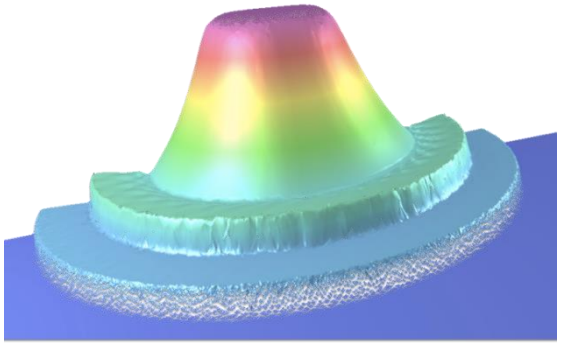
A local, O(N), asynchronous solution scheme

Direct discretization of spacetime

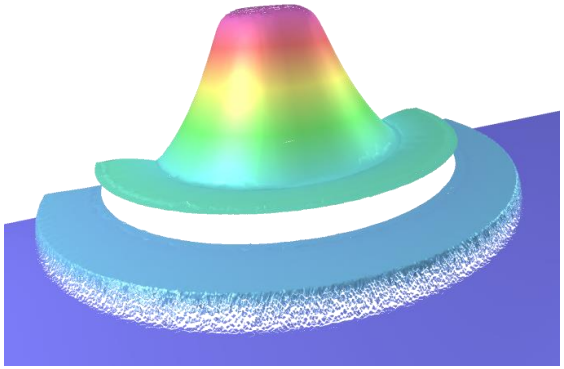
- Replaces a separate time integration; no global time step constraint
- Unstructured meshes in spacetime
- No tangling in moving boundaries
- Arbitrarily high and local order of accuracy in time
- Unambiguous numerical framework for boundary conditions



shock capturing more expensive, less accurate



Shock tracking in spacetime: more accurate and efficient



Results by Scott Miller

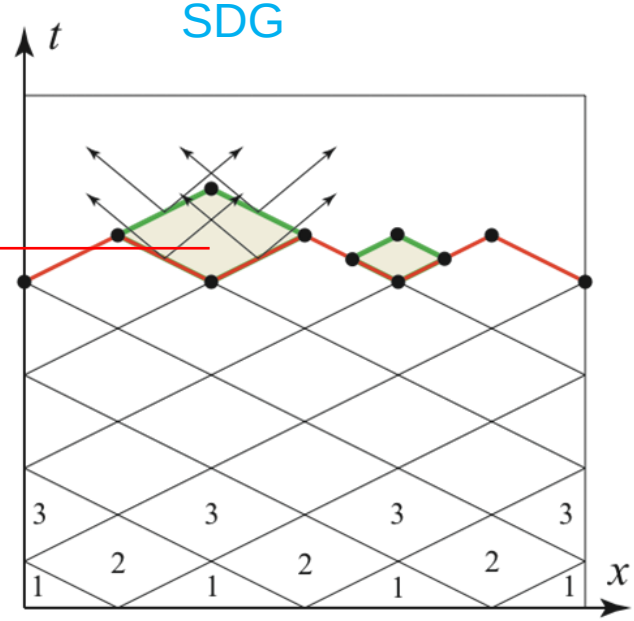
Spacetime Discontinuous Galerkin (SDG) Finite Element Method

DG + spacetime meshing + causal meshes for hyperbolic problems:

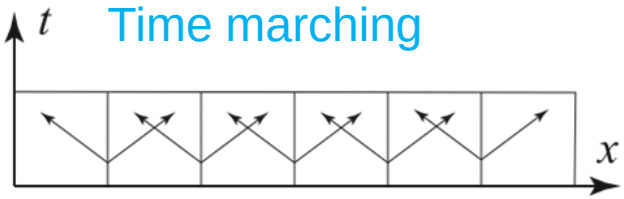
- Local solution property
- O(N) complexity (solution cost scales linearly vs. number of elements N)
- Asynchronous patch-by-patch solver

  - 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

SDG



Time marching



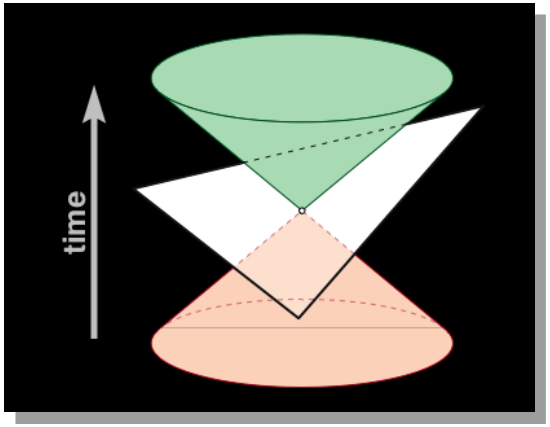
Time marching or the use of extruded meshes imposes a global coupling that is not intrinsic to a hyperbolic problem

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.

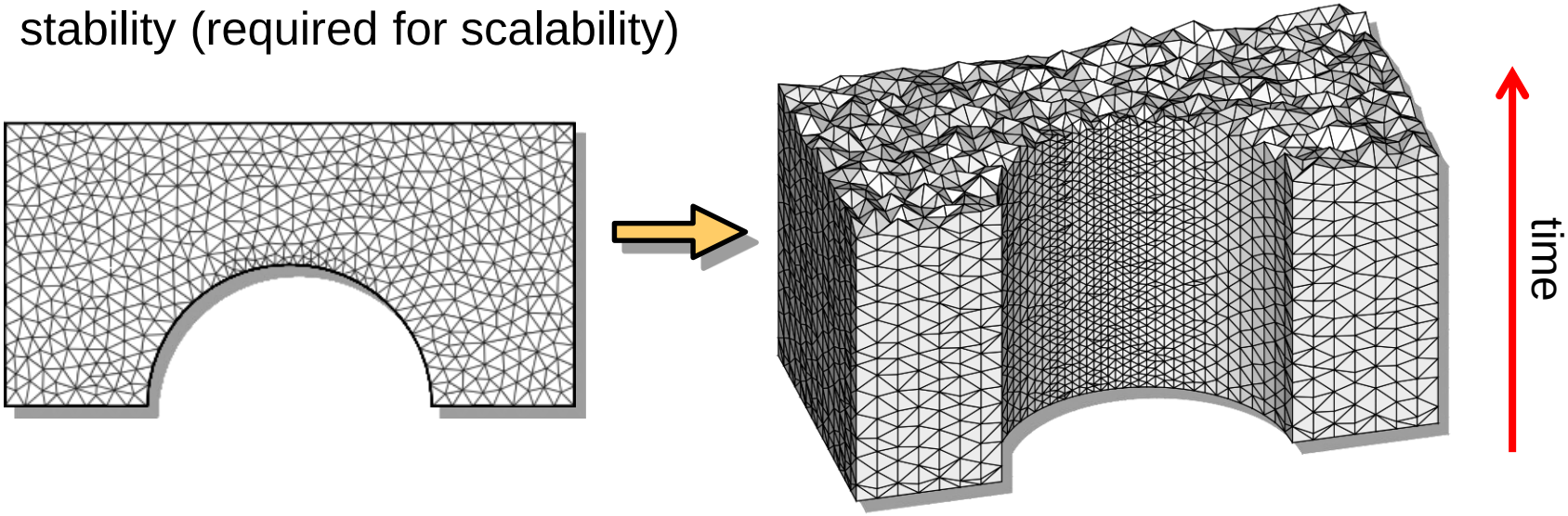
Tent Pitcher: Causal spacetime meshing

- 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)

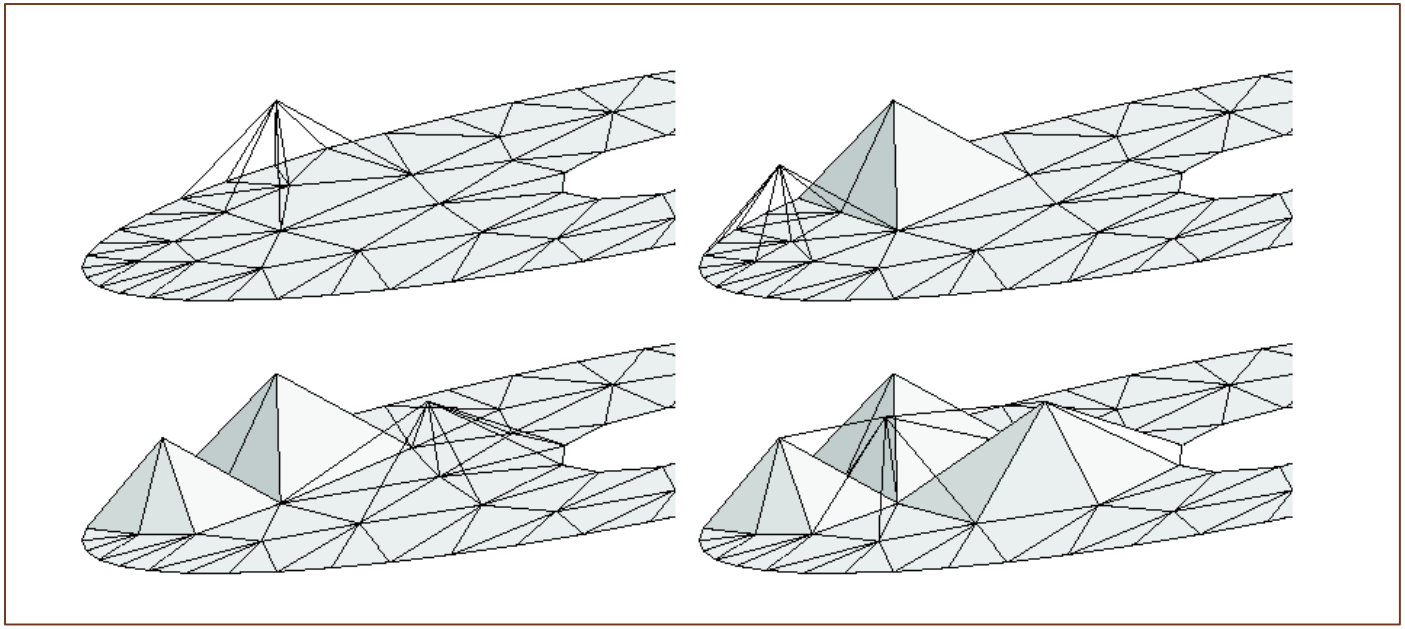


causality constraint



Tent Pitcher: Patch–by–patch meshing

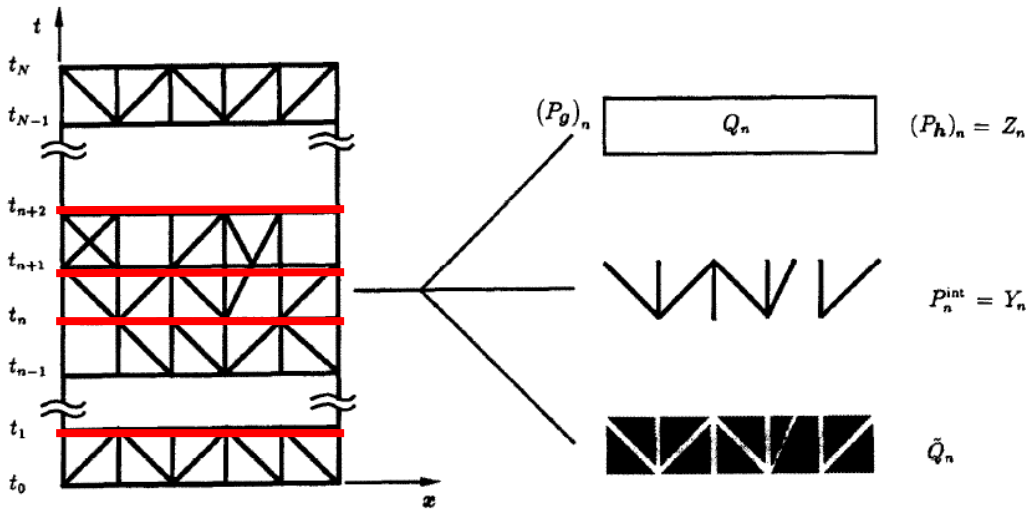
- meshing and solution are interleaved
  - patches (‘tents’) of tetrahedra are solve immediately ⇨ O(N) property
  - rich parallel structure: patches can be created and solved in parallel

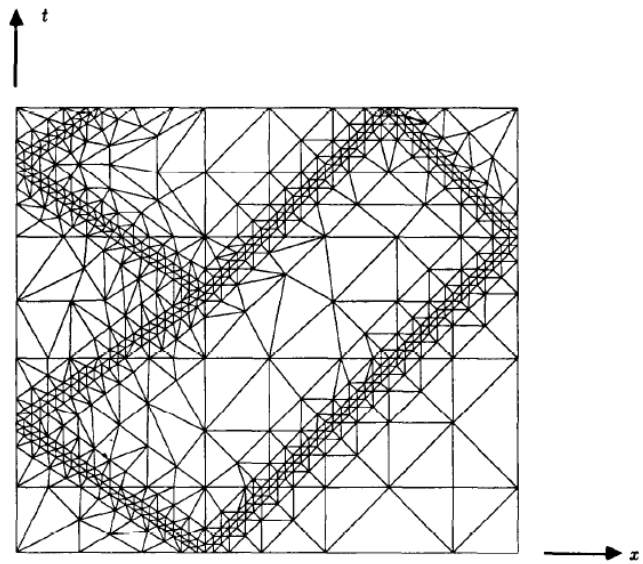


tent–pitching sequence

A few other spacetime DG methods

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

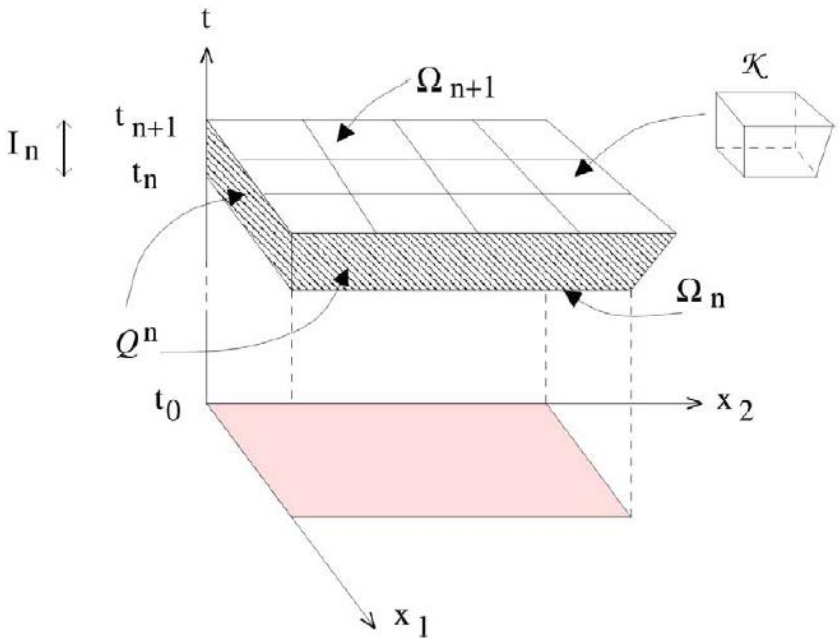




- Elements are arranged in spacetime slabs
- Discontinuities are only between spacetime slabs
- Elements within slabs are solved simultaneously

A few other spacetime DG methods

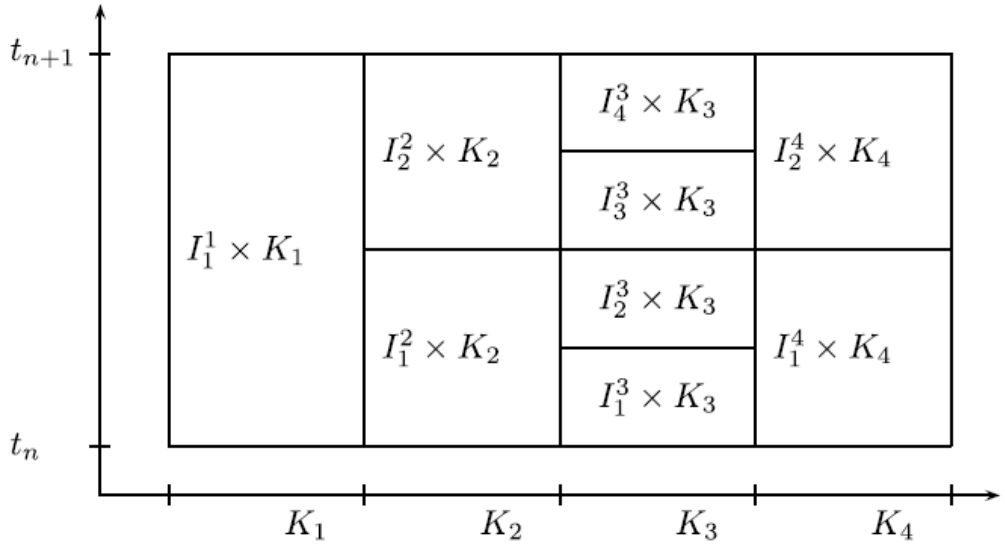
- Spacetime discontinuous Galerkin method (JJW Van der Vegt, H Van der Ven, *et al*)



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

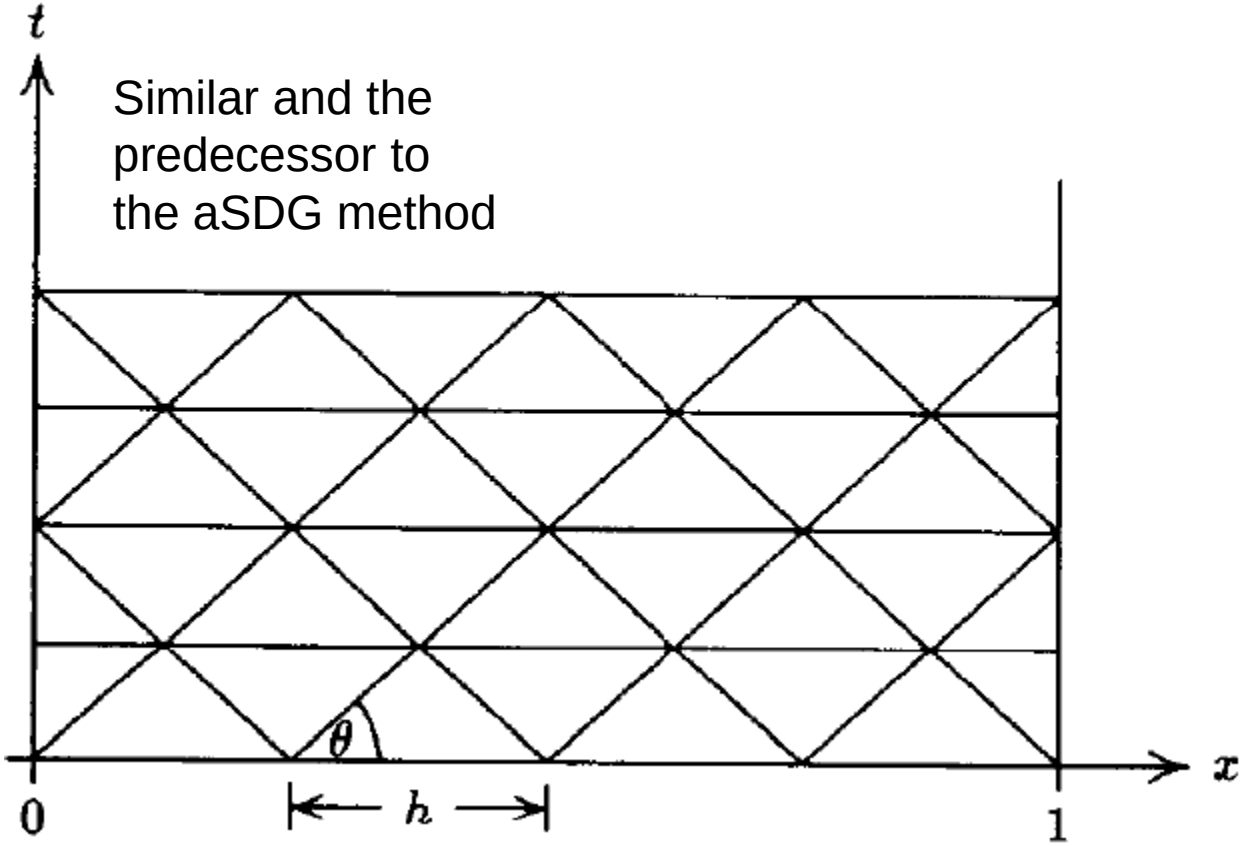
A few other spacetime DG methods

- hp-adaptive Spacetime discontinuous Galerkin method, Discontinuous in space, continuous in time (
  - M. Lilienthal, S.M. Schnepp, and T.Weiland. Non-dissipative space-time hp-discontinuous Galerkin method for the time-dependent Maxwell equations. Journal of Computational Physics, 275:589 –607, 2014.)
  - Bo Wang, Ziqing Xie, and Zhimin Zhang. Space-time discontinuous Galerkin method for Maxwell equations in dispersive media. Acta Mathematica Scientia, 34(5):1357–76, 2014.



A few other spacetime DG methods

- Causal spacetime meshing (Richter, Falk, etc.)
  Gerard R. Richter, An explicit finite element method for the wave equation, Applied Numerical Mathematics 16 (1994) 65-80

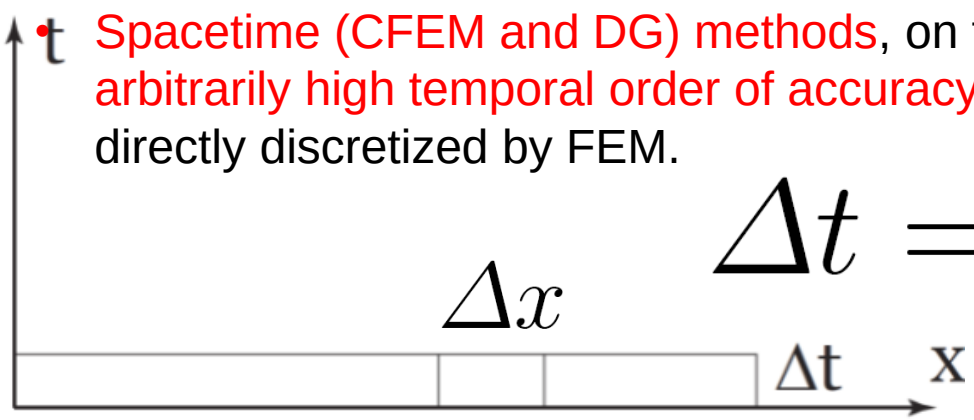


Advantages of Spacetime discontinuous Galerkin (SDG) Finite element method

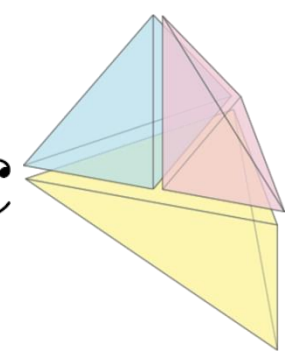
1. Arbitrarily high temporal order of accuracy

- 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 ⇨ 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.



$$\Delta t = \mathcal{C}(p)\Delta x / c$$

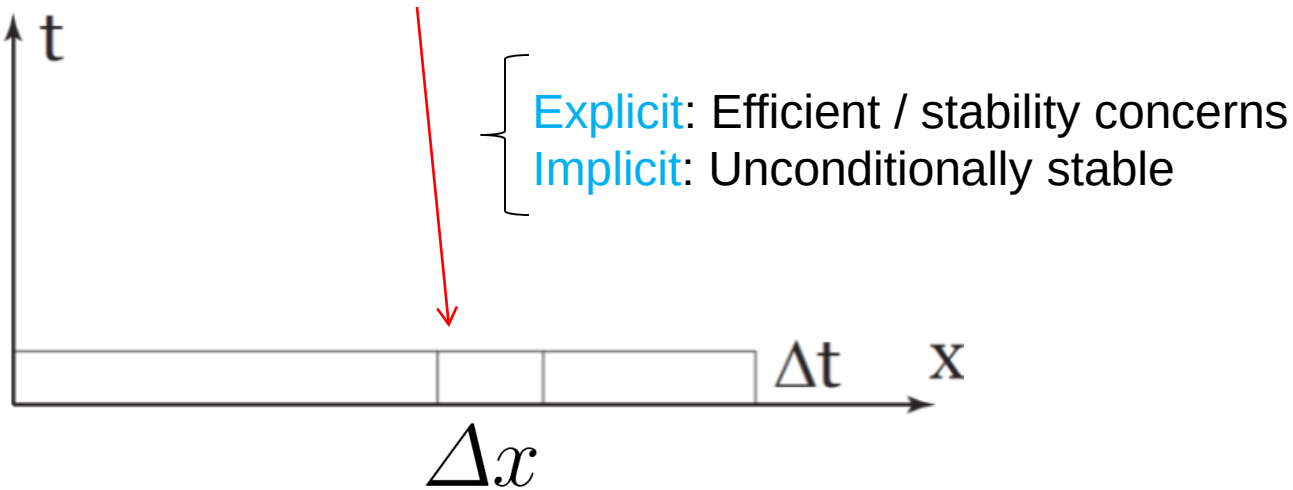


2. Asynchronous / no global time step

- 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.

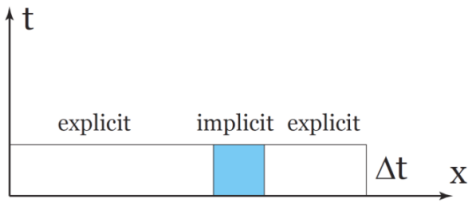
Time-marching methods

- **Time step is limited by smallest elements for explicit methods**

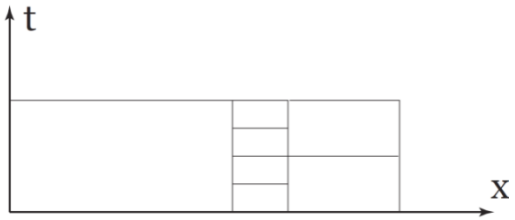


2. Asynchronous / no global time step

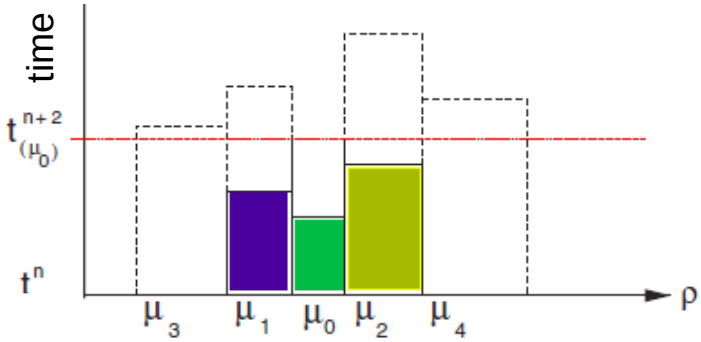
- **Improvements:**
  - **Implicit-Explicit (IMEX)** methods increase the time step by geometry splitting (implicit method for small elements) or operator splitting.



  - **Local time-stepping (LTS)**: subcycling for smaller elements enables using larger global time steps



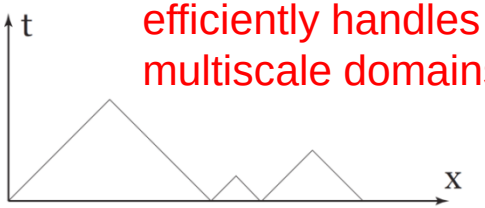
A. Taube, M. Dumbser, C.D. Munz and R. Schneider, A high-order discontinuous Galerkin method with time accurate
local time stepping for the Maxwell equations, Int. J. Numer. Model. 2009; 22:77–103



SDGFEM

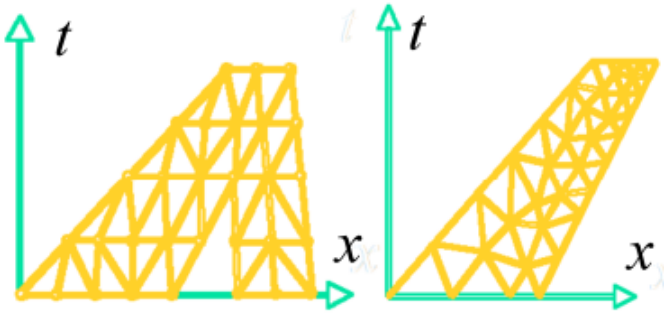
- Small elements locally have smaller progress in time (no global time step constrains)
- None of the complicated “improvements” of time marching methods needed

SDGFEM graciously and efficiently handles highly multiscale domains



3. Spacetime grids and Moving interfaces

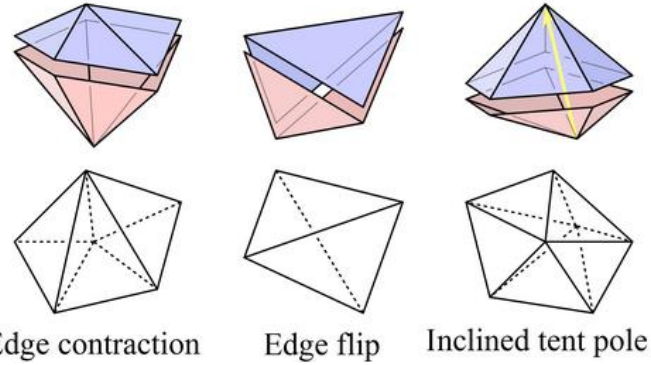
- Problems with moving interfaces:
  * Solid-fluid interaction * Non-linear free surface water waves
  * Helicopter rotors /forward fight * Flaps and slats on wings and piston engines
- Derivation of a conservative scheme is very challenging:
  - Even Arbitrary Lagrangian Eulerian (ALE) methods do not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



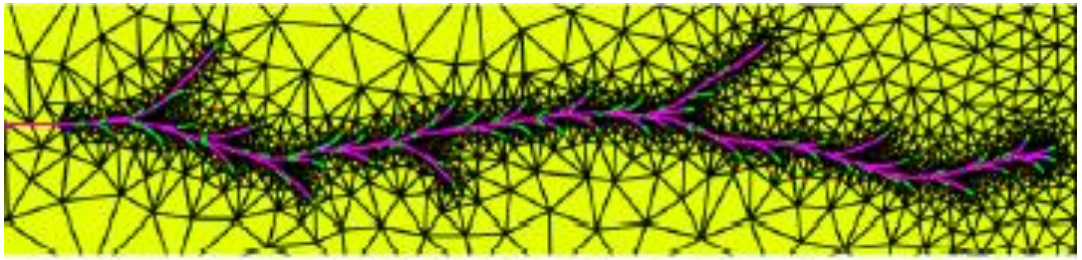
Tracking moving boundaries in spacetime

- Spacetime mesh adaptive operations

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

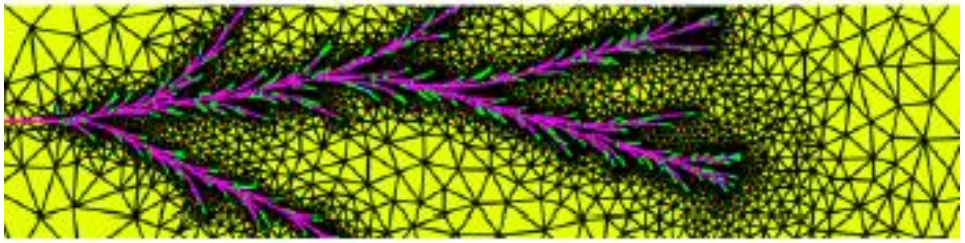


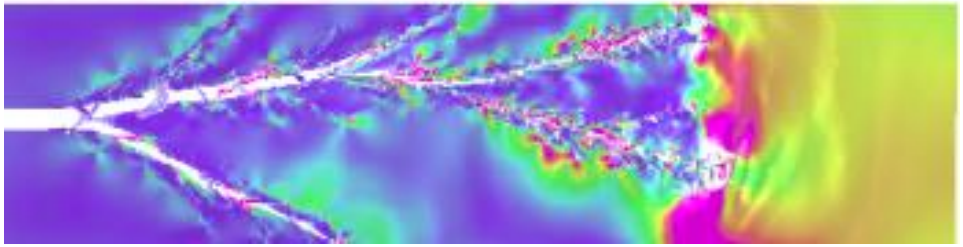
Examples from solid mechanics: Solution dependent crack propagation



Low load

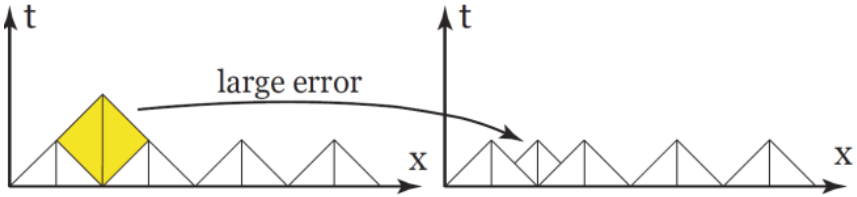
High load





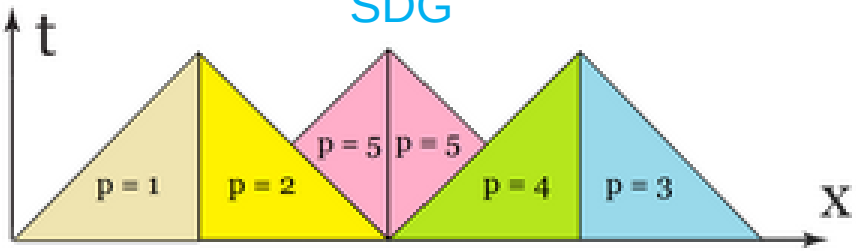
4. Adaptive mesh operations

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



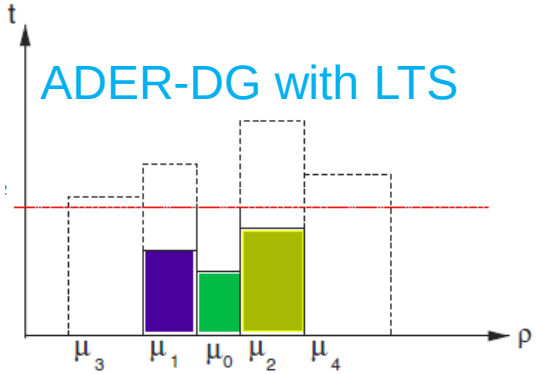
- Arbitrary order and size in time:

SDG



Example: LTS by Dumbser, Munz, Toro, Lorcher, et. al.

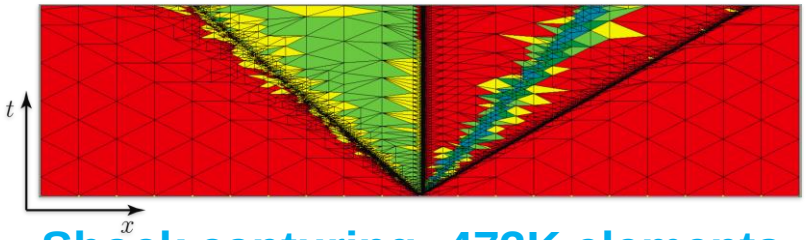
ADER-DG with LTS



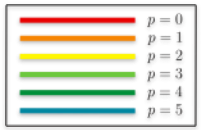
- Adaptive operations in spacetime:
  - Front-tracking better than shock capturing
  - *hp*-adaptivity better than *h*-adaptivity

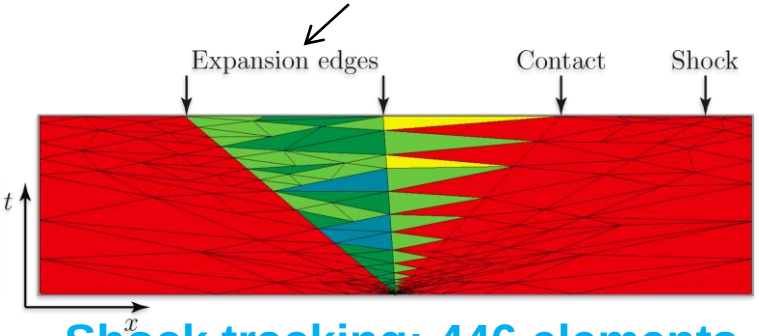
Sod's shock tube problem

Results by Scott Miller



Shock capturing: 473K elements

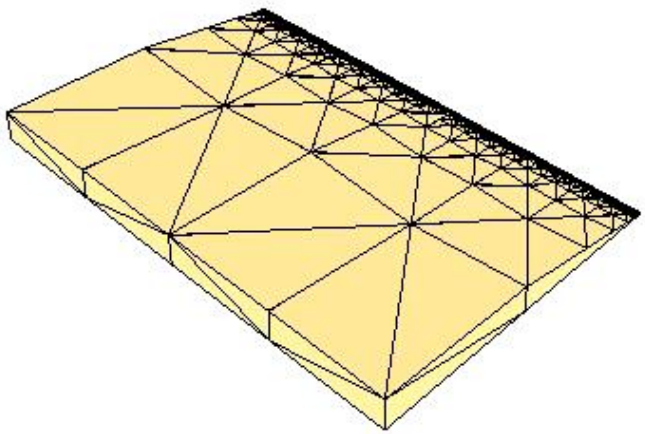


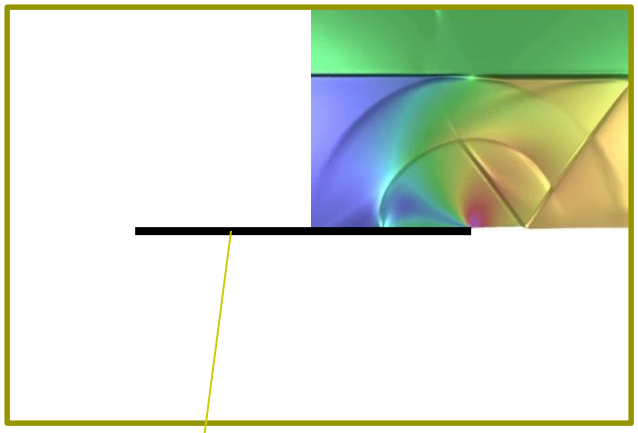


Shock tracking: 446 elements

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

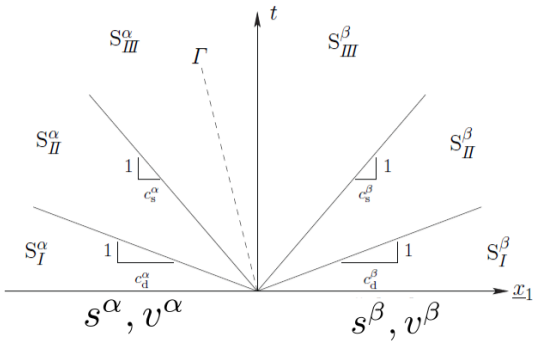
Time in up direction

5. Riemann-solution free scheme

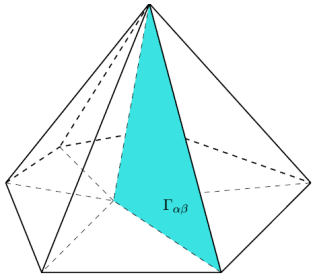
- Reimann solutions are often complicated, expensive, and even difficult to derive particularly for nonlinear and anisotropic materials.
  Example: Simple linear elastodynamic problem

$$\underline{s}_I^1 = \frac{\underline{w}^{(1)^\alpha}\rho^\beta c_\mathrm{d}^\beta + \underline{w}^{(1)^\beta}\rho^\alpha c_\mathrm{d}^\alpha}{\rho^\alpha c_\mathrm{d}^\alpha + \rho^\beta c_\mathrm{d}^\beta} = \frac{\check{\underline{s}}^{1^\alpha}\rho^\beta c_\mathrm{d}^\beta + \check{\underline{s}}^{1^\beta}\rho^\alpha c_\mathrm{d}^\alpha}{\rho^\alpha c_\mathrm{d}^\alpha + \rho^\beta c_\mathrm{d}^\beta} + \frac{\rho^\alpha\rho^\beta c_\mathrm{d}^\alpha c_\mathrm{d}^\beta}{\rho^\alpha c_\mathrm{d}^\alpha + \rho^\beta c_\mathrm{d}^\beta}[\![\check{\underline{v}}_1]\!]$$

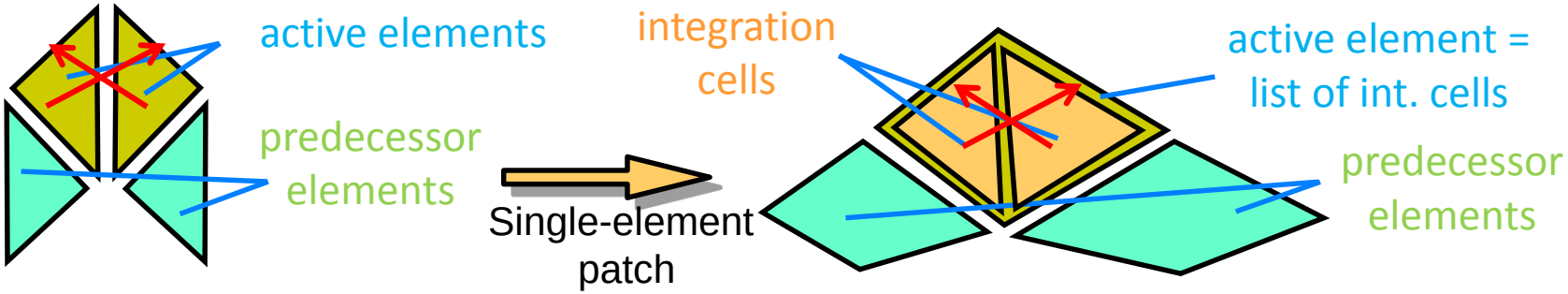
(regions III and IV)



- Riemann solutions required for inter-element noncausal boundaries



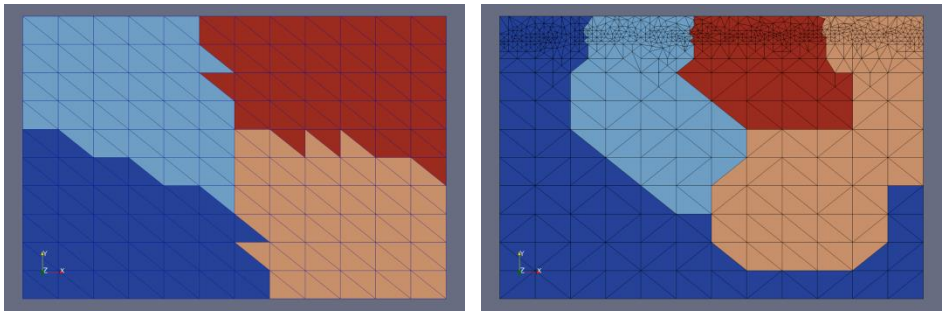
- If interior facets are eliminated we obtain a Riemann-solver free method ⇨

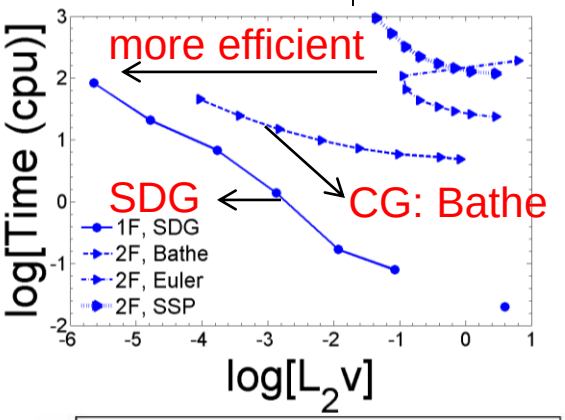


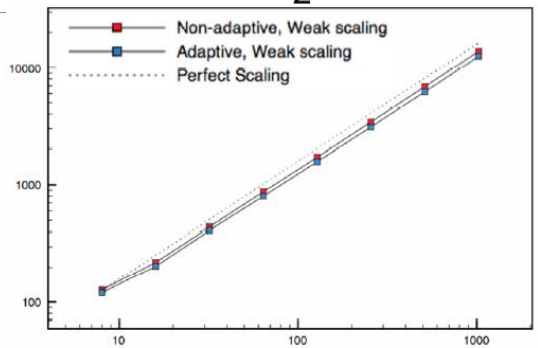
- Riemann-solution free scheme can also be more efficient

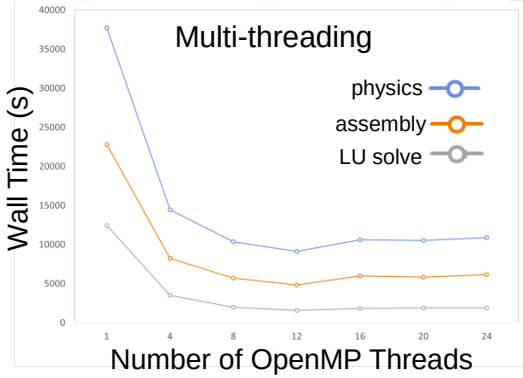
5. parallel computing (asynchronous structure)

- 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
  4,5.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





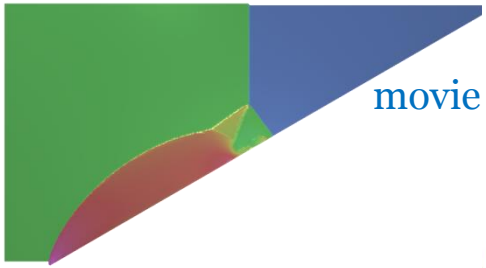




Multi-threading & Vectorization UIUC

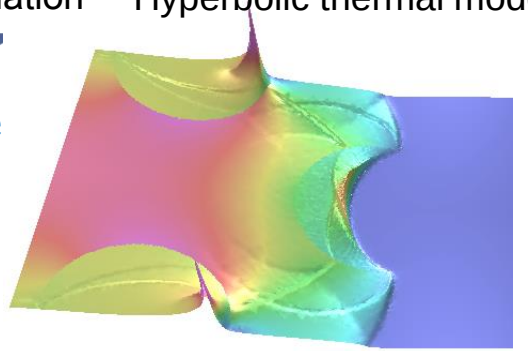
Other Applications

Fluid mechanics: Euler's equation



movie

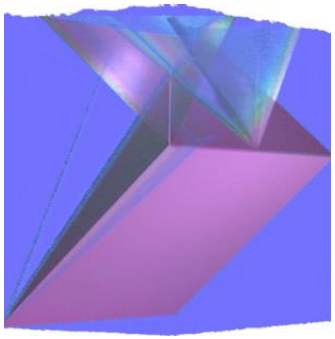
Hyperbolic thermal model



Solid mechanics

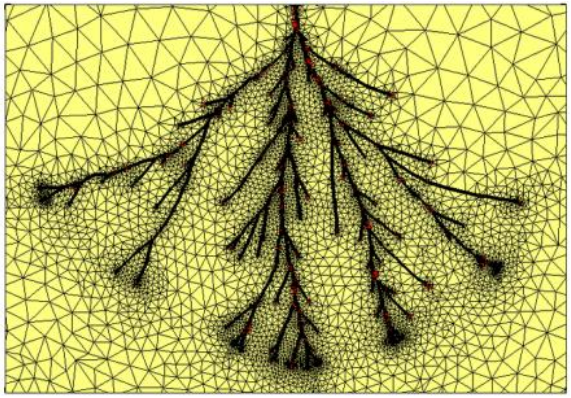
movie

YouTube link



Multiscale & Probabilistic Fracture

- Probabilistic crack nucleation.
- Exact tracking of crack interfaces.

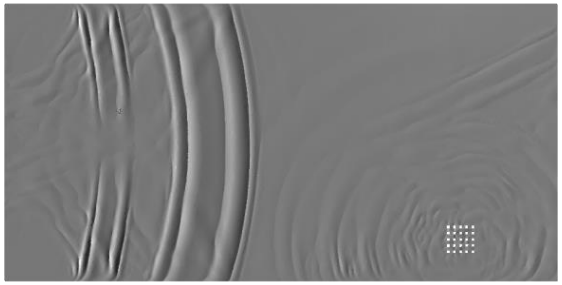


Click here to play movie

YouTube link

Structural Health Monitoring

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

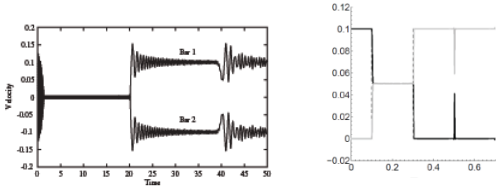


Click here to play movie

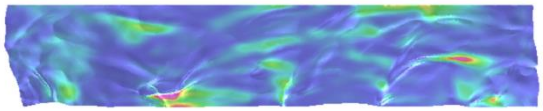
YouTube link

Dynamic Contact/Fracture

- SDGFEM eliminates common artifacts at contact transitions



High resolution slip-stick-separation waves



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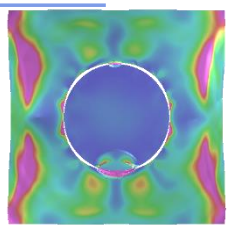


Click here to play movie

YouTube link

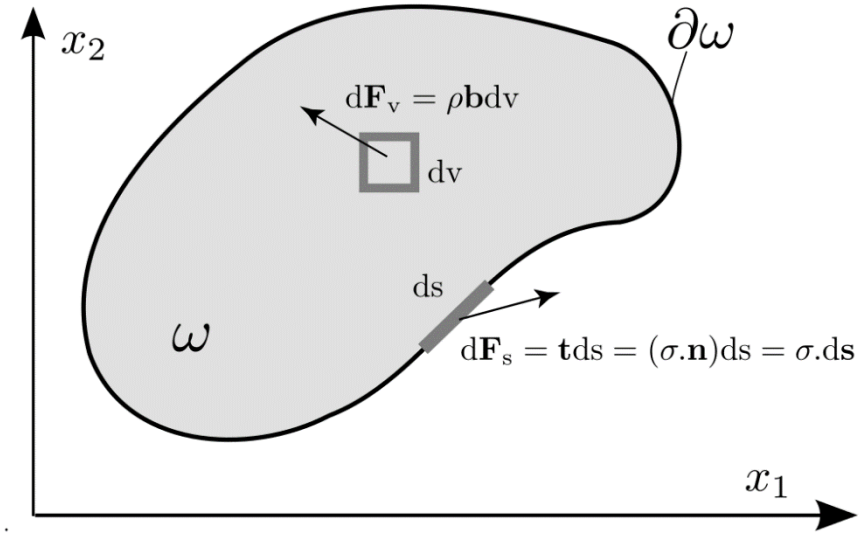
2. Electromagnetics

Balance laws in spacetime: Differential forms

Balance laws for dynamic problems

For a general conservation law let:

- $\mathbf{f}_t$: conserved quantity = temporal flux
- $\mathbf{f}_x$: total outward spatial flux
- $\mathbf{r}$: source term



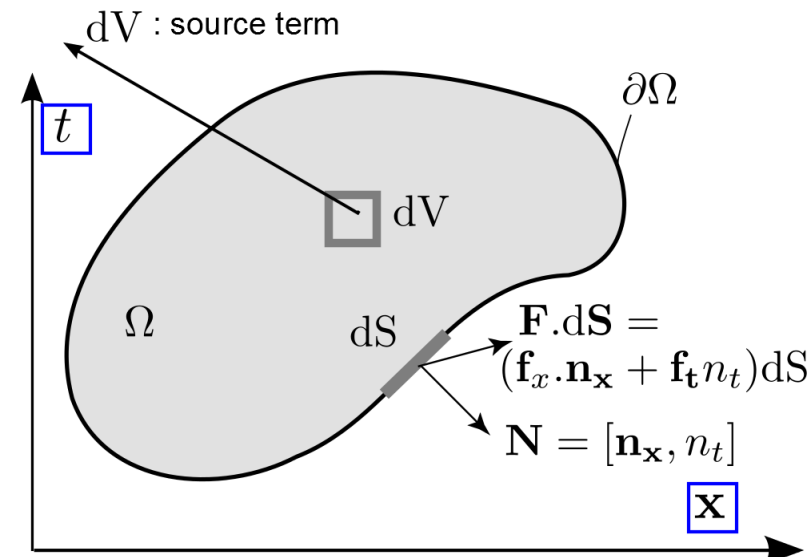
Balance law reads as

$$\forall\omega \qquad \int_\omega \mathbf{r}\,\mathrm{dv} - \int_{\partial\omega} \mathbf{f}_x.\mathrm{ds} = \int_\omega \mathbf{r}\,\mathrm{dv} - \int_{\partial\omega} (\mathbf{f}_x.\mathbf{n})\,\mathrm{ds} = \frac{\mathrm{d}}{\mathrm{d}t}\int_\omega \mathbf{f}_t\,\mathrm{dv}$$

Spacetime expression of balance law: Sloppy way!

$$\mathbf{F} = \underbrace{[\mathbf{f}_x | \mathbf{f}_t]}$$

Spatial & temporal fluxes are Combined.



- Balance law for arbitrary Ω in spacetime:

$$\forall \Omega \subset \mathcal{D} : \int_{\partial\Omega} \mathbf{F}.\,\mathrm{d}\mathbf{S} - \int_{\Omega} \mathbf{s}\ \mathrm{dV} =$$

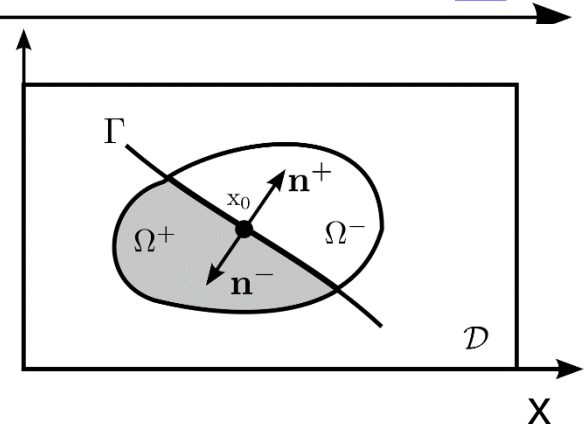
$$\int_{\partial\Omega} (\mathbf{f}_x.\mathbf{n_x} + \mathbf{f_t} n_t)\mathrm{dS} - \int_{\Omega} \mathbf{s}\ \mathrm{dV} = \mathbf{0}$$

- Strong form:

$$\forall \mathbf{x} \in \mathcal{D} \setminus \Gamma : \nabla_{\mathrm{st}}.\mathbf{F} - \mathbf{s} = \frac{\mathrm{d}\mathbf{f}_t}{\mathrm{d}t} + \nabla.\mathbf{f}_x - \mathbf{s} = \mathbf{0}$$ PDE

$$\forall \mathbf{x} \in \Gamma : \ [\![\mathbf{F}]\!]_{\mathbf{N}} = (\mathbf{F}^* - \mathbf{F}))_{\mathbf{N}} =$$

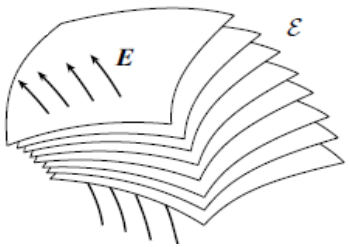
$$(\mathbf{f}_x^* - \mathbf{f}_x).\mathbf{n}_x + (\mathbf{f}_t^* - \mathbf{f}_t).n_t = \mathbf{0}$$ Jump (Rankin-Hugoniot) conditions



Exterior calculus: 0 to 3-forms

- f: 0-form [*e.g.*, electric potential f] $\Rightarrow$
  $\boldsymbol{d}f$: 1-form

$$\boldsymbol{d}f = f_1 \mathrm{d}x_1 + f_2 \mathrm{d}x_2 + f_3 \mathrm{d}x_3 = f_i \mathrm{d}x_i = \nabla f \mathrm{d}\mathbf{x}$$

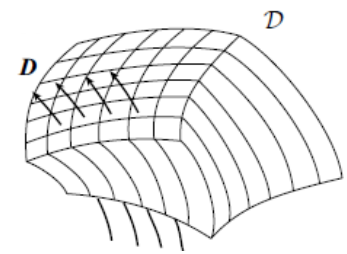


Russer 2004

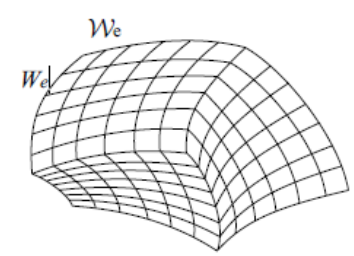
- $\boldsymbol{v}$: 1-form [*e.g.*, electric field $\mathbf{E}$]
  $(\boldsymbol{v} = v^i \mathrm{d}x_i = \mathbf{v}\mathrm{d}\mathbf{x})$ $\Rightarrow$
  $\boldsymbol{d}\boldsymbol{v}$: 2-form

$$\begin{aligned}\boldsymbol{d}\boldsymbol{v} &= \underbrace{(v^3_{,2} - v^2_{,3})}_{(\nabla\times\mathbf{v})_1}\underbrace{\mathrm{d}x_2 \wedge \mathrm{d}x_3}_{\star\mathrm{d}x^1} + \underbrace{(v^1_{,3} - v^3_{,1})}_{(\nabla\times\mathbf{v})_2}\underbrace{-\mathrm{d}x_1 \wedge \mathrm{d}x_3}_{\star\mathrm{d}x^2} + \underbrace{(v^2_{,1} - v^1_{,2})}_{(\nabla\times\mathbf{v})_3}\underbrace{\mathrm{d}x_1 \wedge \mathrm{d}x_2}_{\star\mathrm{d}x^3} \\ &= \nabla \times \mathbf{v} \star\mathrm{d}\mathbf{x}\end{aligned}$$

- $\boldsymbol{w}$: 2-form [*e.g.*, electric flux density $\mathbf{D}$]
  $(\boldsymbol{w} = w_i \star\mathrm{d}x^i = \mathbf{w}\star\mathrm{d}\mathbf{x} = w_1 \mathrm{d}x_2 \wedge \mathrm{d}x_3 - w_2 \mathrm{d}x_1 \wedge \mathrm{d}x_3 + w_3 \mathrm{d}x_1 \wedge \mathrm{d}x_2)$ $\Rightarrow$
  $\boldsymbol{d}\boldsymbol{w}$: 3-form



$$\boldsymbol{d}\boldsymbol{w} = \boldsymbol{d}(w_i \star\mathrm{d}x^i) = \underbrace{(w_{1,1} + w_{2,2} + w_{3,3})}_{\nabla.\mathbf{w}}\underbrace{\mathrm{d}x_1 \wedge \mathrm{d}x_2 \wedge \mathrm{d}x_3}_{\boldsymbol{\Omega}} = \nabla.\mathbf{w}\ \boldsymbol{\Omega}$$



- 3-form: [*e.g.*, electric charge density] $\rho\boldsymbol{\Omega}$ $\Rightarrow \boldsymbol{d}\rho\boldsymbol{\Omega} = 0$

Forms in spacetime

d: spatial dimension. $\star$: Hodge star operator.

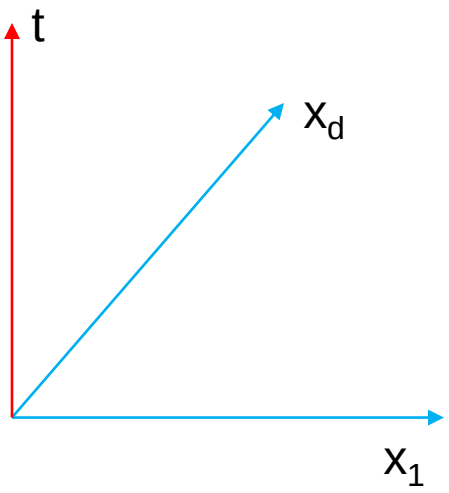
- 1-forms: $\{\mathrm{d}x_1, \ldots, \mathrm{d}x_d, \mathrm{d}t\}$. Specific Definition:

$$\mathbf{dx} := \mathbf{e}^i \mathrm{d}x_i$$

- $(d+1)$-form: $\boldsymbol{\Omega} := \mathrm{d}x_1 \wedge \ldots \wedge \mathrm{d}x_d \wedge \mathrm{d}t$.

- d-forms: $\{\star\mathrm{d}x^j, \star\mathrm{d}t\}$.
  Identities: $\mathrm{d}x_i \wedge \star\mathrm{d}x^j = \delta_i^{\ j}\boldsymbol{\Omega}$, $\mathrm{d}t \wedge \star\mathrm{d}x^j = \mathbf{0}$, $\mathrm{d}t \wedge \star\mathrm{d}t = \boldsymbol{\Omega}$ and $\mathrm{d}x_i \wedge \star\mathrm{d}t = \mathbf{0}$
  Example ($d = 3$):

$$\star\mathrm{d}x^1 = \mathrm{d}x_2 \wedge \mathrm{d}x_3 \wedge \mathrm{d}t$$
$$\star\mathrm{d}x^2 = \mathrm{d}x_3 \wedge \mathrm{d}x_1 \wedge \mathrm{d}t$$
$$\star\mathrm{d}x^3 = \mathrm{d}x_1 \wedge \mathrm{d}x_2 \wedge \mathrm{d}t$$



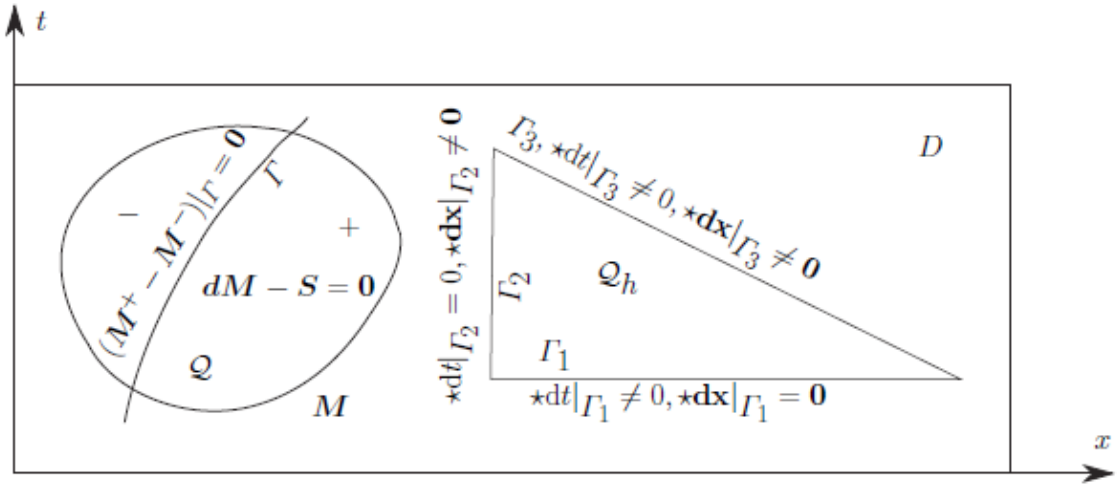
Specific Definition:

$$\star\mathbf{dx} := \mathbf{e}_i \star\mathrm{d}x^i$$

Spacetime expression of balance law: Using differential forms

- Spacetime flux $\boldsymbol{F}$:
  - Temporal flux: $\boldsymbol{f}_t = \mathbf{f}_t \star \mathrm{d}t$
  - Spatial flux: $\boldsymbol{f}_x = \mathbf{f}_x \star \mathrm{d}x$

$$\boxed{\boldsymbol{F} = \boldsymbol{f}_t + \boldsymbol{f}_x}$$



- Source term $\boldsymbol{s} = \mathbf{s}\boldsymbol{\Omega}$
- Balance law

$$\forall \Omega \subset \mathcal{D}: \qquad \int_{\partial\Omega} \boldsymbol{F} = \int_{\Omega} \boldsymbol{s}$$

- Strong form (application of Stokes theorem):

$$\int_{\Omega} (\boldsymbol{dF} - \boldsymbol{s}) = 0 \qquad \Rightarrow \qquad \begin{cases} \boldsymbol{dF} - \boldsymbol{s} = (\mathbf{f}_{t,t} + \nabla.\mathbf{f}_x - \mathbf{s})\boldsymbol{\Omega} = 0 & \text{PDE} \\ [\![\boldsymbol{F}]\!]_\Gamma = 0 & \text{Jump part} \end{cases}$$

Elastodynamics

Elastodynamic formulation in spacetime: Fields, fluxes and sources

- Kinematic fields

$$\mathbf{u} = u^i \boldsymbol{e}_i \qquad \Rightarrow$$

$$\boldsymbol{\varepsilon} := \boldsymbol{v} + \boldsymbol{E} \text{ velocity–strain 1-form, where } \begin{cases} \boldsymbol{v} & = \mathbf{v}\mathrm{d}t = v^i \boldsymbol{e}_i \mathrm{d}t \\ \boldsymbol{E} & = \mathbf{E} \wedge \mathbf{dx} = E^i_j e_i \mathrm{d}x^j \end{cases}$$

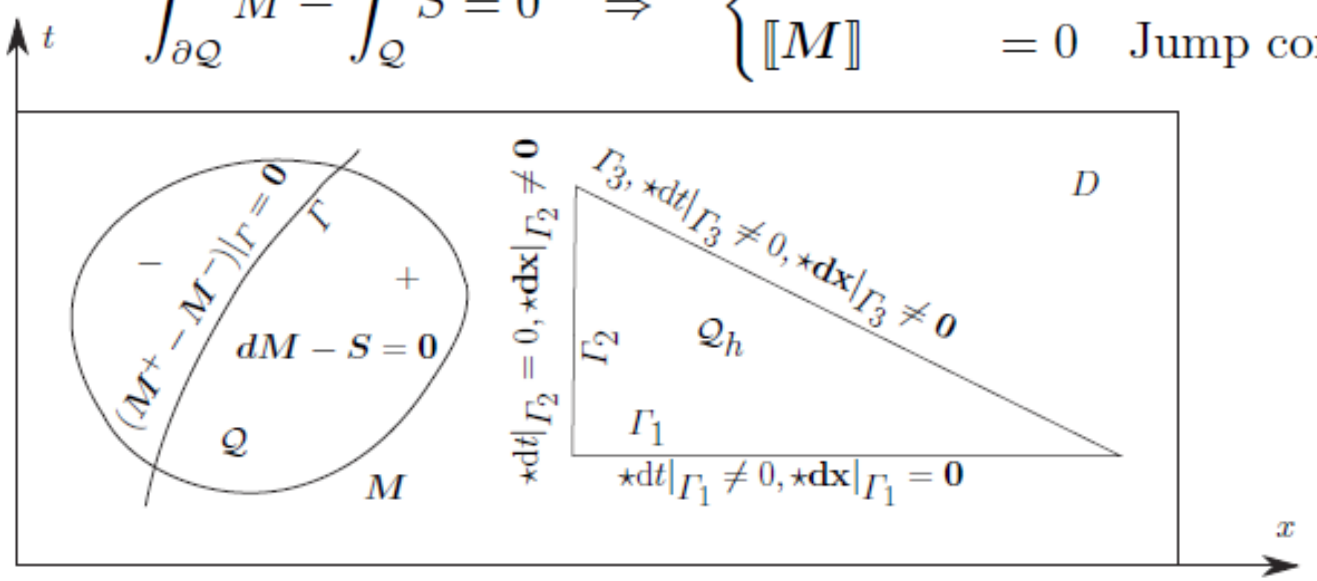
- Force-like fields

$$\boldsymbol{M} := \boldsymbol{p} - \boldsymbol{s} \text{ spacetime momentum flux, where } \begin{cases} \boldsymbol{p} & = \mathbf{p} \star \mathrm{d}t = p_i \boldsymbol{e}^i \star \mathrm{d}t \\ \boldsymbol{s} & = \mathbf{s} \wedge \star \mathbf{dx} = s_{ij} e^i \star \mathrm{d}x_j \end{cases}$$

- Balance law

$$\int_{\partial \mathcal{Q}} \boldsymbol{M} - \int_{\mathcal{Q}} \boldsymbol{S} = 0 \quad \Rightarrow \quad \begin{cases} \mathbf{d}\boldsymbol{M} - \boldsymbol{S} & = 0 \quad \text{PDE} \\ [\![\boldsymbol{M}]\!] & = 0 \quad \text{Jump conditions} \end{cases}$$

$\nabla . s - S = \dot{p}$



Electromagnetics

Electromagnetics formulation in spacetime: Fields, fluxes and sources

- Electromagnetic fields

$$\boldsymbol{U} = \begin{bmatrix} \boldsymbol{E} \\ \boldsymbol{H} \end{bmatrix} \quad \begin{aligned} \boldsymbol{E} &= \mathbf{E}\mathbf{dx} \wedge \mathrm{d}t = E^1 \mathrm{d}x_1 \wedge \mathrm{d}t + E^2 \mathrm{d}x_2 \wedge \mathrm{d}t + E^3 \mathrm{d}x_3 \wedge \mathrm{d}t \\ \boldsymbol{H} &= \mathbf{H}\mathbf{dx} \wedge \mathrm{d}t = H^1 \mathrm{d}x_1 \wedge \mathrm{d}t + H^2 \mathrm{d}x_2 \wedge \mathrm{d}t + H^3 \mathrm{d}x_3 \wedge \mathrm{d}t \end{aligned}$$

- Electromagnetic (total) flux densities

$$\boldsymbol{F}^t = \begin{bmatrix} \boldsymbol{D}^t \\ \boldsymbol{B}^t \end{bmatrix} \quad \begin{aligned} \boldsymbol{D}^t &= \mathbf{D}^t \star \mathbf{dx} \wedge \mathrm{d}t = D_1^t \mathrm{d}x_2 \wedge \mathrm{d}x_3 + D_2^t \mathrm{d}x_3 \wedge \mathrm{d}x_1 + D_3^t \mathrm{d}x_1 \wedge \mathrm{d}x_2 \\ \boldsymbol{B}^t &= \mathbf{B}^t \star \mathbf{dx} \wedge \mathrm{d}t = B_1^t \mathrm{d}x_2 \wedge \mathrm{d}x_3 + B_2^t \mathrm{d}x_3 \wedge \mathrm{d}x_1 + B_3^t \mathrm{d}x_1 \wedge \mathrm{d}x_2 \end{aligned}$$

- Constitutive equation

$$\bar{\boldsymbol{F}}^{t\mathcal{I}} = \sum_{\mathcal{J}=1}^{2} \bar{\epsilon}^{\mathcal{I}\mathcal{J}}(\omega) \star \bar{\boldsymbol{U}}_{\mathcal{J}}$$

$$\bar{\epsilon}^{\mathcal{I}\mathcal{J}}(\omega) := \epsilon_\infty^{\mathcal{I}\mathcal{J}} + \frac{\sigma^{\mathcal{I}\mathcal{J}}}{j\omega} + \bar{\epsilon}_d^{\mathcal{I}\mathcal{J}}(\omega)$$

$$\boldsymbol{F} = \begin{bmatrix} \boldsymbol{D} \\ \boldsymbol{B} \end{bmatrix}, \mathbf{J} = \mathbf{J}_\sigma + \mathbf{J}_{\epsilon_d}$$

Inductive | **Conductive** | **Dispersive**

$\begin{aligned} \boldsymbol{D} &= \epsilon_\infty^{11} \star \boldsymbol{E} + \epsilon_\infty^{12} \star \boldsymbol{H} \\ \boldsymbol{B} &= \epsilon_\infty^{21} \star \boldsymbol{E} + \epsilon_\infty^{22} \star \boldsymbol{H} \end{aligned}$	$\begin{aligned} \mathbf{J}_{E\sigma} &= \sigma^{11}\mathbf{E} + \sigma^{12}\mathbf{H} \\ \mathbf{J}_{H\sigma} &= \sigma^{21}\mathbf{E} + \sigma^{22}\mathbf{H} \end{aligned}$	$\bar{\mathbf{J}}_{\epsilon_d}^{\mathcal{I}} := \sum_{\mathcal{J}=1}^{2} \{j\omega\bar{\epsilon}_d^{\mathcal{I}\mathcal{J}}(\omega)\}\bar{\mathbf{U}}_{\mathcal{J}}$

Spacetime electromagnetic flux

Spacetime electromagnetic flux density $\boldsymbol{M} = \boldsymbol{F} + \mathbb{J}\boldsymbol{U}$

$$\mathbb{J} := \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}$$

$$\begin{cases} \boldsymbol{M}^E & := \boldsymbol{D} - \boldsymbol{H} \\ \boldsymbol{M}^H & := \boldsymbol{B} + \boldsymbol{E} \end{cases}$$

2-form fluxes in spacetime for EM problem

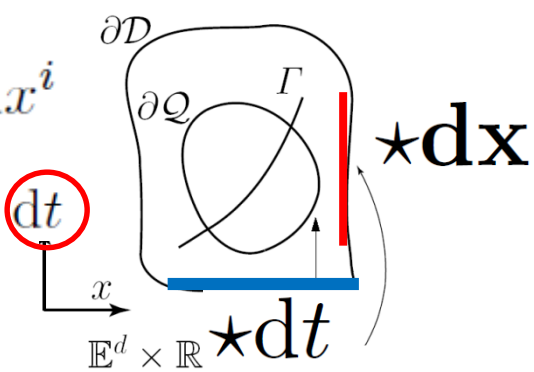
$$\boldsymbol{U} = \begin{bmatrix} \boldsymbol{E} \\ \boldsymbol{H} \end{bmatrix} = \begin{bmatrix} E^1 \mathrm{d}x_1 \wedge \mathrm{d}t + E^2 \mathrm{d}x_2 \wedge \mathrm{d}t + E^3 \mathrm{d}x_3 \wedge \mathrm{d}t \\ H^1 \mathrm{d}x_1 \wedge \mathrm{d}t + H^2 \mathrm{d}x_2 \wedge \mathrm{d}t + H^3 \mathrm{d}x_3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

$$\boldsymbol{F} = \begin{bmatrix} \boldsymbol{D} \\ \boldsymbol{B} \end{bmatrix} = \begin{bmatrix} D_1 \mathrm{d}x_2 \wedge \mathrm{d}x_3 + D_2 \mathrm{d}x_3 \wedge \mathrm{d}x_1 + D_3 \mathrm{d}x_1 \wedge \mathrm{d}x_2 \\ B_1 \mathrm{d}x_2 \wedge \mathrm{d}x_3 + B_2 \mathrm{d}x_3 \wedge \mathrm{d}x_1 + B_3 \mathrm{d}x_1 \wedge \mathrm{d}x_2 \end{bmatrix}$$

Comparison with d-form fluxes in spacetime

Acting on time-like ("vertical") boundaries $\star\mathbf{dx} := \mathbf{e}^i \star \mathrm{d}x^i$

$$= \mathbf{e}^1 \mathrm{d}x^2 \wedge \mathrm{d}x^3 \wedge \mathrm{d}t + \mathbf{e}^2 \mathrm{d}x^3 \wedge \mathrm{d}x^1 \wedge \mathrm{d}t + \mathbf{e}^3 \mathrm{d}x^1 \wedge \mathrm{d}x^2 \wedge \mathrm{d}t$$



Acting on space-like ("horizontal") boundaries

$$\star\mathrm{d}t = -\mathrm{d}x^1 \wedge \mathrm{d}x^2 \wedge \mathrm{d}x^3$$

Spacetime flux

Comparison with other differential form formulation of EM problem

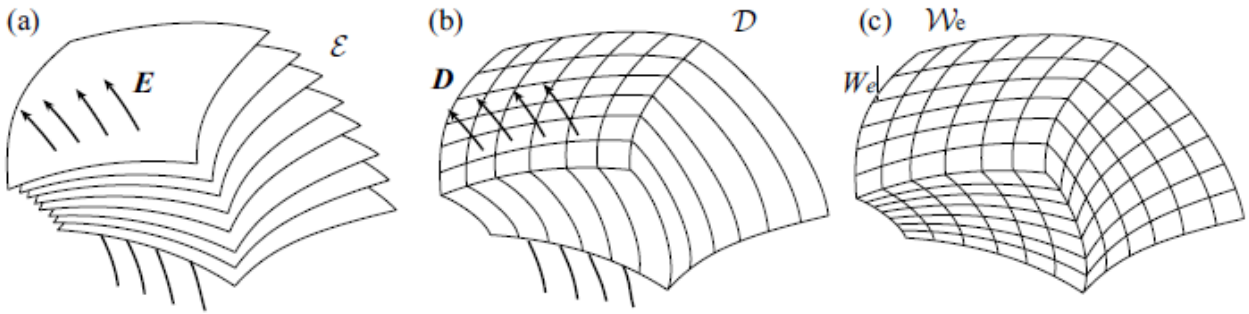


Fig. 2. Geometric representation of (a) a 1-form, (b) a 2-form, (c) a 3-form.

p	Quantity	Differential Form
0	Electric Potential	$f(\boldsymbol{x},t)$
1	Electric Field	$\mathcal{E}(\boldsymbol{x},t) = E_x\,\mathrm{d}x + E_y\,\mathrm{d}y + E_z\,\mathrm{d}z$
1	Magnetic Field	$\mathcal{H}(\boldsymbol{x},t) = H_x\,\mathrm{d}x + H_y\,\mathrm{d}y + H_z\,\mathrm{d}z$
2	Electric Flux Density	$\mathcal{D}(\boldsymbol{x},t) = D_x\,\mathrm{d}y \wedge \mathrm{d}z + D_y\,\mathrm{d}z \wedge \mathrm{d}x + D_z\,\mathrm{d}x \wedge \mathrm{d}y$
2	Magnetic Flux Density	$\mathcal{B}(\boldsymbol{x},t) = B_x\,\mathrm{d}y \wedge \mathrm{d}z + B_y\,\mathrm{d}z \wedge \mathrm{d}x + B_z\,\mathrm{d}x \wedge \mathrm{d}y$
2	Current Density	$\mathcal{J}(\boldsymbol{x},t) = J_x\,\mathrm{d}y \wedge \mathrm{d}z + J_y\,\mathrm{d}z \wedge \mathrm{d}x + J_z\,\mathrm{d}x \wedge \mathrm{d}y$

Source: Peter Russer, Exterior Differential Forms in Teaching Electromagnetics, 2004.

Our electromagnetic fields have an extra **d***t*

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

$$\boldsymbol{E} = \mathcal{E} \wedge \mathrm{d}t$$
$$\boldsymbol{H} = \mathcal{H} \wedge \mathrm{d}t$$

Balance laws in spacetime

Spacetime electromagnetic flux density

$$\boldsymbol{M} = \boldsymbol{F} + \mathbb{J}\boldsymbol{U} \qquad \mathbb{J} := \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}$$

Source terms: current and charge densities

$$\boldsymbol{R}_M := \boldsymbol{J} + \rho = \begin{bmatrix} J_1^E \star\mathrm{d}x^1 + J_2^E \star\mathrm{d}x^2 + J_3^E \star\mathrm{d}x^3 + \rho^E \star\mathrm{d}t \\ J_1^H \star\mathrm{d}x^1 + J_2^H \star\mathrm{d}x^2 + J_3^H \star\mathrm{d}x^3 + \rho^H \star\mathrm{d}t \end{bmatrix}$$

Integral form of Maxwell equations

$$-\int_{\partial\mathcal{Q}} \boldsymbol{f} \wedge \boldsymbol{M} + \int_{\mathcal{Q}} \boldsymbol{f} \wedge \boldsymbol{R}_M = \boldsymbol{0}$$

(***f*** is a 1-form)

Stokes' theorem

Strong form of Maxwell equations

$$\boldsymbol{dM} + \boldsymbol{R}_M = \boldsymbol{0}$$

Diffuse part (Provides **PDEs**)

$$\boldsymbol{f} \wedge [\![\boldsymbol{M}]\!] = 0$$

Jump part (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)

$$\begin{cases} \left(\dot{\mathbf{D}} + \boldsymbol{J}^E - \nabla \times \mathbf{H}\right) \star \mathrm{d}x & = \mathbf{0} \quad \text{Ampère's law} \\ \left(\dot{\mathbf{B}} + \boldsymbol{J}^H + \nabla \times \mathbf{E}\right) \star \mathrm{d}x & = \mathbf{0} \quad \text{Faraday law} \end{cases}$$

$$\begin{cases} \left(\nabla.\mathbf{D} - \rho^E\right) \star \mathrm{d}t & = \mathbf{0} \quad \text{Gauss law for electric field} \\ \left(\nabla.\mathbf{B} - \rho^H\right) \star \mathrm{d}t & = \mathbf{0} \quad \text{Gauss law for magnetic field} \end{cases}$$

b. Jump equations (BCs, interfaces, *etc.*) $\boldsymbol{f} \wedge [\![\boldsymbol{M}]\!] = 0$

- Weighted residual statement (WRS)

Stokes' theorem

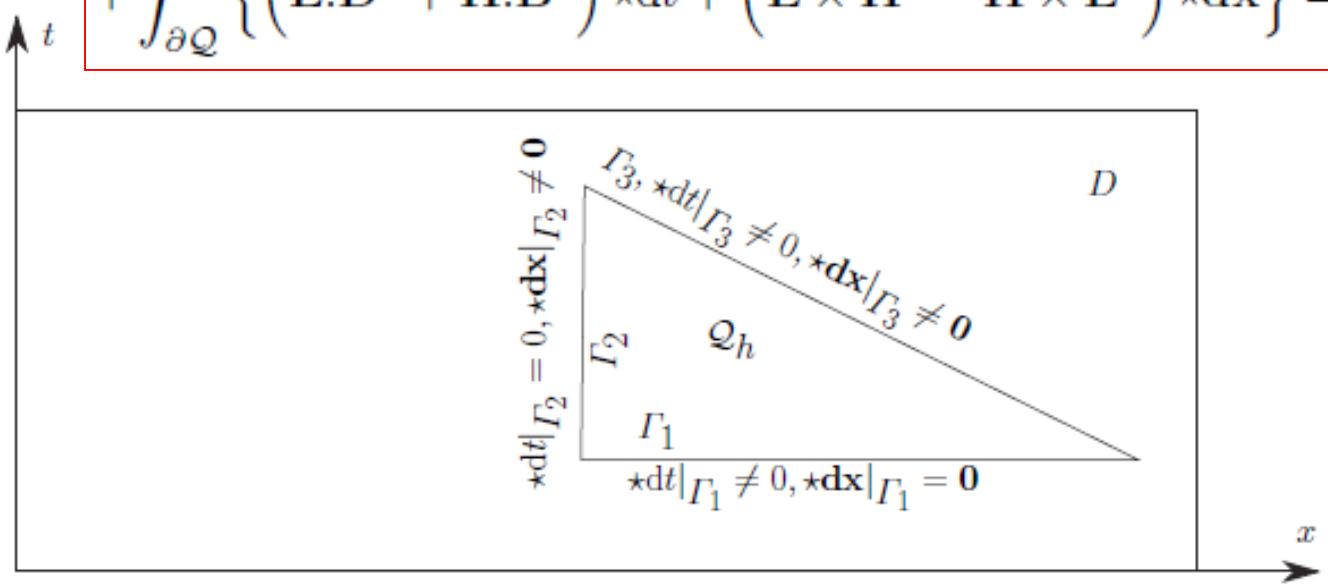
$$-\int_{\mathcal{Q}} \mathrm{i}\,\hat{U} \wedge (d\boldsymbol{M}^h + \boldsymbol{R}_M^h) + \int_{\partial\mathcal{Q}} \mathrm{i}\,\hat{U} \wedge [\![\boldsymbol{M}]\!]_h = \mathbf{0}$$

Strong Form to weak form and FEM formulation

- Weak statement (WKS)

$$-\int_{\mathcal{Q}} \left\{ d\mathbf{i}\,\hat{\boldsymbol{U}} \wedge \boldsymbol{M}^h + \mathbf{i}\,\hat{\boldsymbol{U}} \wedge \boldsymbol{R}_M^h \right\} + \int_{\partial\mathcal{Q}} \mathbf{i}\,\hat{\boldsymbol{U}} \wedge \boldsymbol{M}^* = 0 \Longrightarrow$$

$$\boxed{\begin{aligned} &\int_{\mathcal{Q}} \left\{ \left(-\dot{\hat{\mathbf{E}}}.\mathbf{D}^h - \nabla \times \hat{\mathbf{E}}.\mathbf{H}^h + \hat{\mathbf{E}}.\boldsymbol{J}^{h^E} \right) + \left(-\dot{\hat{\mathbf{H}}}.\mathbf{B}^h + \nabla \times \hat{\mathbf{H}}.\mathbf{E}^h + \hat{\mathbf{H}}.\boldsymbol{J}^{h^H} \right) \right\} \boldsymbol{\Omega} \\ &+ \int_{\partial\mathcal{Q}} \left\{ \left(\hat{\mathbf{E}}.\mathbf{D}^* + \hat{\mathbf{H}}.\mathbf{B}^* \right) \star \mathrm{d}t + \left(\hat{\mathbf{E}} \times \mathbf{H}^* - \hat{\mathbf{H}} \times \mathbf{E}^* \right) \star \mathbf{dx} \right\} = 0 \end{aligned}}$$



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

- Energy stability proof (dissipative method) $\boldsymbol{N} := \boldsymbol{u} + \boldsymbol{S}$

$$\Delta_{\mathcal{D}} := \int_{\partial\mathcal{Q}} \boldsymbol{N}(\boldsymbol{U}^*) + \int_{\mathcal{Q}} \boldsymbol{R}_N = \int_{\partial\mathcal{Q}} \boldsymbol{N}([\![\boldsymbol{U}]\!]_h) \geq 0$$

$\boldsymbol{u} := -\frac{1}{2}\mathrm{i}\,\boldsymbol{U}_{\mathcal{I}} \wedge \boldsymbol{F}^{\mathcal{I}} = \frac{1}{2}(\mathrm{E.D} + \mathrm{H.B}) \star \mathrm{d}t$	$\boldsymbol{S} := -\mathrm{i}\,\boldsymbol{E} \wedge \boldsymbol{H} = \mathrm{E} \times \mathrm{H} \star \mathrm{dx}$	$\boldsymbol{R}_N := -\mathrm{i}\,\boldsymbol{U} \wedge \boldsymbol{R}_M = \left\{\mathrm{E.J}^E + \mathrm{H.J}^H\right\} \Omega$

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

$$\begin{aligned}
a_{\mathcal{Q}}(\boldsymbol{U}^h, \hat{\boldsymbol{U}}) &:= -\int_{\mathcal{Q}} \mathrm{i}\,\hat{\boldsymbol{U}} \wedge (d\boldsymbol{M}^h + \boldsymbol{R}_M^h) + \int_{\partial\mathcal{Q}} \mathrm{i}\,\hat{\boldsymbol{U}} \wedge [\![\boldsymbol{M}]\!]_h \\
&= -\int_{\mathcal{Q}} \left\{ d\mathrm{i}\,\hat{\boldsymbol{U}} \wedge \boldsymbol{M}^h + \mathrm{i}\,\hat{\boldsymbol{U}} \wedge \boldsymbol{R}_M^h \right\} + \int_{\partial\mathcal{Q}} \mathrm{i}\,\hat{\boldsymbol{U}} \wedge \boldsymbol{M}^* \quad \Rightarrow \\
2a_{\mathcal{Q}}(\boldsymbol{U}^h, \hat{\boldsymbol{U}}) &= -2\int_{\mathcal{Q}} \mathrm{i}\,\hat{\boldsymbol{U}} \wedge \boldsymbol{R}_M^h - \int_{\mathcal{Q}} \left\{ \mathrm{i}\,\hat{\boldsymbol{U}} \wedge d\boldsymbol{M}^h + d\mathrm{i}\,\hat{\boldsymbol{U}} \wedge \boldsymbol{M}^h \right\} + \int_{\partial\mathcal{Q}} \mathrm{i}\,\hat{\boldsymbol{U}} \wedge \{[\![\boldsymbol{M}]\!]_h + \boldsymbol{M}^*\}
\end{aligned}$$

  - By showing $\hat{\mathbf{U}}_{\mathcal{I}}.\mathbf{F}^{*\mathcal{I}} = \mathbf{U}^*_{\mathcal{I}}.\hat{\mathbf{F}}^{\mathcal{I}}$ (interchanging * and ^ on fields and flux densities)

  and manipulation of bilinear form we can show:

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

$$
\begin{aligned}
2a_{\mathcal{Q}}(\boldsymbol{U}^h,\hat{\boldsymbol{U}}) &= -2\int_{\mathcal{Q}} \mathbf{i}\,\hat{\boldsymbol{U}}\wedge \boldsymbol{R}_M^h + \int_{\partial\mathcal{Q}} \mathbf{U}_{\mathcal{I}}^*.\mathbf{F}^{*\mathcal{I}}\star\mathrm{d}t + 2\mathbf{E}^*\times\mathbf{H}^*\star\mathrm{d}x \\
&- \int_{\partial\mathcal{Q}} \left[\mathbf{U}_{\mathcal{I}}^*.\left(\mathbf{F}^{*\mathcal{I}}-\hat{\mathbf{F}}^{\mathcal{I}}\right) - \hat{\mathbf{U}}_{\mathcal{I}}.\left(\mathbf{F}^{*\mathcal{I}}-\mathbf{F}^{h\mathcal{I}}\right)\right]\star\mathrm{d}t \\
&- \int_{\partial\mathcal{Q}} \left\{\left[\left(\mathbf{E}^*-\hat{\mathbf{E}}\right)\times\mathbf{H}^* - \left(\mathbf{E}^*-\mathbf{E}^h\right)\times\hat{\mathbf{H}}\right] + \left[\mathbf{E}^*\times\left(\mathbf{H}^*-\hat{\mathbf{H}}\right) - \hat{\mathbf{E}}\times\left(\mathbf{H}^*-\mathbf{H}^h\right)\right]\right\}\star\mathrm{d}\mathbf{x} \\
&+ \int_{\mathcal{Q}} \left\{\left(\hat{\mathbf{H}}.\nabla\times\mathbf{E}^h - \mathbf{H}^h.\nabla\times\hat{\mathbf{E}}\right) - \left(\hat{\mathbf{E}}.\nabla\times\mathbf{H}^h - \mathbf{E}^h.\nabla\times\hat{\mathbf{H}}\right)\right\}\boldsymbol{\Omega}
\end{aligned}
$$

By choosing weight functions equal to solution $\hat{\mathbf{U}} = \mathbf{U}^h$ and noting $a_{\mathcal{Q}}(\boldsymbol{U}^h,\hat{\boldsymbol{U}}) = 0$

$$
\int_{\partial\mathcal{Q}} \frac{1}{2}\mathbf{U}_{\mathcal{I}}^*.\mathbf{F}^{*\mathcal{I}}\star\mathrm{d}t + \mathbf{E}^*\times\mathbf{H}^*\star\mathrm{d}x - \int_{\mathcal{Q}} \mathbf{i}\,\hat{\boldsymbol{U}}\wedge\boldsymbol{R}_M^h =
$$

$$
\int_{\partial\mathcal{Q}} \frac{1}{2}[\![\mathbf{U}_{\mathcal{I}}]\!]_h.[\![\mathbf{F}^{\mathcal{I}}]\!]_h\star\mathrm{d}t + [\![\mathbf{E}]\!]_h\times[\![\mathbf{H}]\!]_h\star\mathrm{d}x
$$

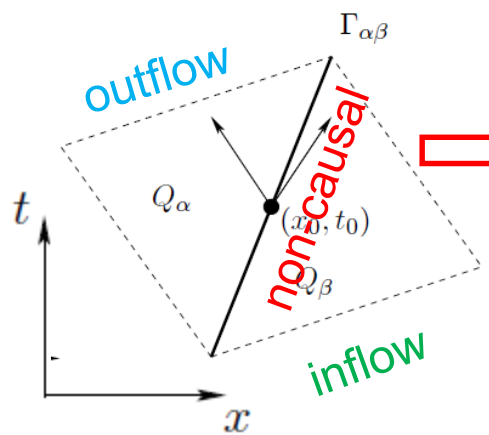
That is

$$
\boxed{\Delta_{\mathcal{D}} := \int_{\partial\mathcal{Q}} \boldsymbol{N}(\boldsymbol{U}^*) + \int_{\mathcal{Q}} \boldsymbol{R}_N = \int_{\partial\mathcal{Q}} \boldsymbol{N}([\![\boldsymbol{U}]\!]_h)}
$$

But,

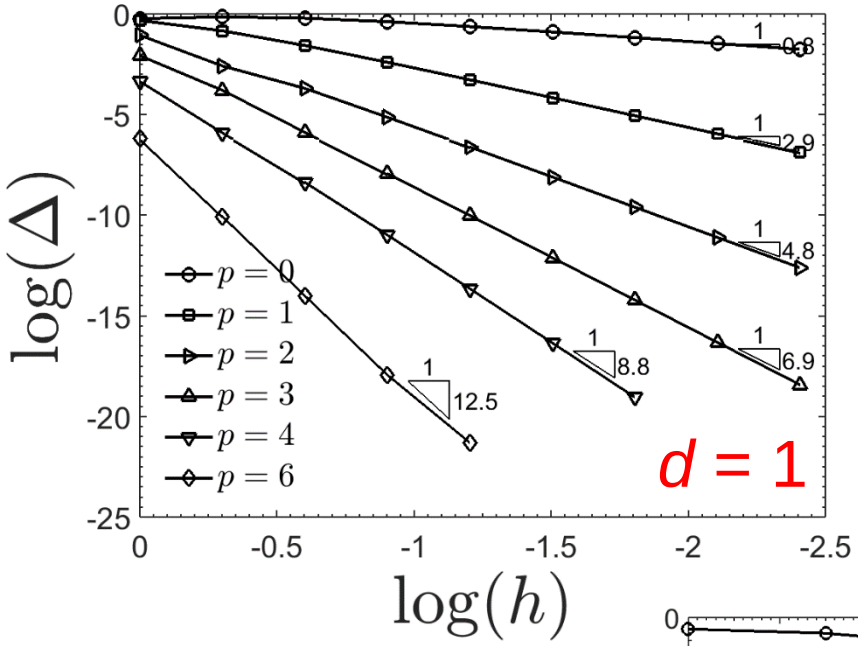
$$
\int_{\partial\mathcal{Q}} \boldsymbol{N}([\![\boldsymbol{U}]\!]_h)
$$

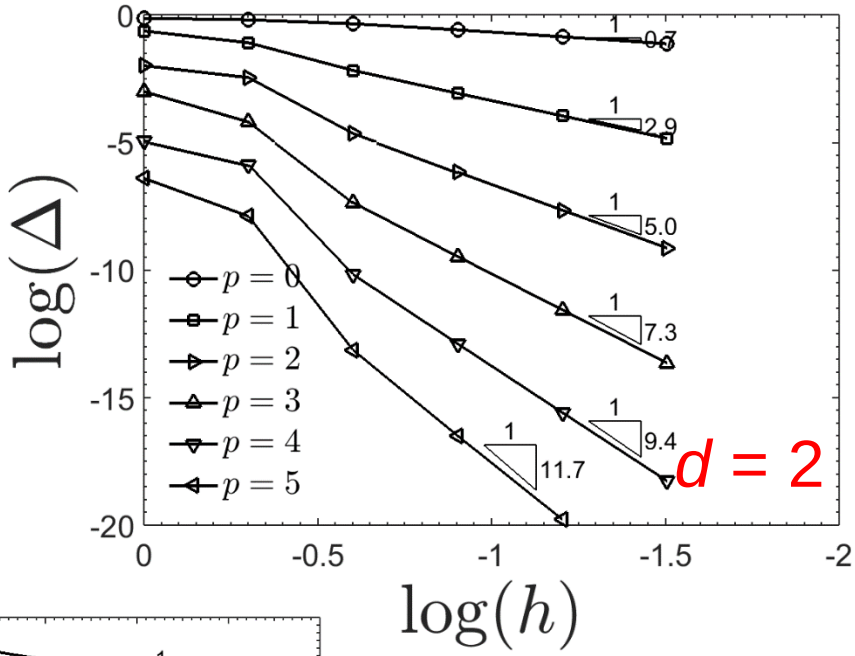
- = 0 outflow
- > 0 inflow
- > 0 non-causal (using Riemann values, *etc.*)

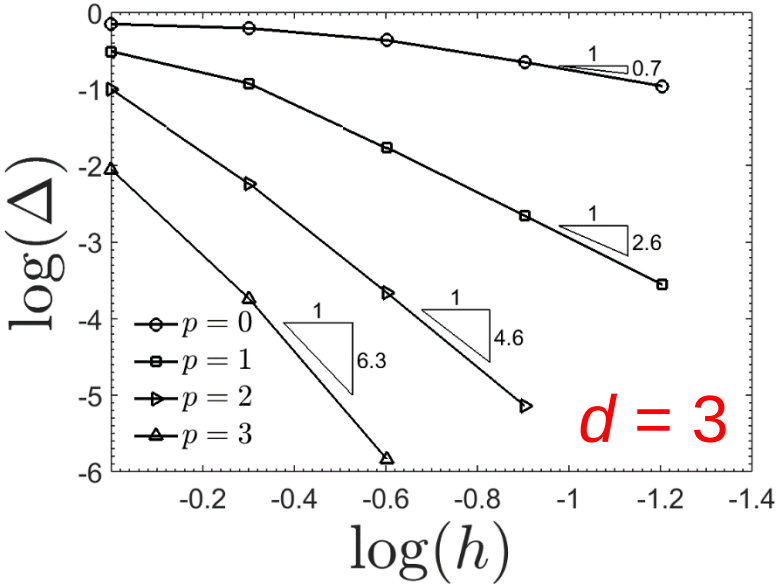


$$
\boxed{\begin{aligned}\Delta &:= \int_{\partial\mathcal{D}} \boldsymbol{N}(\boldsymbol{U}^*) + \int_{\mathcal{D}} \boldsymbol{R}_N \\ &= \sum_{\mathcal{Q}\in\mathcal{P}_h} \Delta_{\mathcal{Q}} \geq 0\end{aligned}}
$$

Convergence studies: Energy Dissipation





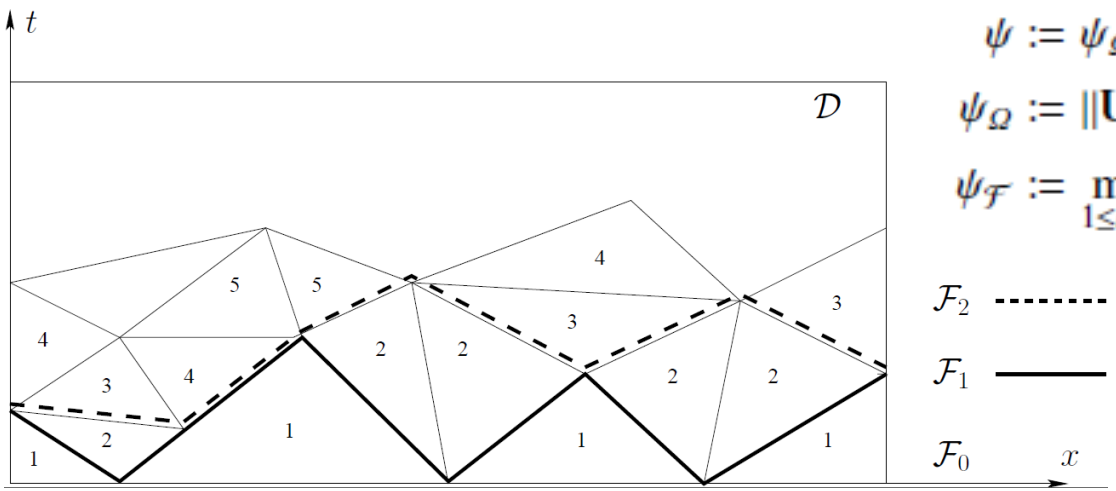


Energy dissipation:

Convergence rate:

$2p + 1$

Convergence studies: Error w.r.t. exact solution



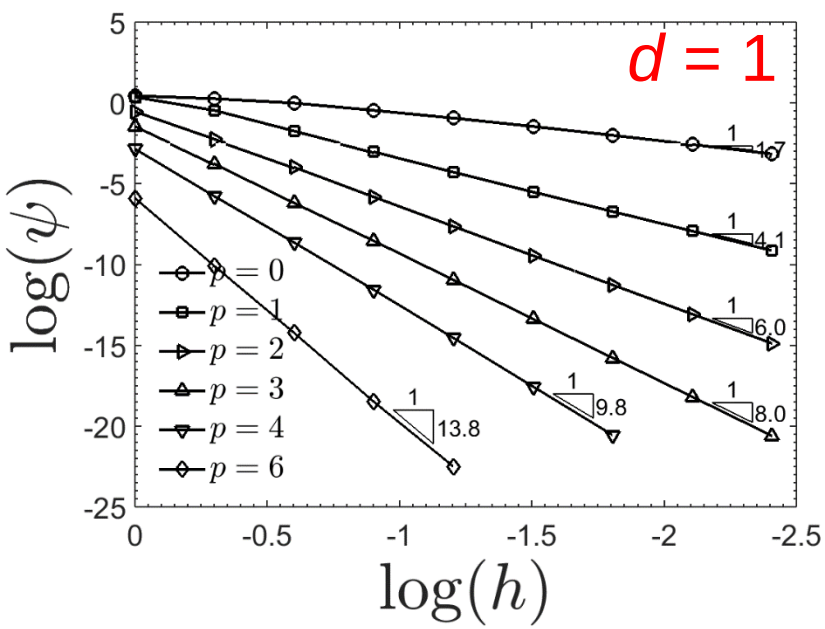
$$\psi := \psi_\Omega + \psi_\mathcal{F}, \quad \text{where}$$

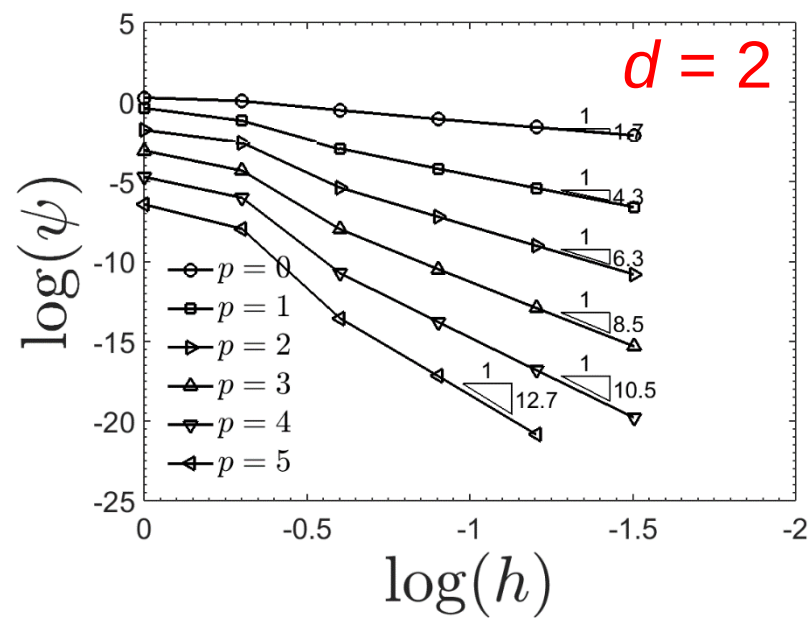
$$\psi_\Omega := \|\mathbf{U}^h - \mathbf{U}\|^2_{e,\mathcal{D}}$$ Error inside elements

$$\psi_\mathcal{F} := \max_{1\le k\le M} |\mathbf{U}^h - \mathbf{U}|^2_{e,\mathcal{F}_k}$$ Error on fronts

Convergence rate:

$2p + 2$





Other types of error:
1. Divergence errors

Balance laws exactly satisfied:

$$\begin{cases} \left(\dot{\mathbf{D}} + \boldsymbol{J}^E - \nabla \times \mathbf{H}\right) \star \mathrm{d}x &= \mathbf{0} \quad \text{Ampère's law} \\ \left(\dot{\mathbf{B}} + \boldsymbol{J}^H + \nabla \times \mathbf{E}\right) \star \mathrm{d}x &= \mathbf{0} \quad \text{Faraday law} \end{cases}$$

in balance law form:

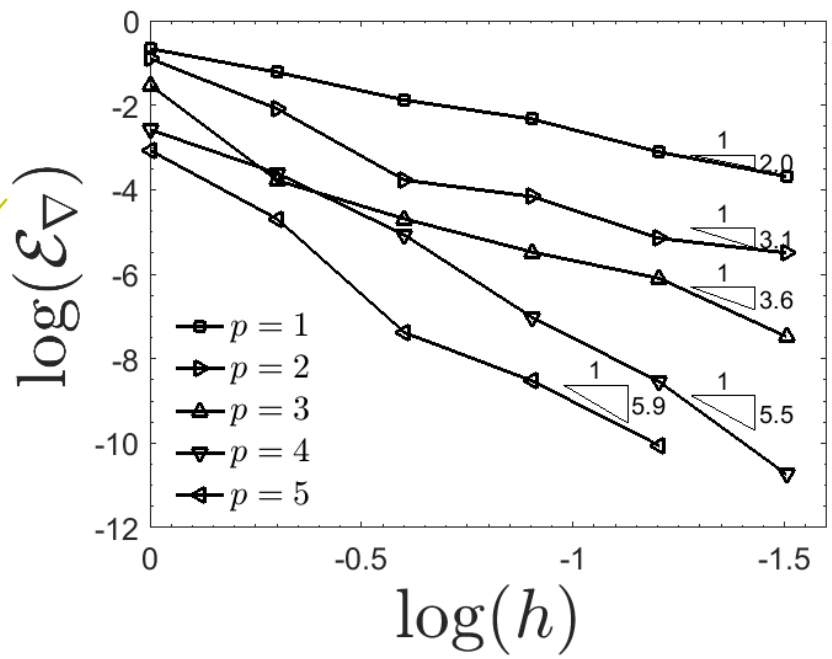
$$-\int_{\mathcal{Q}} \left\{ \boldsymbol{d}\mathbf{i}\,\hat{\boldsymbol{U}} \wedge \boldsymbol{M}^h + \mathbf{i}\,\hat{\boldsymbol{U}} \wedge \boldsymbol{R}_M^h \right\} + \int_{\partial\mathcal{Q}} \mathbf{i}\,\hat{\boldsymbol{U}} \wedge \boldsymbol{M}^* = \mathbf{0}$$

BUT divergence laws are not even weakly enforced!

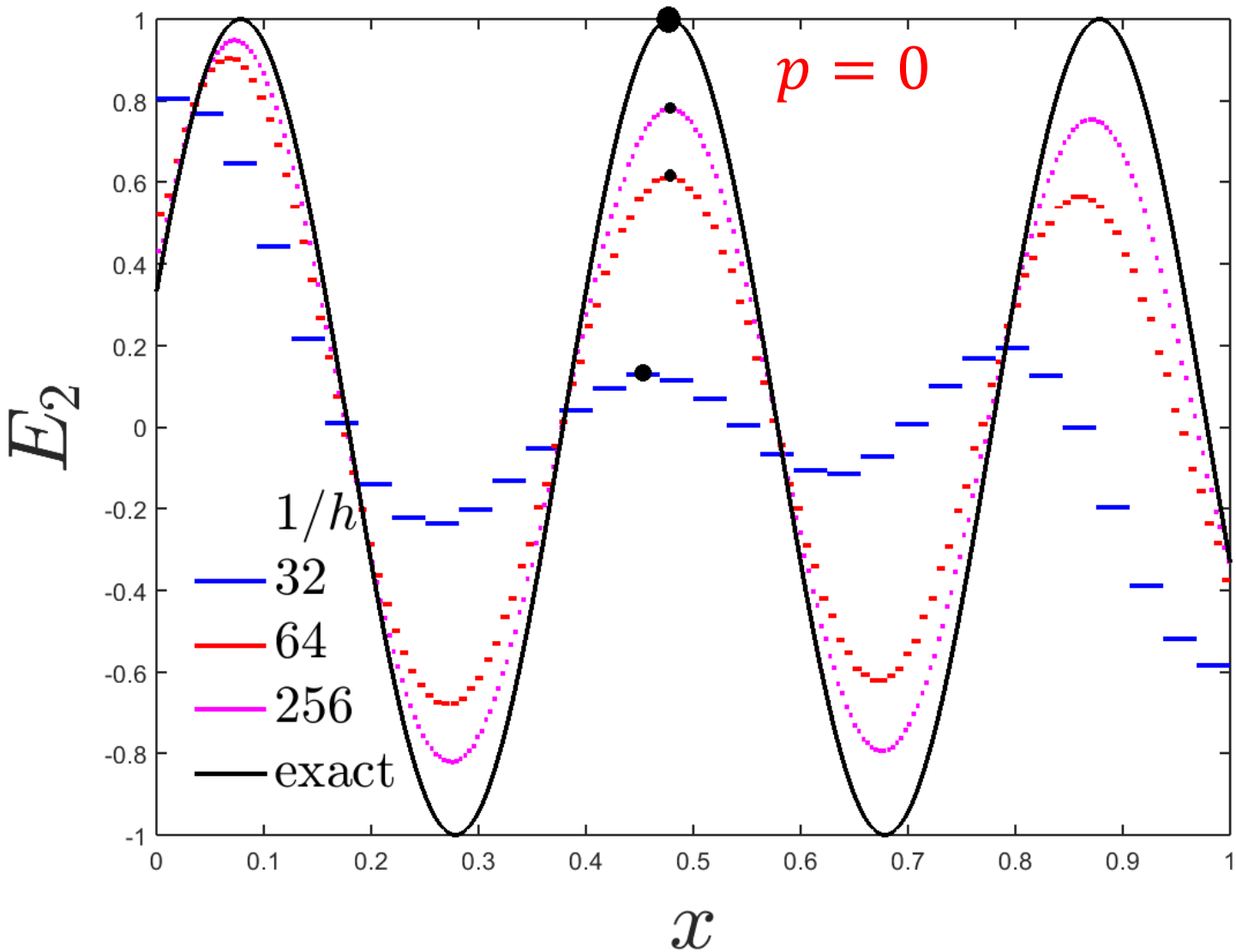
$$\begin{cases} (\nabla.\mathbf{D} - \rho^E) \star \mathrm{d}t &= \mathbf{0} \quad \text{Gauss law for electric field} \\ (\nabla.\mathbf{B} - \rho^H) \star \mathrm{d}t &= \mathbf{0} \quad \text{Gauss law for magnetic field} \end{cases}$$

Total divergence errors:
Have convergence rate of

$$p + 1$$



Other types of error:
2. Dispersion error



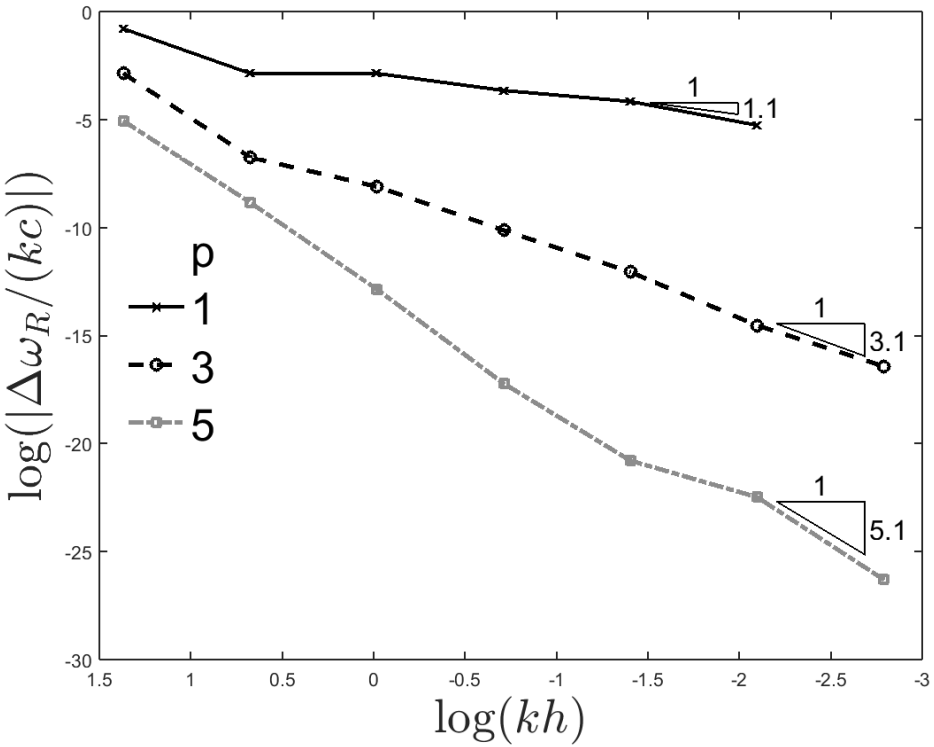
$$\mathbf{E} = \mathcal{E}\cos(\omega t - \mathbf{k}.\mathbf{x})$$

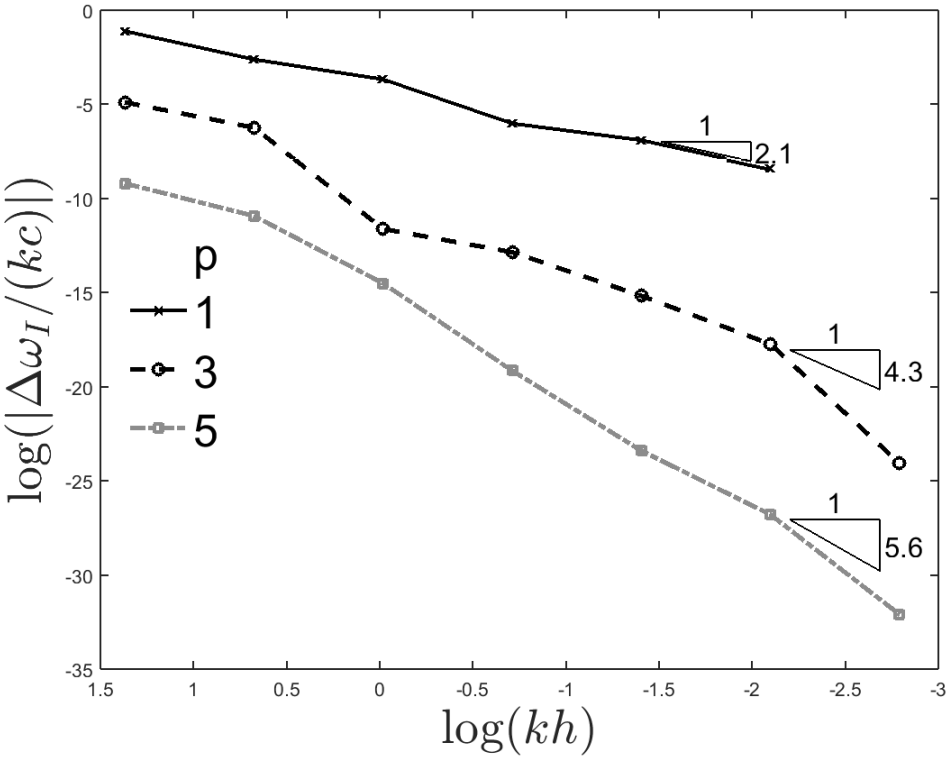
$$\mathbf{H} = \mathcal{H}\cos(\omega t - \mathbf{k}.\mathbf{x})$$

$$\Delta\omega_R := \omega_R^h - \omega_R$$

$$\Delta\omega_I := \omega_I^h - \omega_I$$

Other types of error:
2. Dispersion error





$$\Delta\omega_R := \omega_R^h - \omega_R$$

$$\Delta\omega_I := \omega_I^h - \omega_I$$

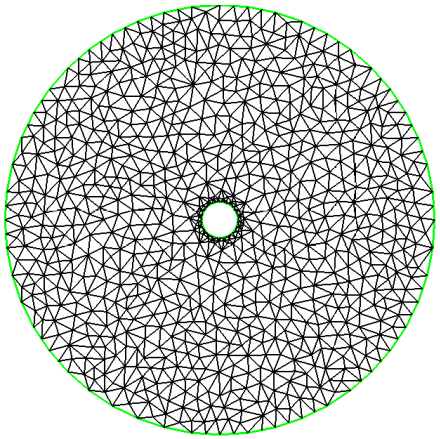
Dispersion error:
Convergence rate (odd *p*):

$$p$$

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

$$p + 1$$

2D scattering problem / meshing in spacetime

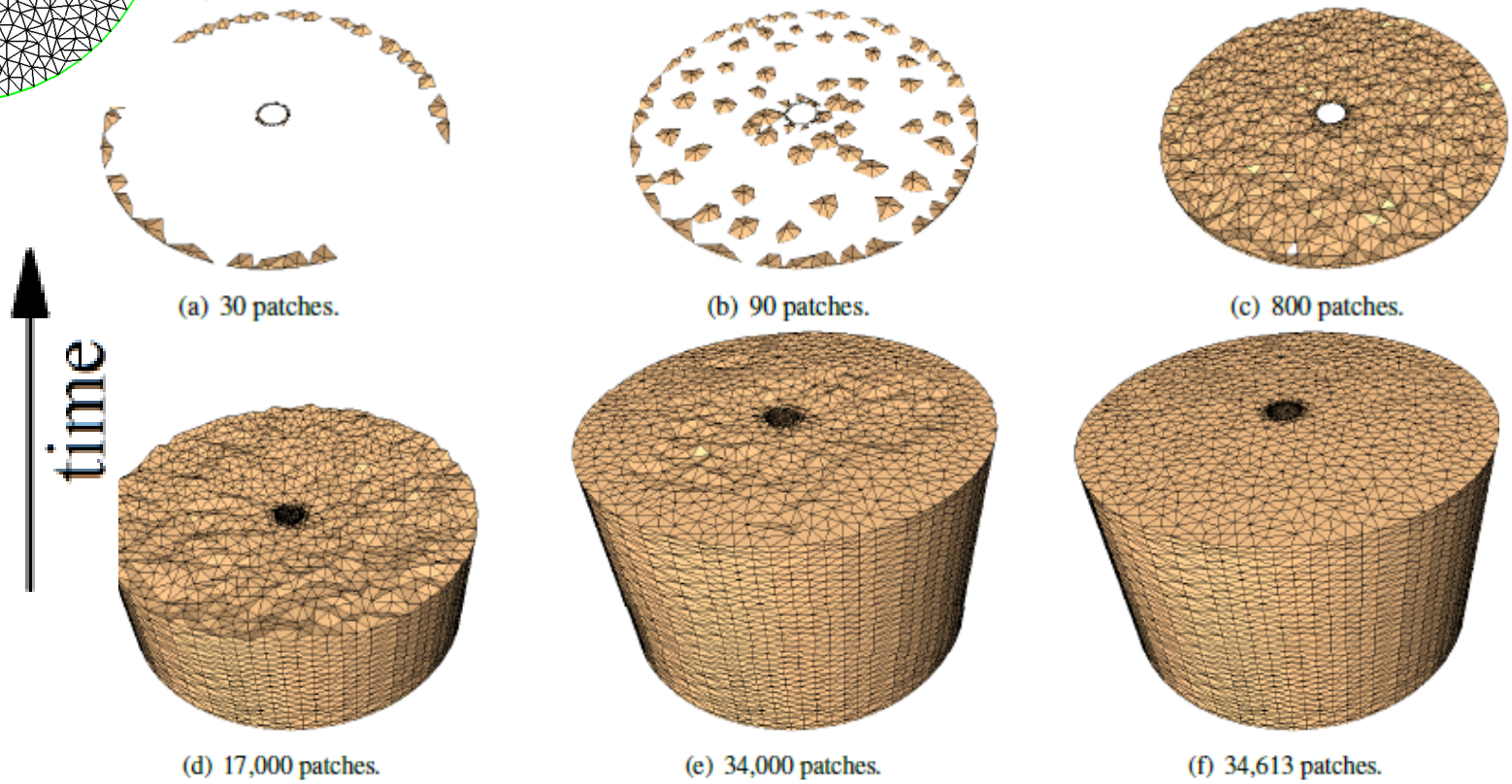


Initial mesh

Transverse Electric (TE) Initial conditions

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

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

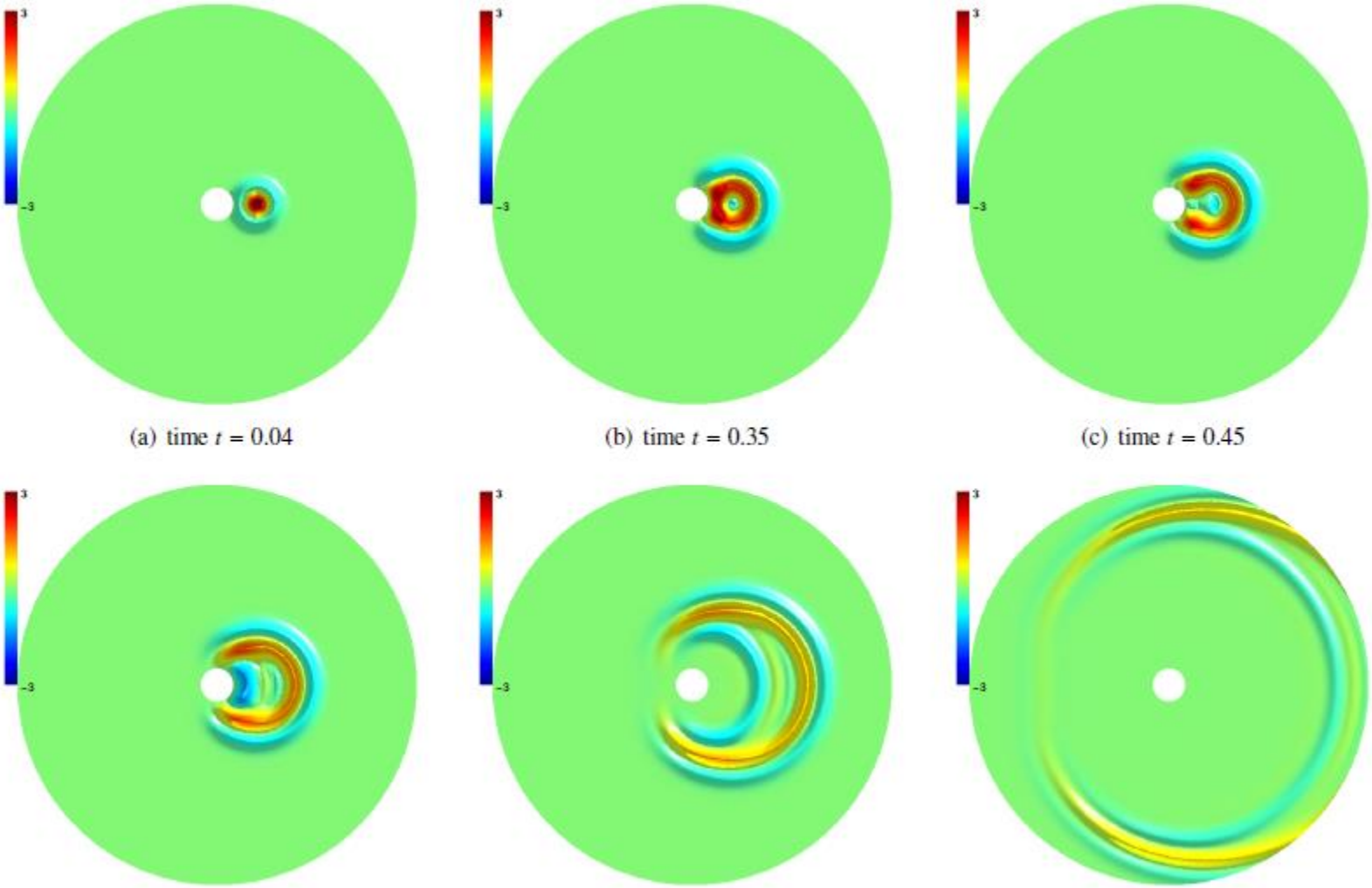


(a) 30 patches. (b) 90 patches. (c) 800 patches.

(d) 17,000 patches. (e) 34,000 patches. (f) 34,613 patches.

Space time meshes

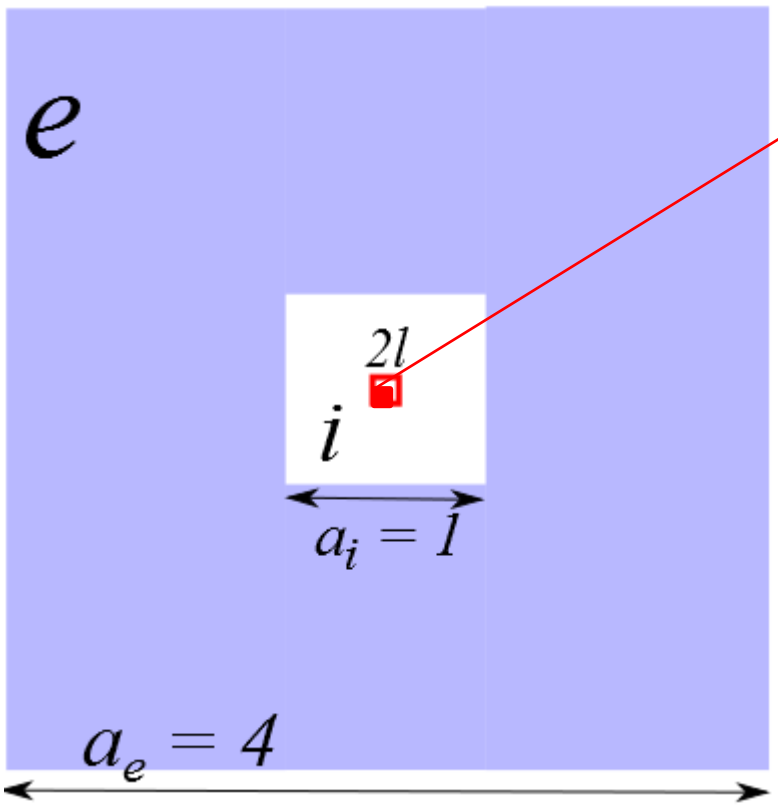
2D scattering problem / solution visualization



(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 $t = 2.70$

2D scattering problem / Nonadaptive meshing



Transverse Magnetic (TM) formulation

Initial condition:

$$H_z = \cos(\frac{\pi}{2}\frac{x}{d_x})\cos(\frac{\pi}{2}\frac{y}{d_y})$$

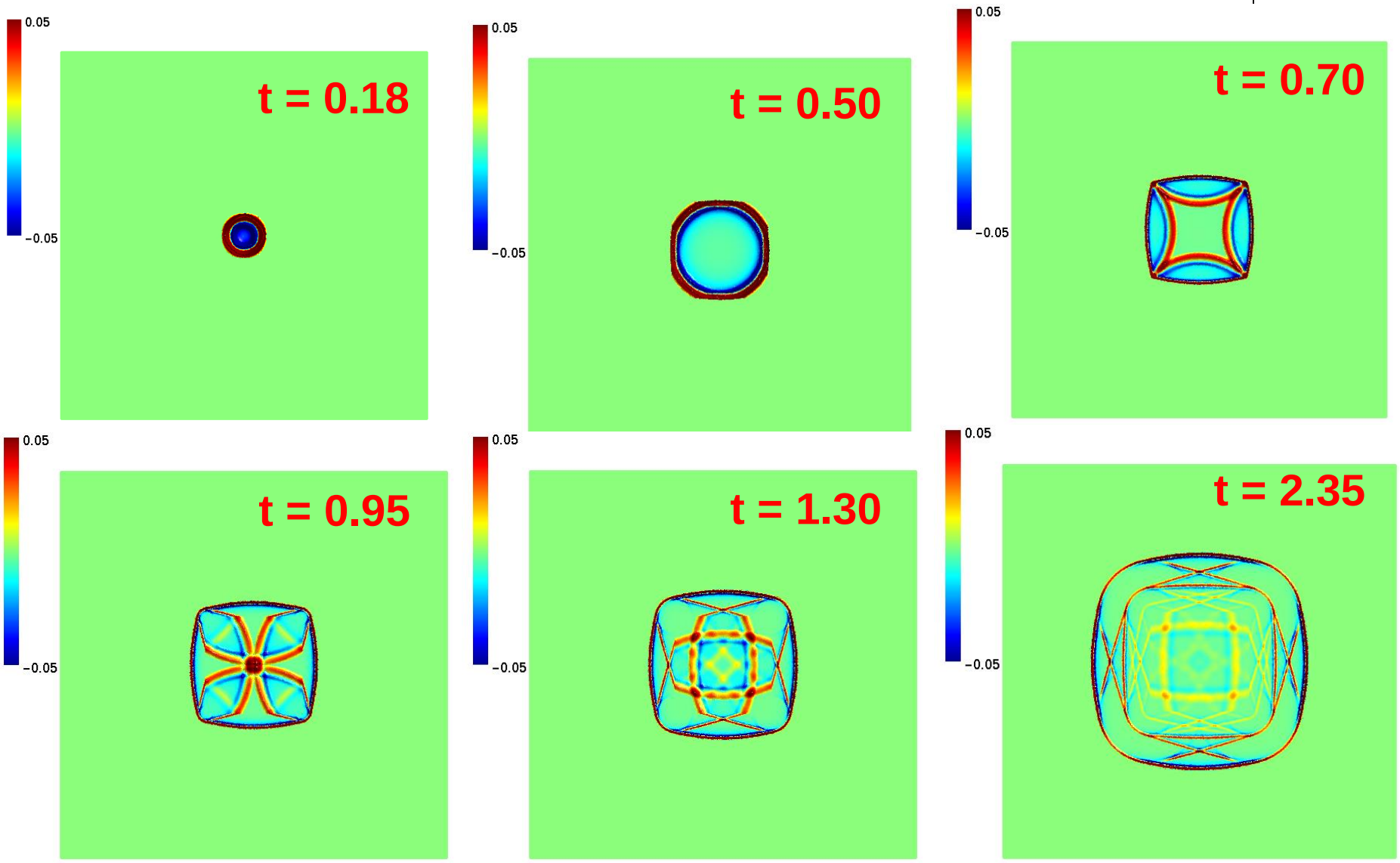
Electric permittivity:

$$\varepsilon_i = 1$$
$$\varepsilon_o = 10$$

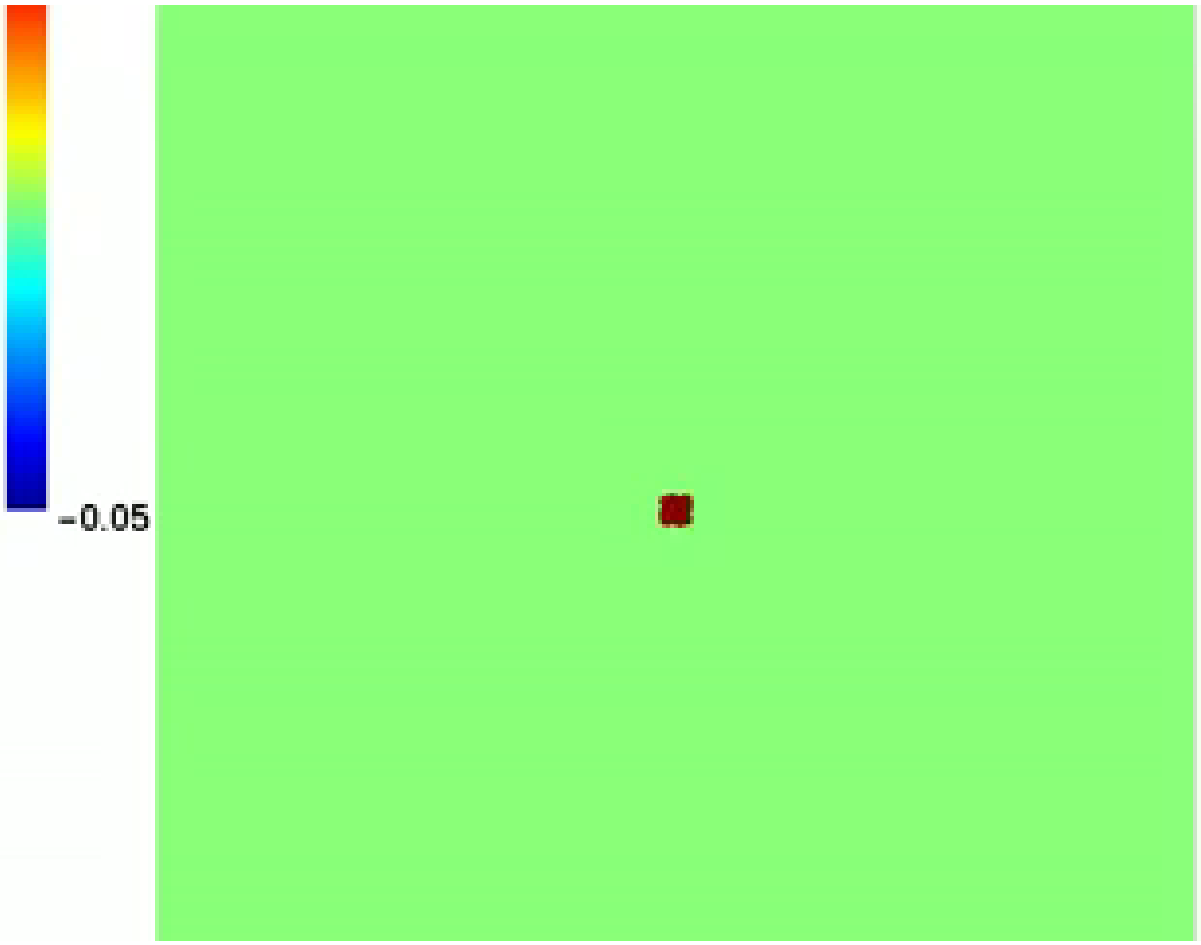
Magnetic permeability:

$$\mu = 1$$

2D scattering problem adaptive meshing

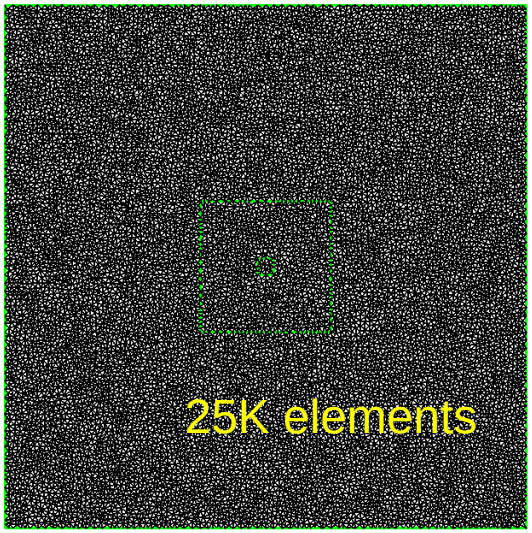


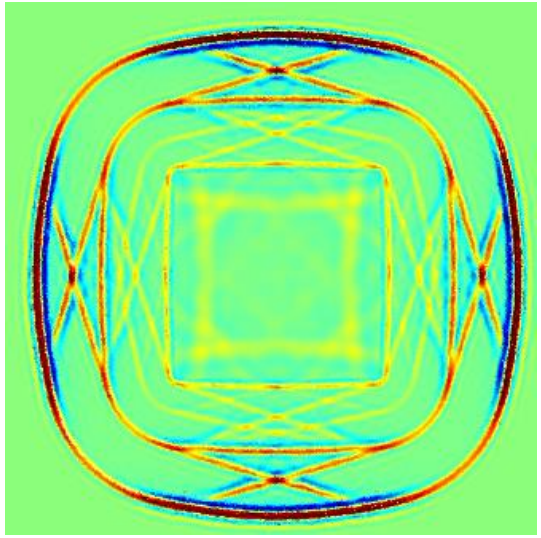
2D scattering problem adaptive meshing



Comparison of Adaptive / nonadaptive schemes

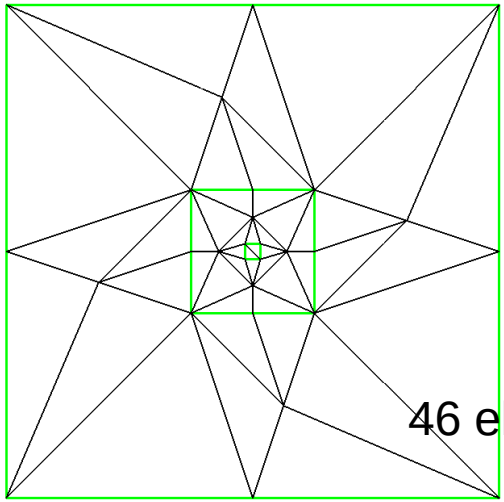
Nonadaptive

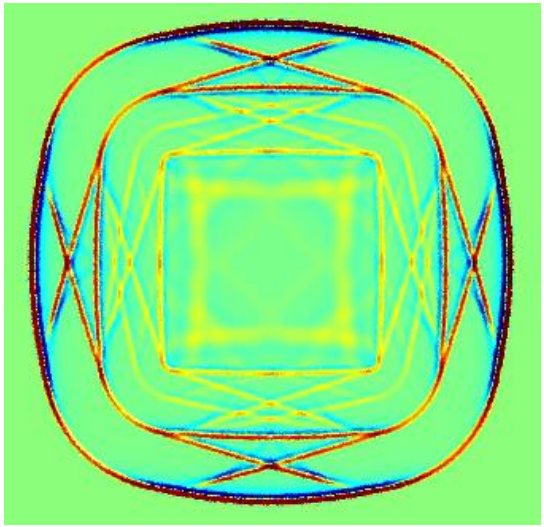




Adaptive

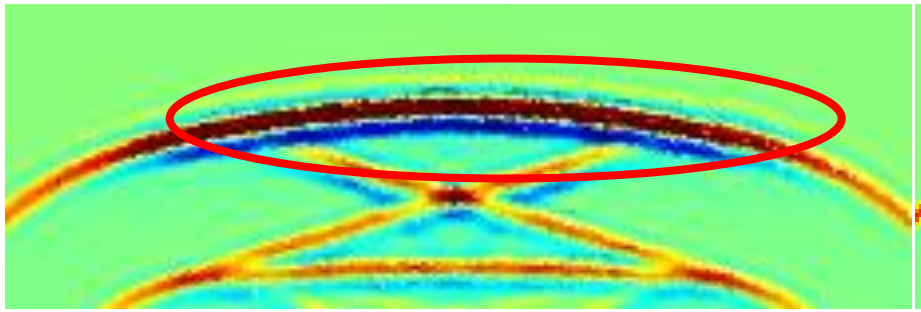
Initial spatial Mesh





Comparison of Adaptive / nonadaptive schemes

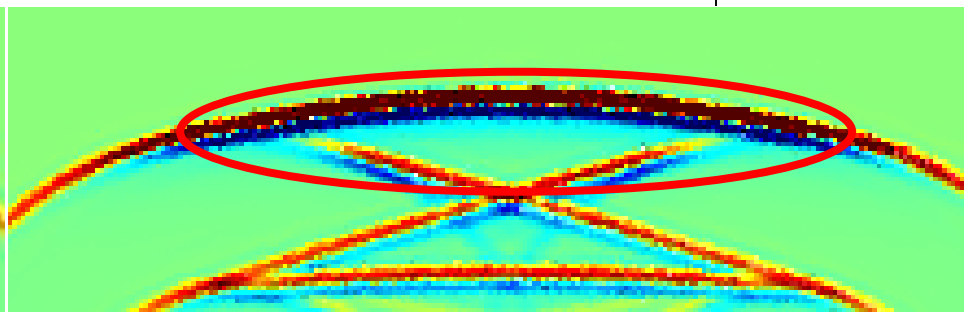
Nonadaptive



93 Hours

Numerical dissipation **$8x10^{-4}$**

Adaptive



72 Hours

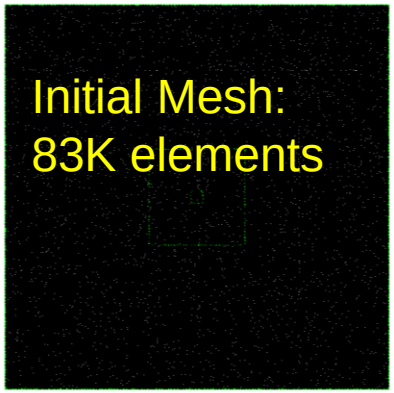
Numerical dissipation **$1x10^{-4}$**

Even finer nonadaptive simulation

> 500 Hours

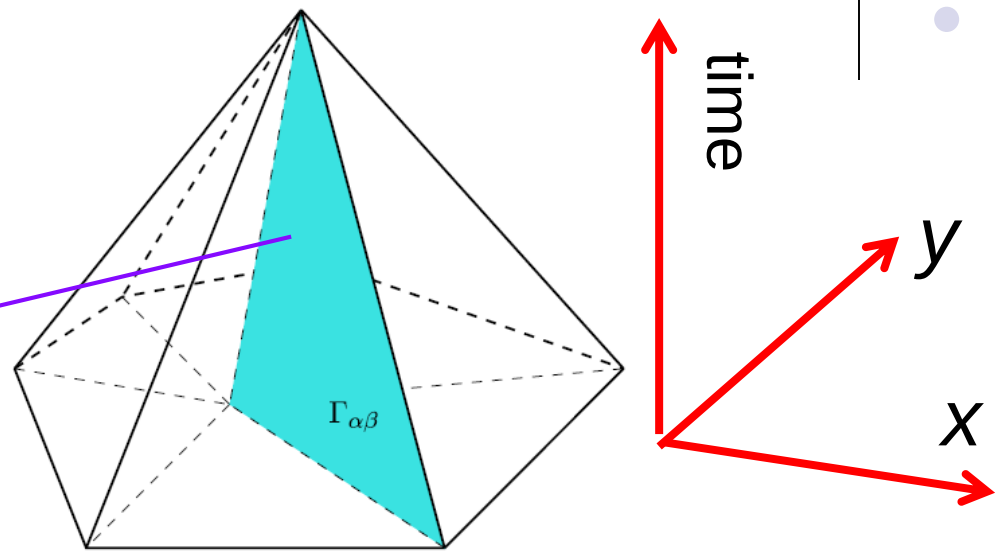
Numerical dissipation **$2x10^{-4}$**

(still larger than adaptive one)



Effect of target values
Riemann versus Average fluxes

Nontrivial target solutions are needed on interior (non-causal) facets of patches



Riemann fluxes (R)

$$\mathbf{E}^* = \frac{(Y\mathbf{E} - \mathbf{n}\times\mathbf{H})^- + (Y\mathbf{E} + \mathbf{n}\times\mathbf{H})^+}{Y^- + Y^+}$$

$$\mathbf{H}^* = \frac{(Z\mathbf{H} + \mathbf{n}\times\mathbf{E})^- + (Z\mathbf{H} - \mathbf{n}\times\mathbf{E})^+}{Z^- + Z^+}$$

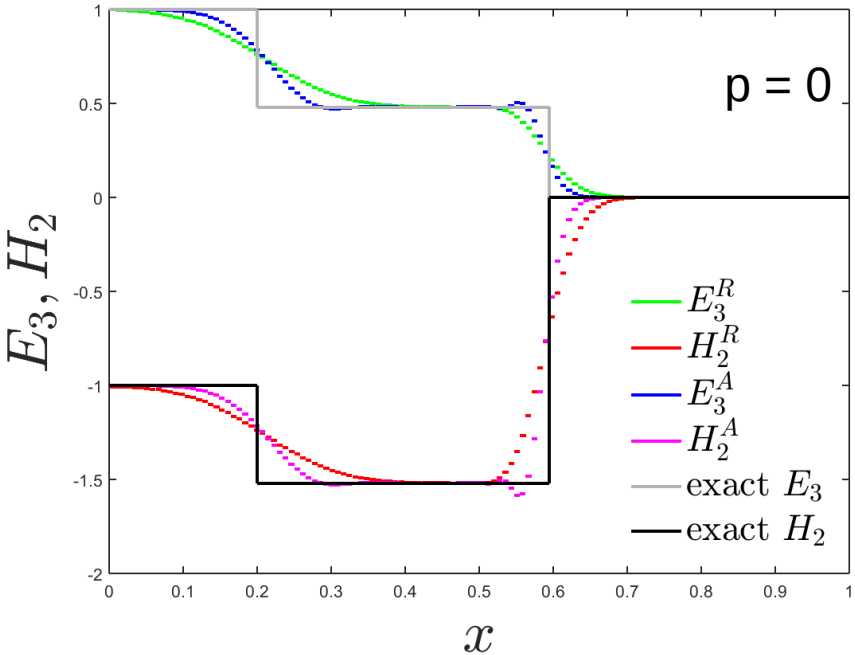
$$\begin{cases} Z = \sqrt{\frac{\mu}{\epsilon}} & \text{impedance} \\ Y = \frac{1}{Z} & \text{admittance} \end{cases}$$

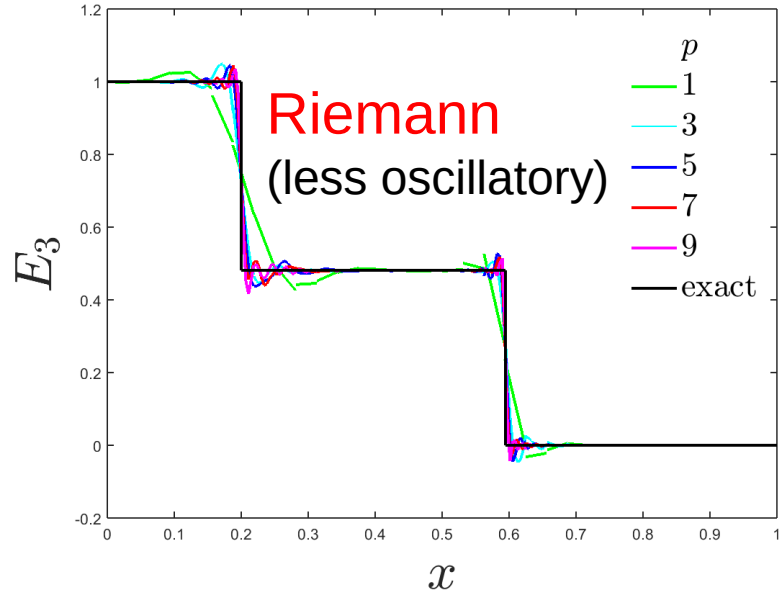
Average fluxes (A)

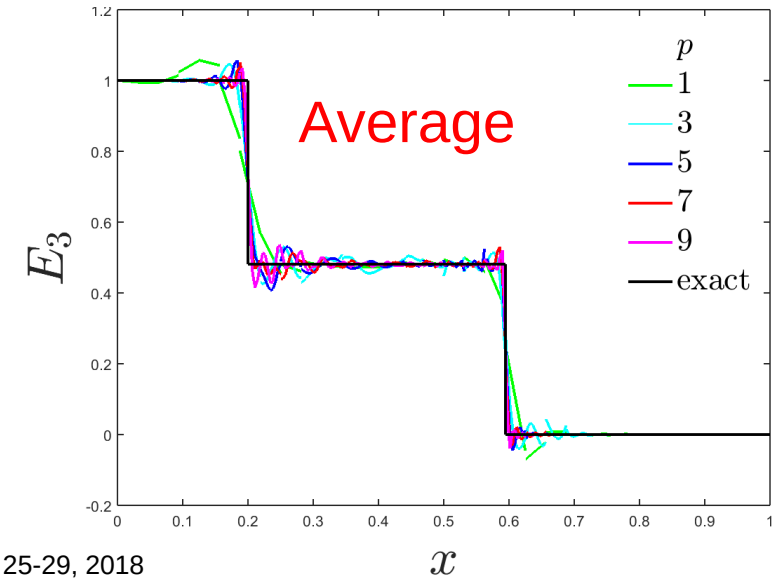
$$\mathbf{E}^* = \frac{\mathbf{E}^- + \mathbf{E}^+}{2}$$

$$\mathbf{H}^* = \frac{\mathbf{H}^- + \mathbf{H}^+}{2}$$

Comparison of Riemann and average fluxes







Riemann solutions:

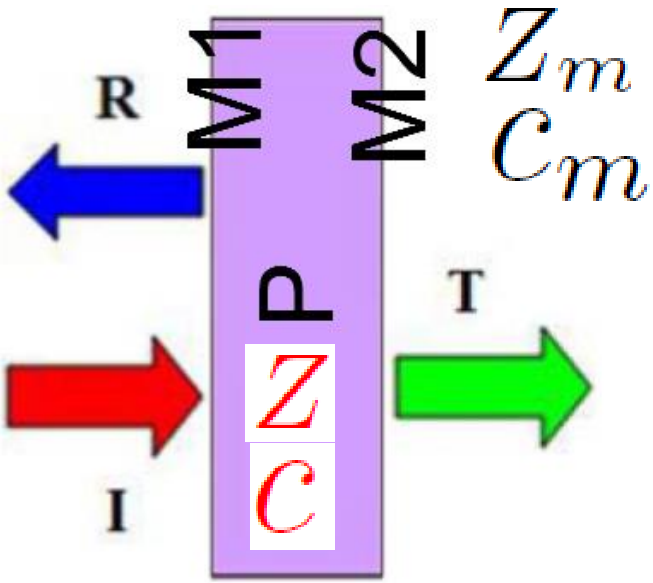
- More dispersive (especially for low p)
- Less oscillatory

Material 1 Material 2

Applied electric field

3. Dispersive media

S-parameters for a slab



Material Properties

$$(\epsilon, \mu)$$

$$\Downarrow$$

$$\begin{cases} Z = \sqrt{\frac{\mu}{\epsilon}} & \text{impedance} \\ c = \frac{1}{\sqrt{\mu\epsilon}} & \text{wave speed} \end{cases}$$

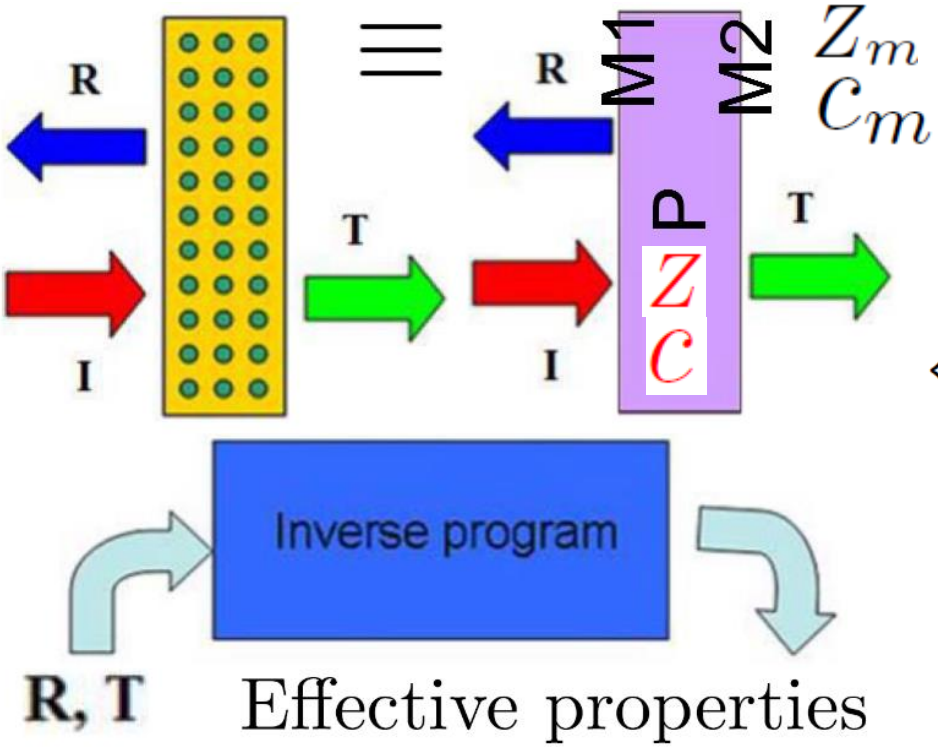
$$\Downarrow$$

Transmission / reflection coefficients

$$\begin{cases} \rho = \frac{Z - Z_m}{Z + Z_m} \\ k = \omega c \end{cases}$$

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

Unit cell to dispersive response (S-parameters) retrieval method



Inverse Problem

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

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

$\Downarrow$

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

$\Downarrow$

Elastodynamics

$$\begin{cases} C = Zc \\ \rho = \frac{Z}{c} \end{cases}$$

Electromagnetics

$$\begin{cases} \epsilon = \frac{1}{Zc} \\ \mu = \frac{Z}{c} \end{cases}$$

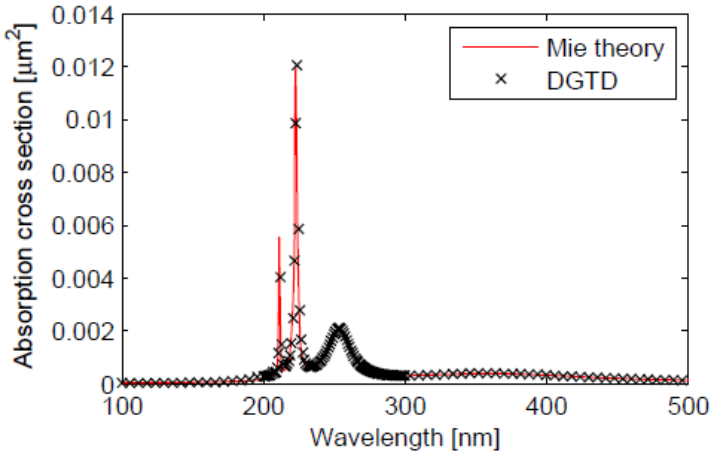
Time Domain vs. Frequency Domain

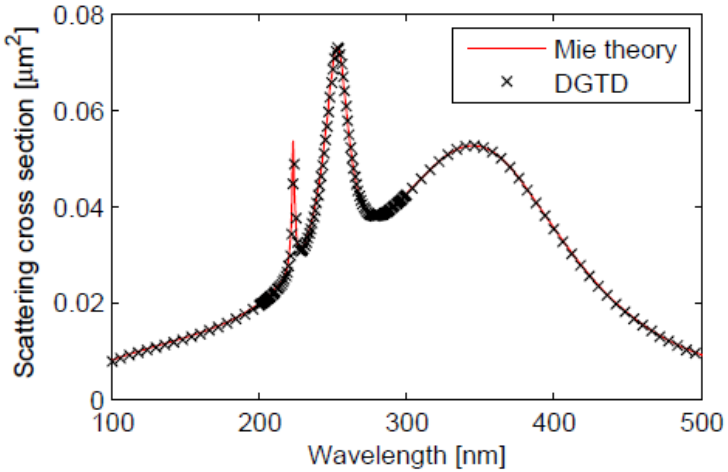
- Time Domain (TD) vs. Frequency Domain (FD) solvers:
  - Transient problems ⇨ TD
  - Steady state and frequency response:
    - Small problem size ⇨ FD
    - **Large problem size ⇨**
      TD (TDDG ≈ $\mathcal{O}(N)$ FD = $\mathcal{O}(N^{\alpha})$, $\alpha \geq 1.5$
  - Material nonlinearities are better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

d	FD	TD
2	$\mathcal{O}(\omega_M^3)$	$\mathcal{O}(\omega_M^3)$
3	$\mathcal{O}(\omega_M^4)$	$\mathcal{O}(\omega_M^6)$

frequency spectrum $[\omega_m \ \omega_M]$

Busch:2009

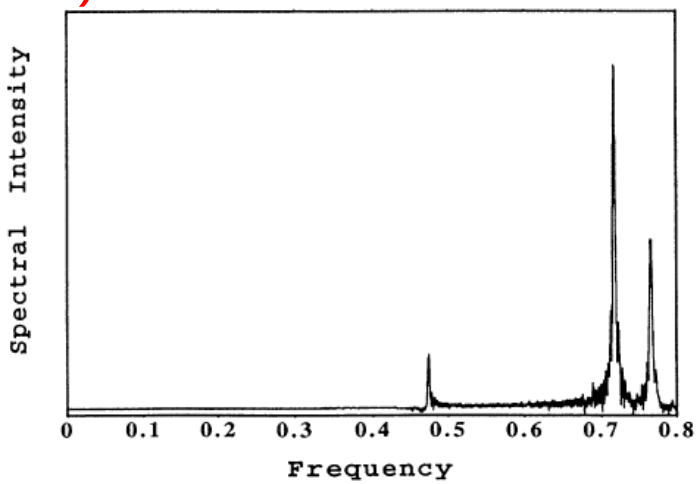


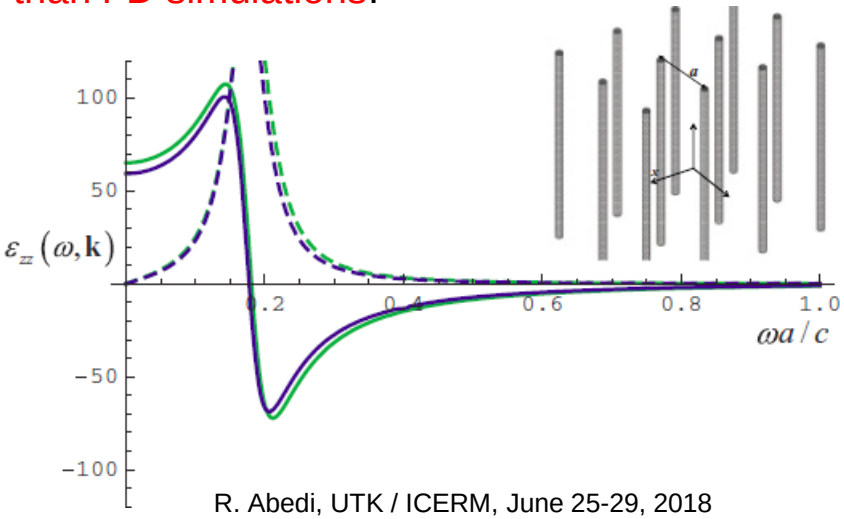


Time Domain vs. Frequency Domain

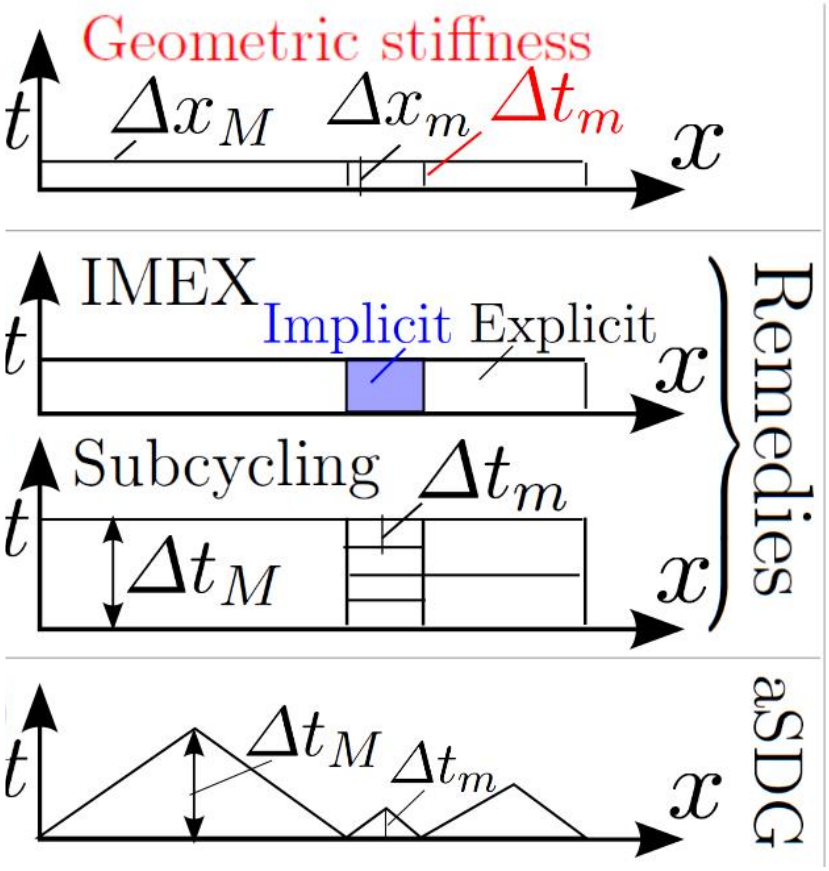
- Time Domain (TD) vs. Frequency Domain (FD) solvers:
  - Eigenmode analysis: Time domain

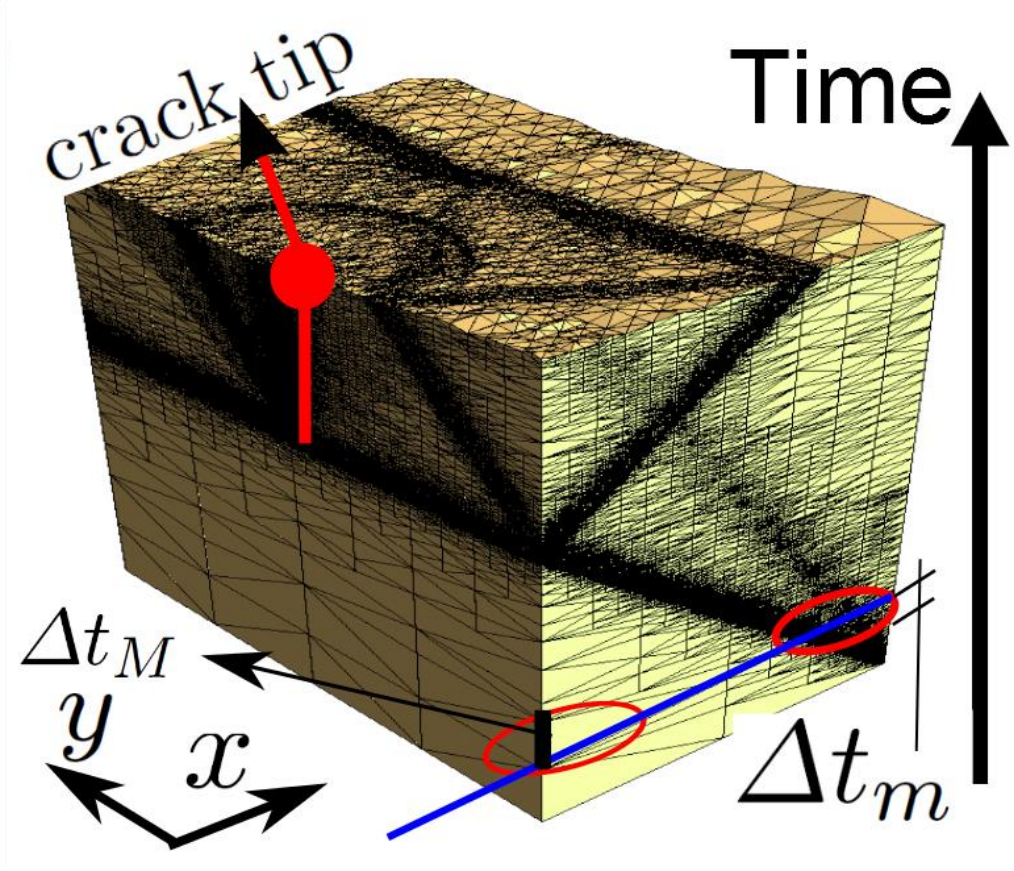
    TD: $\mathcal{O}(N)$ FD: $\mathcal{O}(N^3)$
    - C.T. Chan, Q.L. Yu, and K.M. Ho, Order-N spectral method for electromagnetic waves, PHYSICAL REVIEW B VOLUME 51, 23, 1995
  - Homogenization of dispersive media:
    - Mario G. Silveirinha, PHYSICAL REVIEW B 83, 165104, Time domain homogenization of metamaterials, 2011
  - 3 to 40 times faster than FD simulations.





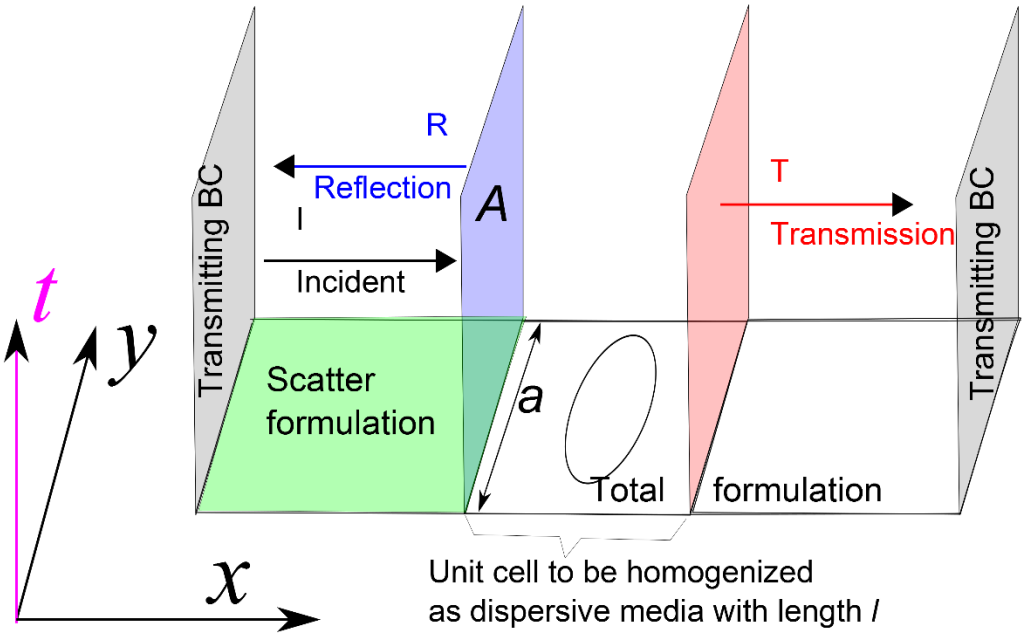
Advantages of SDG method & adaptivity in spacetime





Refinement ratio of 10^4 increases the maximum frequency ω_M captured by 4 order of magnitudes!

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

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

$$\tilde{t} = t - \frac{x}{c} - t_0$$

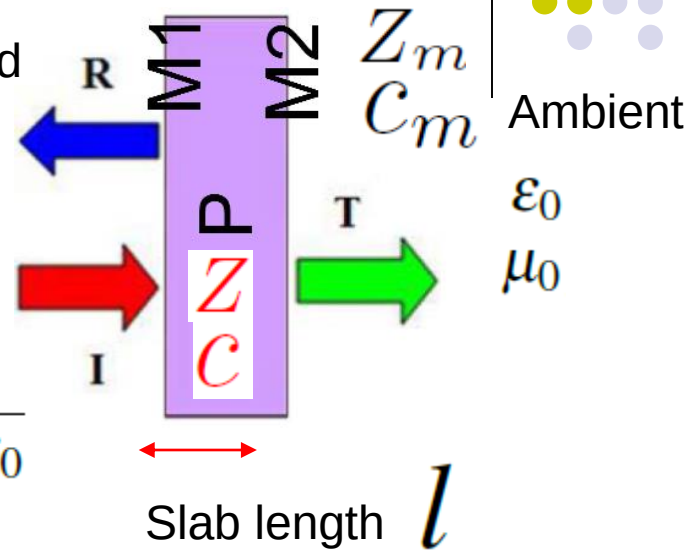
After Fourier transform

$$\bar{r}(\omega) = \frac{\bar{R}(\omega)}{\bar{I}(\omega)}, \quad \bar{t}(\omega) = \frac{\bar{R}(\omega)}{\bar{I}(\omega)}$$

Inverse problem

1. Reflection & Transmission coefficients are computed

$$\bar{r}(\omega) = \frac{\bar{R}(\omega)}{\bar{I}(\omega)}, \quad \bar{t}(\omega) = \frac{\bar{R}(\omega)}{\bar{I}(\omega)}$$



2. Inverse Problem:
Given r & t

$$r = \rho \frac{z^2 - 1}{z^2 - \rho^2}, \quad t = z.\frac{1 - \rho^2}{z^2 - \rho^2}$$

$$z = e^{jkl} \quad \rho = (Z - Z_0)/(Z + Z_0) \quad Z_0 = \sqrt{\mu_0/\varepsilon_0}$$

Find Z (Impedance) and k (wavenumber)

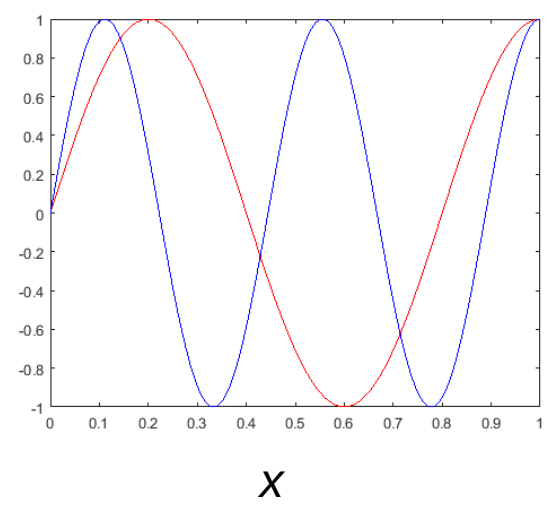
$$Z = Z_0 \sqrt{\frac{(r+1)^2 - t^2}{(r-1)^2 - t^2}}$$

Z is uniquely determined

z is uniquely determined **BUT NOT** k

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

$$\boxed{z = e^{jkl}}$$



3. Once Z and k are knowns $\Rightarrow$
Compute effective material properties

$$\varepsilon = \frac{k}{Z\omega}, \quad \mu = \frac{kZ}{\omega}$$

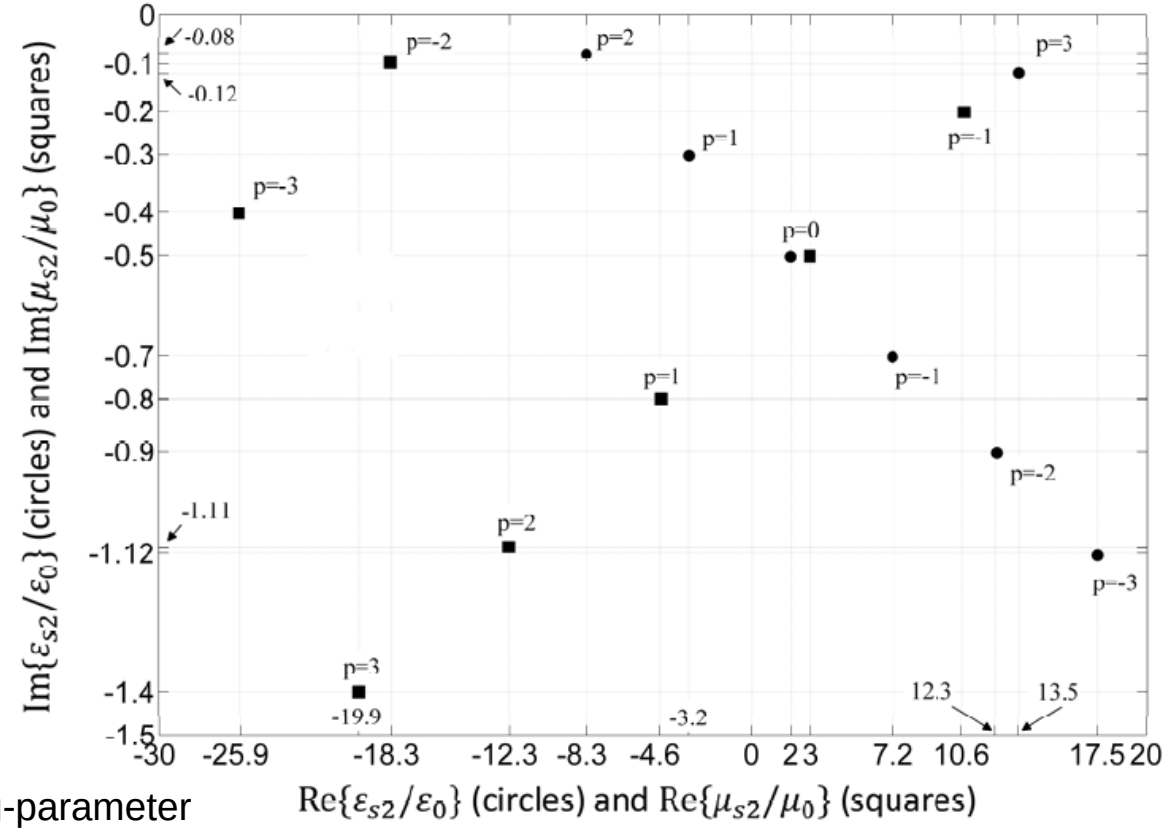
Non-uniqueness

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

$$lk_R \mathrel{+}= 2p\pi$$

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

$$\phi := \theta + 2p\pi$$



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

Addressing: Non-uniqueness

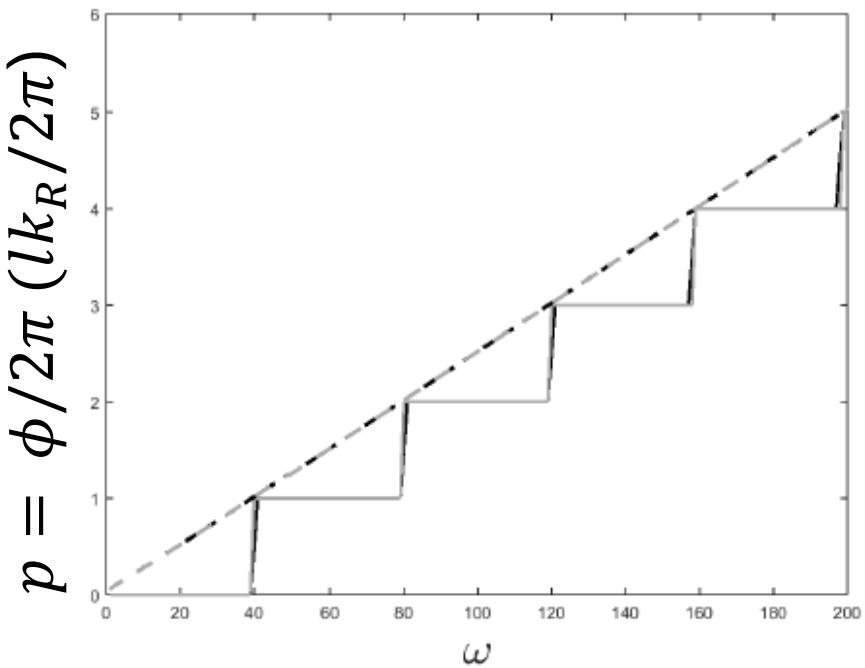
Observation 1: Use continuity of k as ω increases.

As $\omega \to 0 \;\Rightarrow\; k \to 0$

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

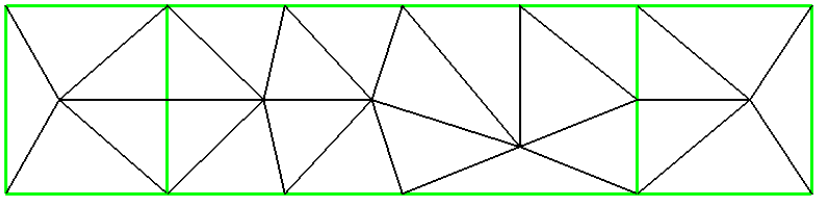
Starts from low frequency where p = 0 and ω increases

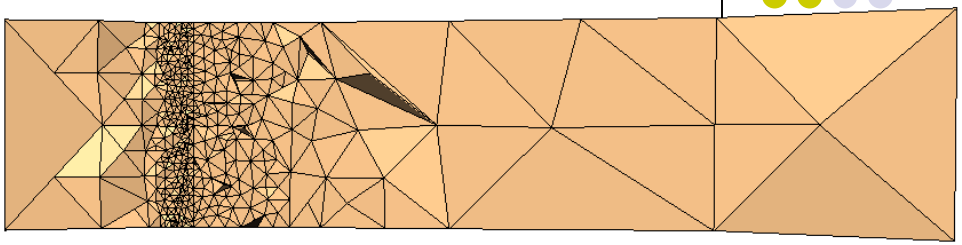
$$\phi := \theta + 2p\pi$$



Test problem:
Retrieval method for solid slab

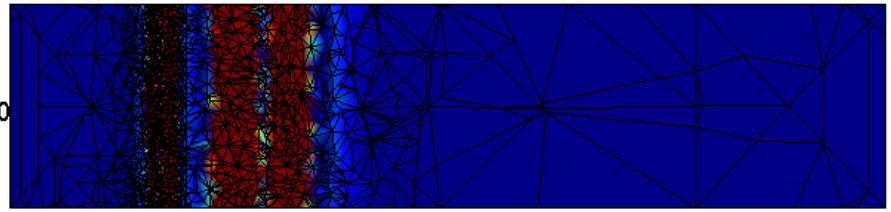
Initial space mesh

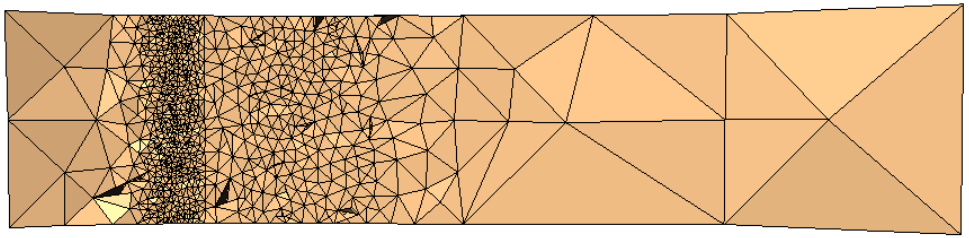


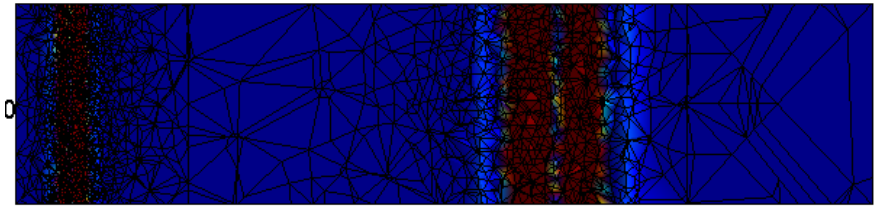


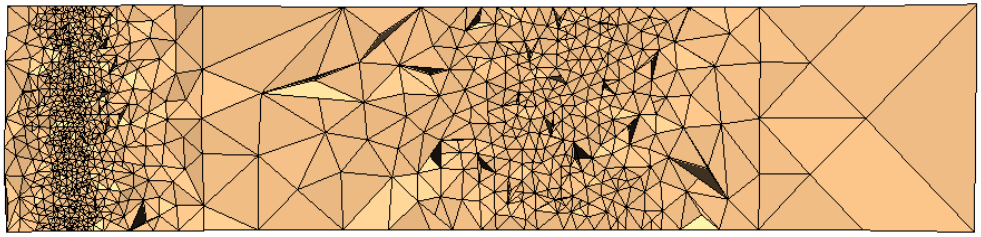
$\varepsilon = 1, \mu = 1$ $\varepsilon = 0.1, \mu = 1$ $\varepsilon = 1, \mu = 1$

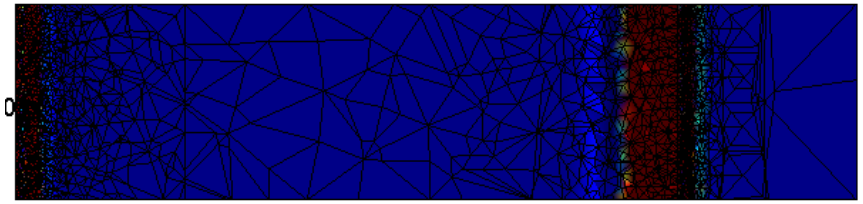
Movie: Solution

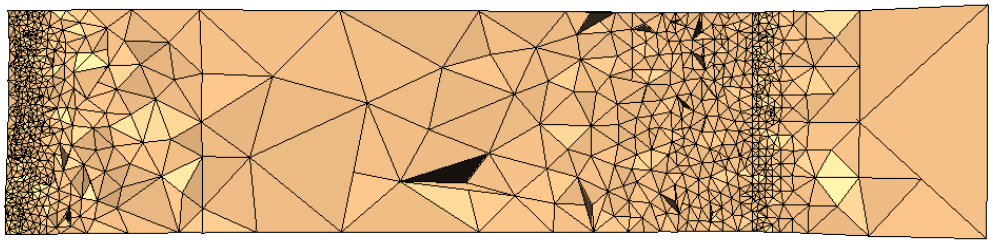




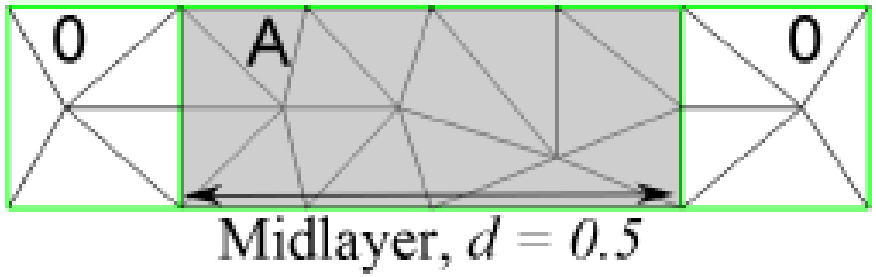




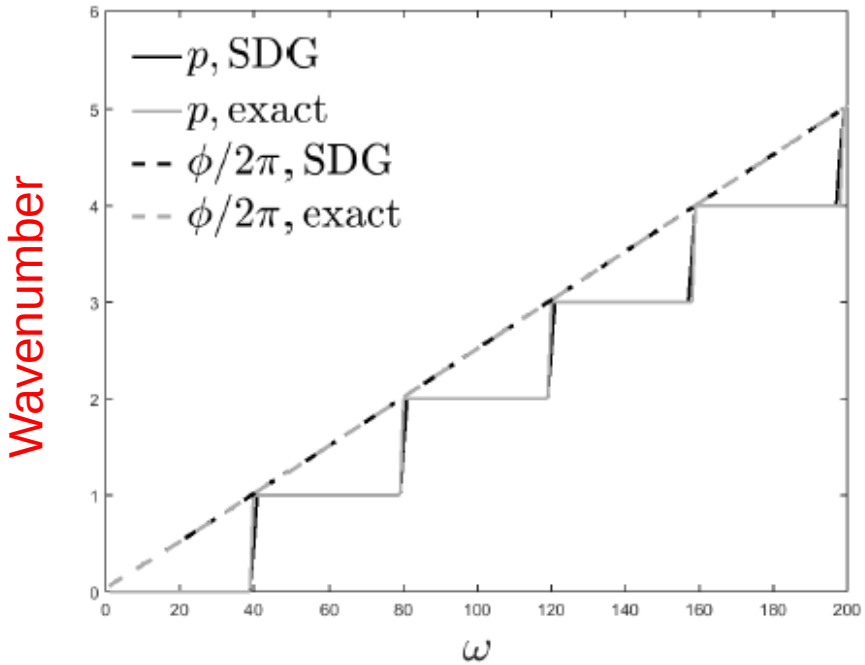


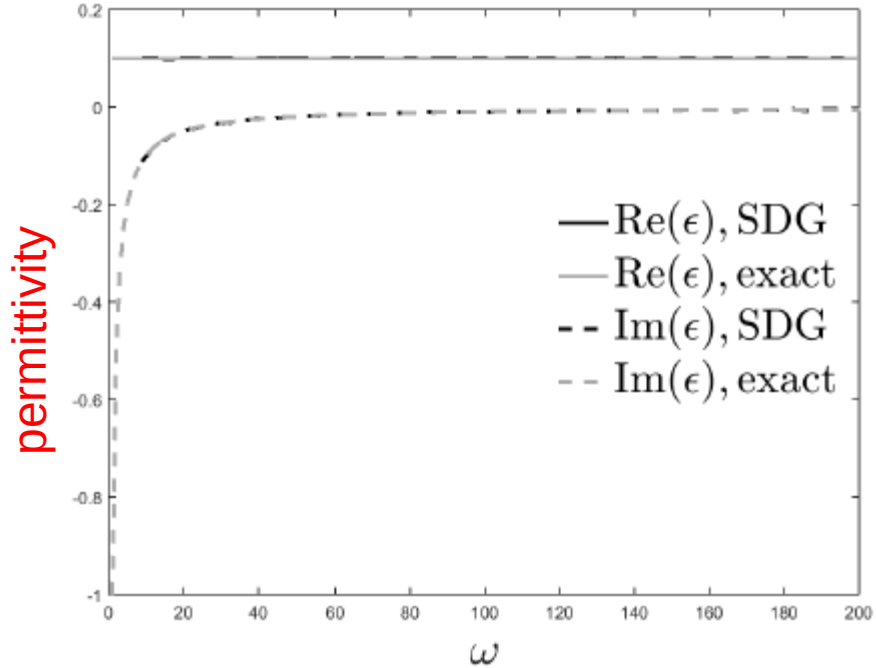


Ambiguity in wave number in parameter retrieval method



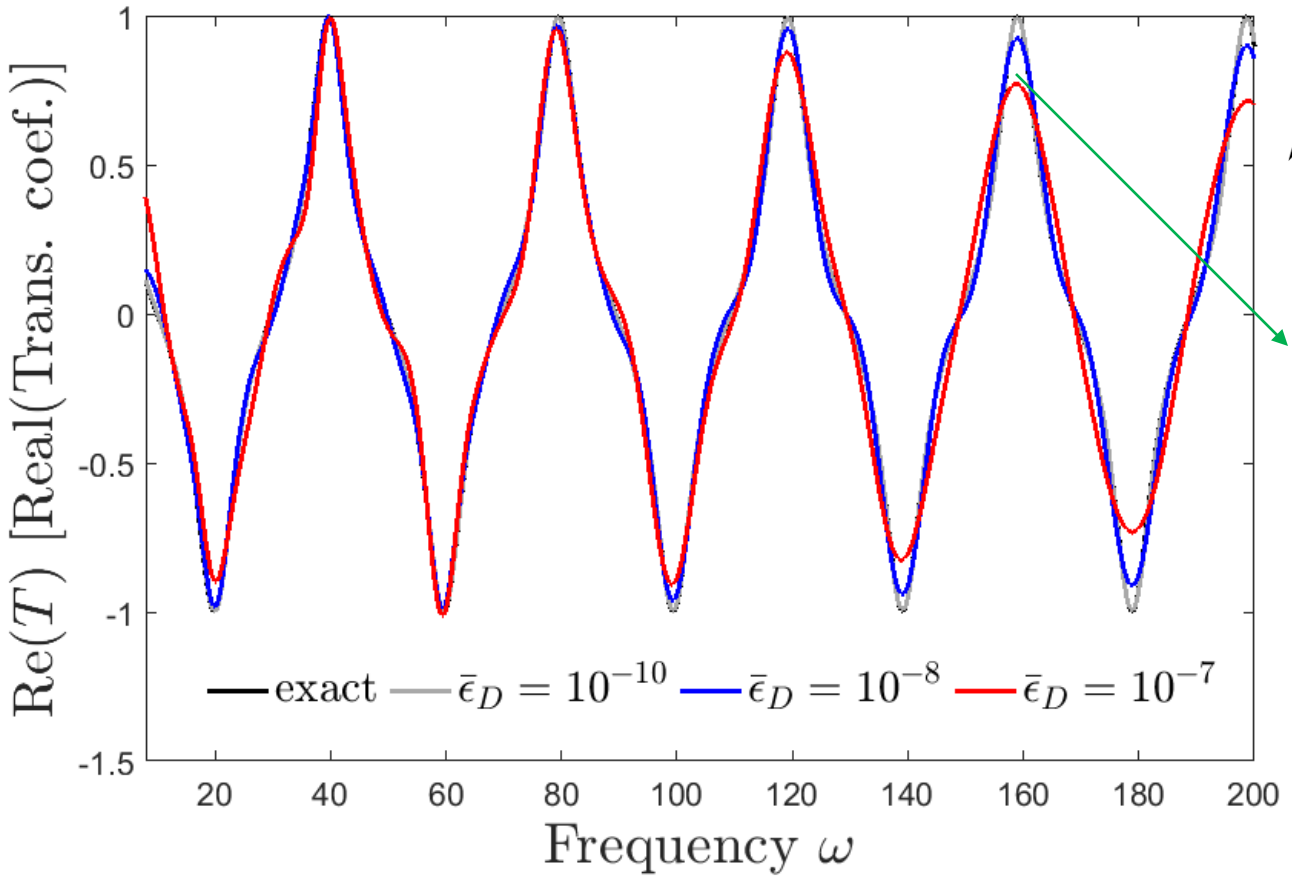
Mid-layer is conductive

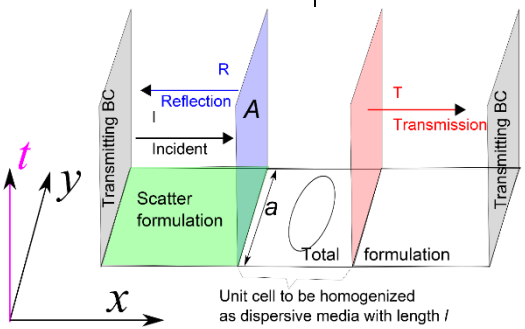




Integer p and scaled phase $\phi/2\pi$ obtained in inverse parameter retrieval stage.

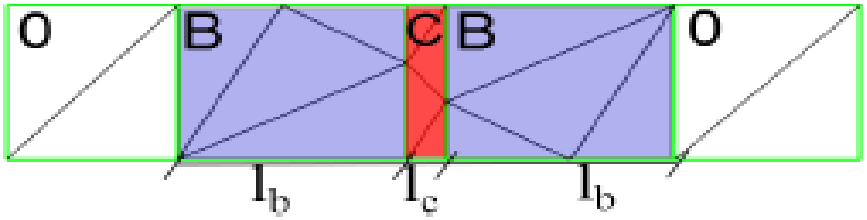
Numerical errors in computing scattering parameters



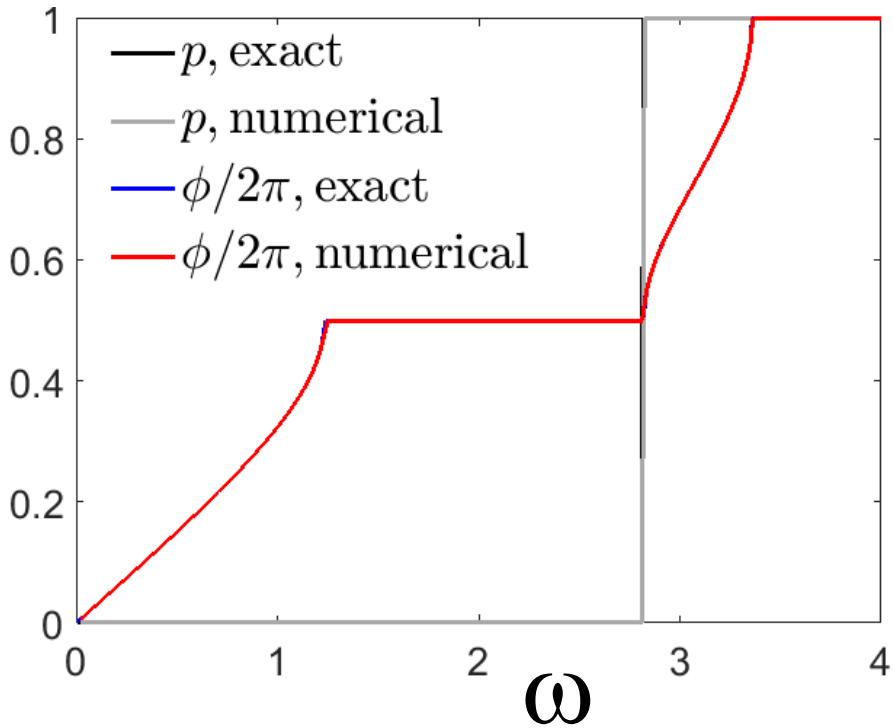


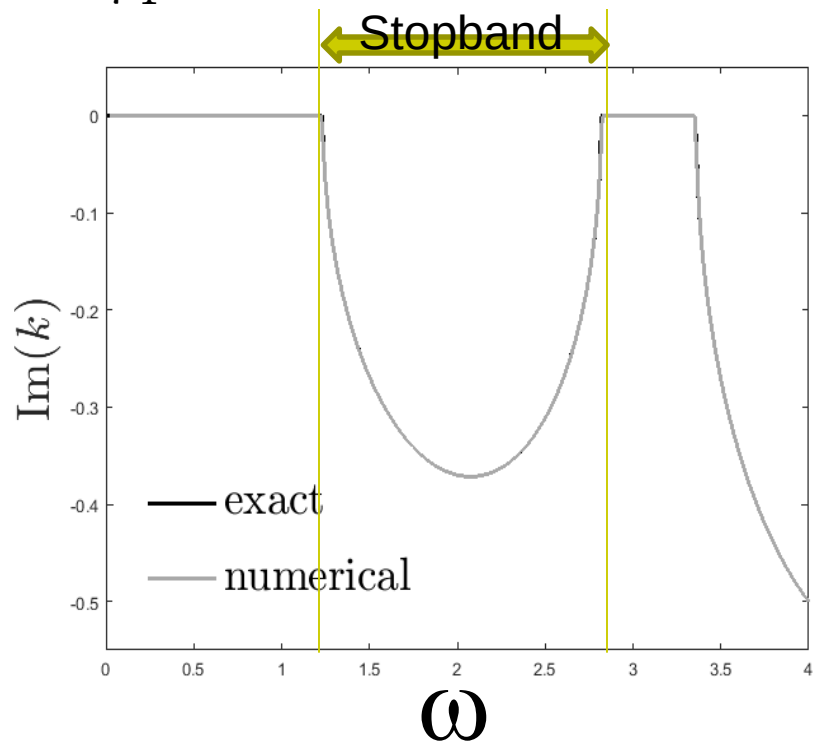
Higher errors in computing R and T at higher frequencies (as expected)

Electromagnetics:
3 layer 1D: Stopbands, *etc.*



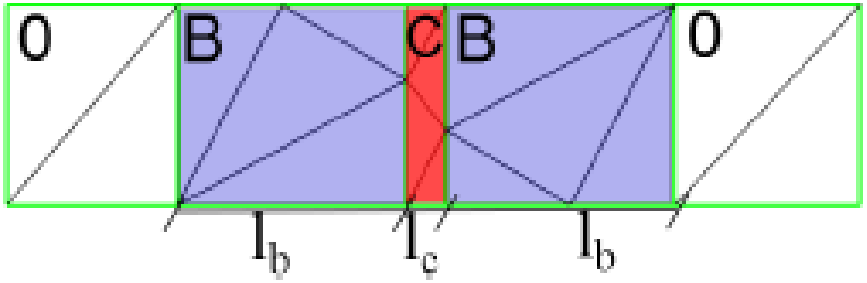
$\epsilon_B = 0.1152$, $\mu_B = 1.18$
$\epsilon_C = 0.003125$, $\mu_C = 7.954$
$\epsilon_0 = 1$, $\mu_1 = 1$





Sia Nemat-Nasser, John R. Willis, Ankit Srivastava, and Alireza V. Amirkhizi. Homogenization of periodic elastic composites and locally resonant sonic materials. Physical Review B, 83(10), March 2011.

Electromagnetics:
3 layer 1D: Stopbands, *etc.*



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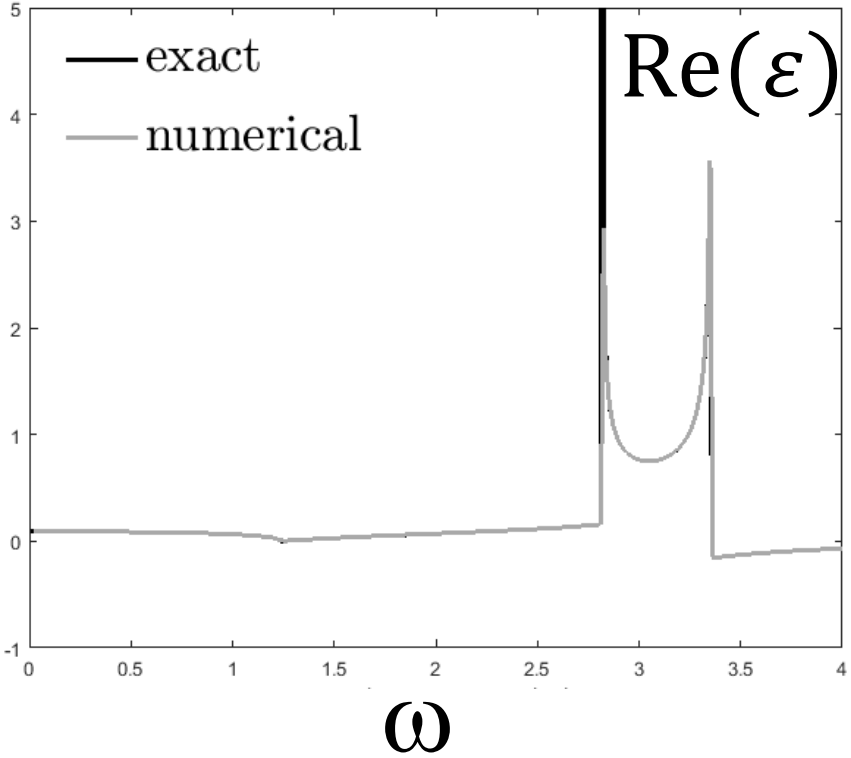
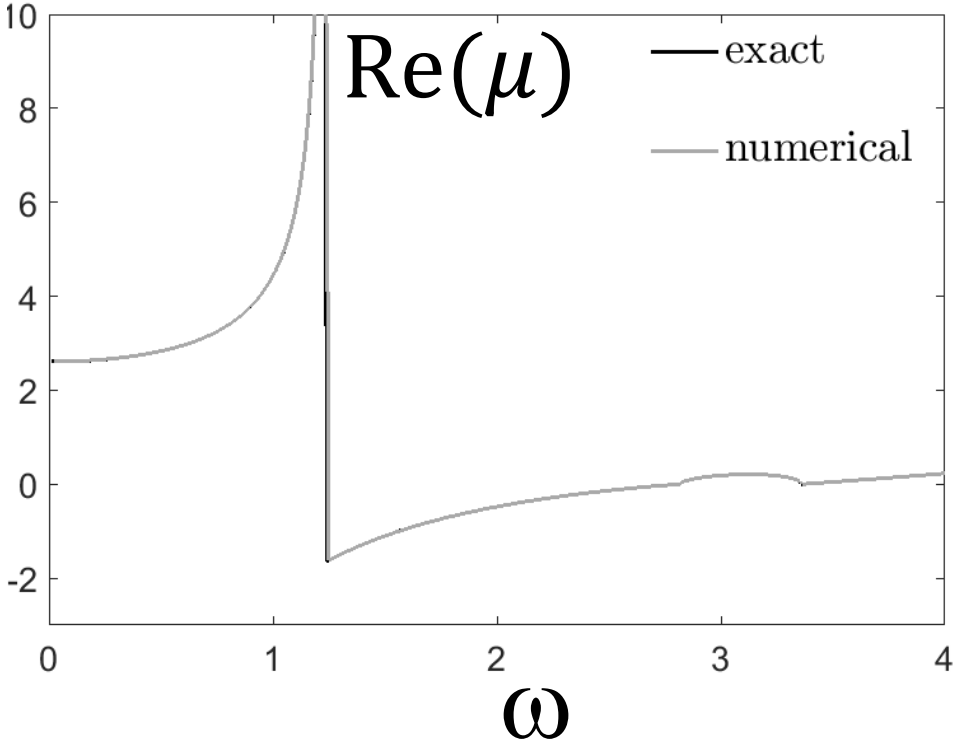
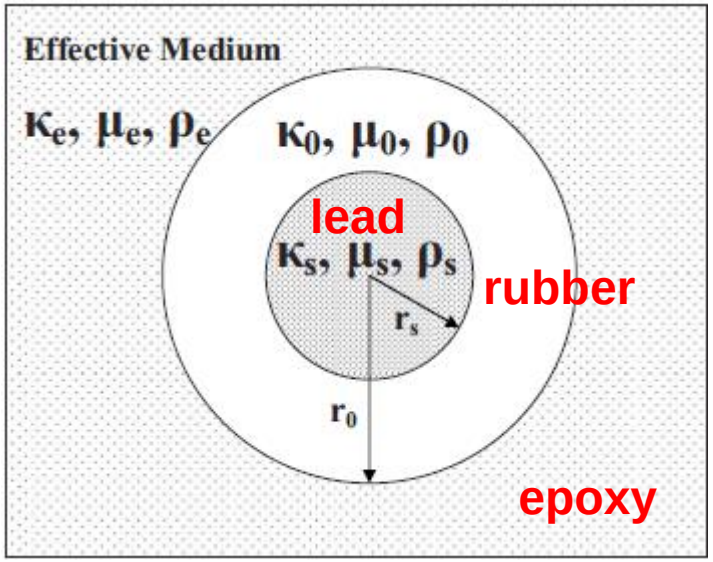
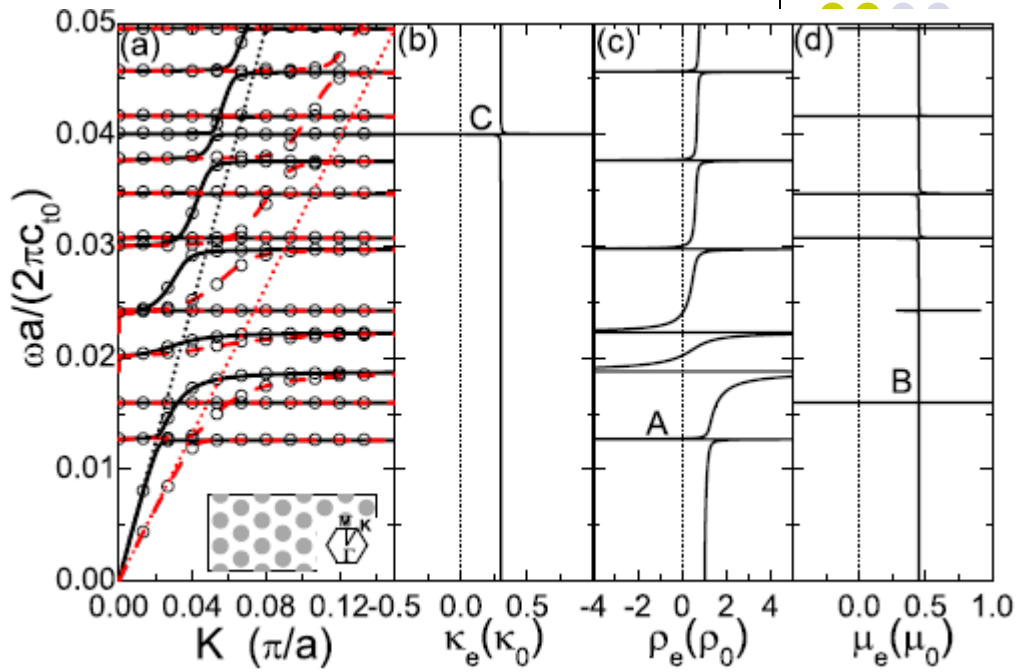




Example from elastodynamics: Retrieval method for 2D unit cells

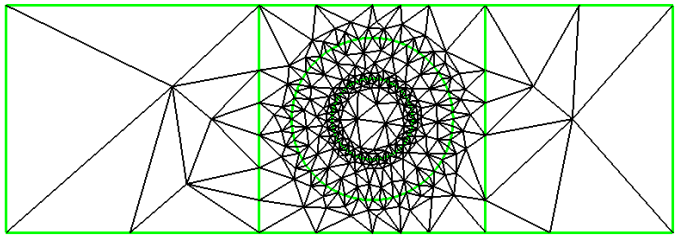


	$\kappa_e+\mu_e>0$ $\mu_e>0$	$\kappa_e+\mu_e>0$ $\mu_e<0$	$\kappa_e+\mu_e<0$ $\mu_e>0$	$\kappa_e+\mu_e<0$ $\mu_e<0$
$\rho_e>0$	$n_l>0$; $n_t>0$	$n_l>0$; t: gap	$n_t>0$; l: gap	l, t: gap
$\rho_e<0$	l, t: gap	$n_t<0$; l: gap	$n_l<0$; t: gap	$n_l<0$; $n_t<0$



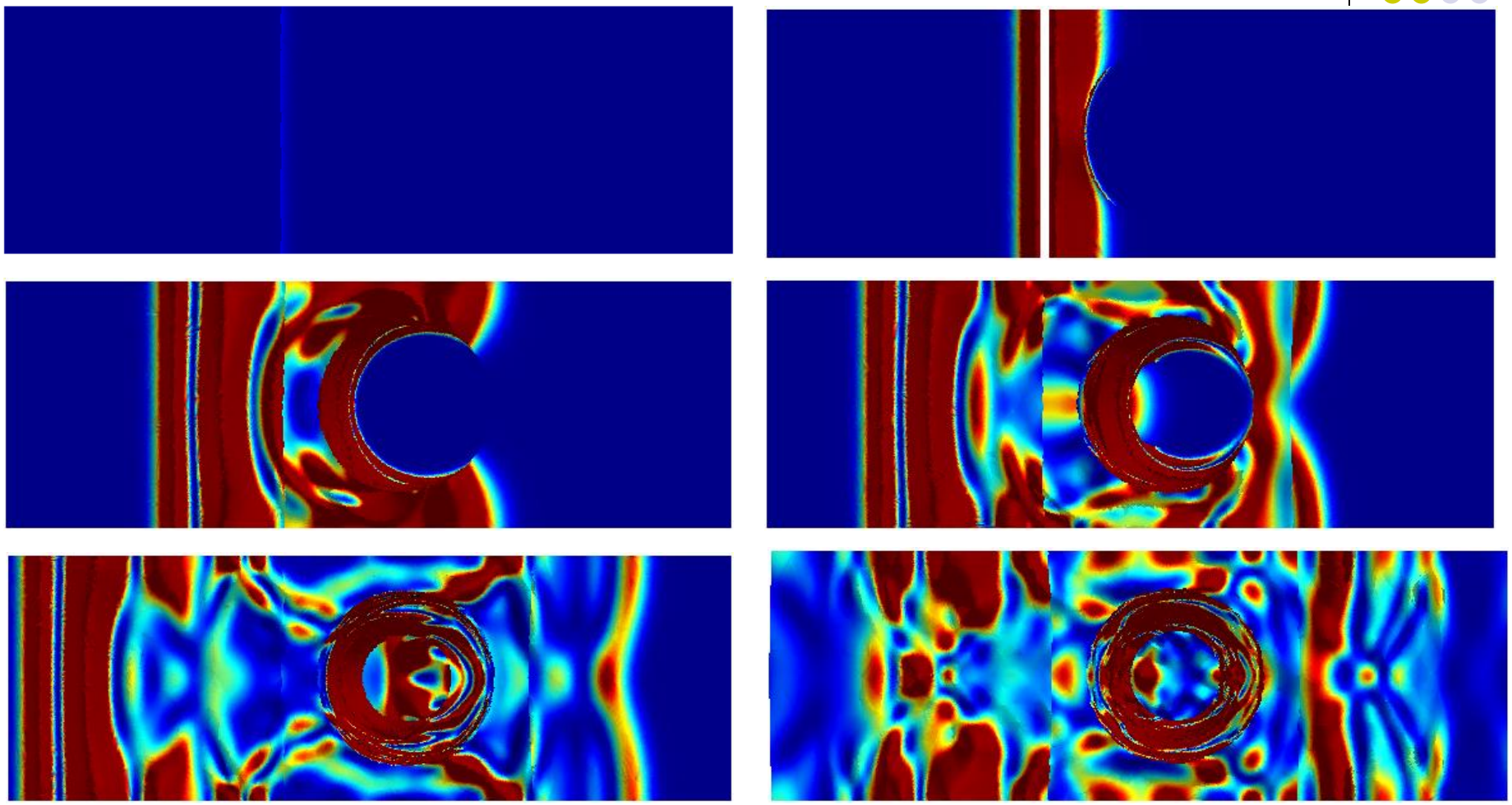
Ying Wu, Yun Lai, and Zhao-Qing Zhang. Effective medium theory for elastic metamaterials in two dimensions. Physical Review B, 2007.

Spatial mesh for the SDG method



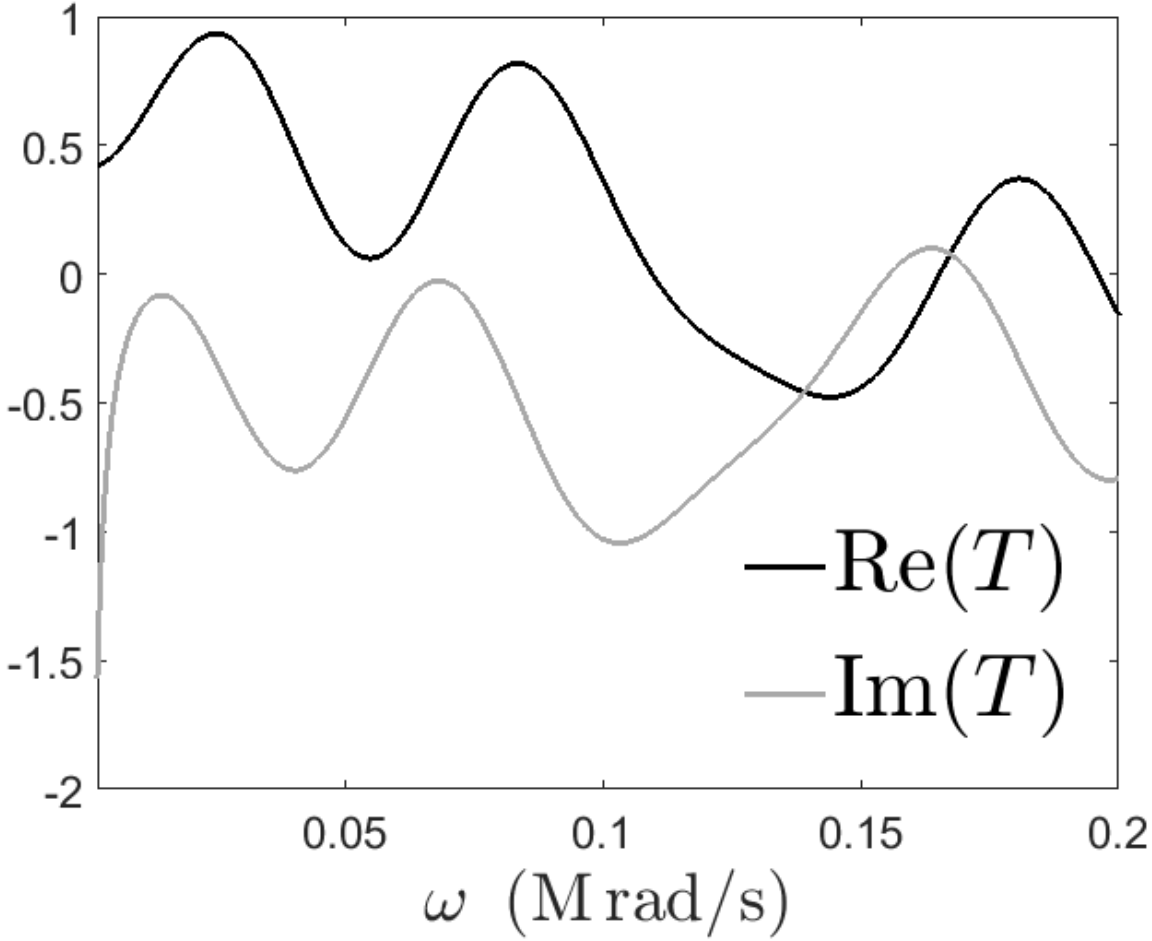
Example from elastodynamics: Retrieval method for 2D unit cells

Example from elastodynamics: Retrieval method for 2D unit cells



Movie: Solution, Mesh

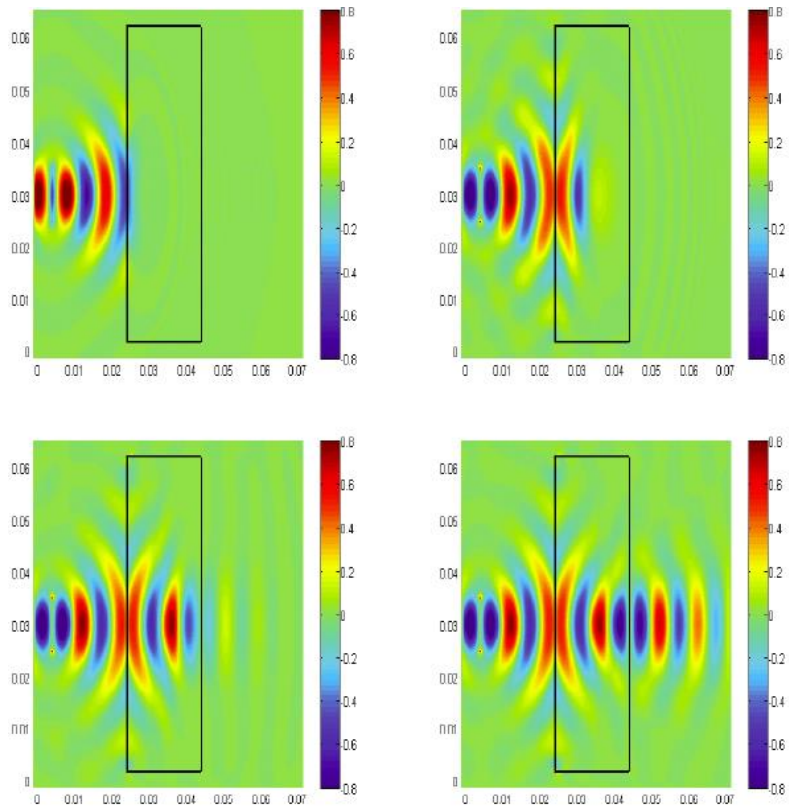
Retrieval method for 2D unit cells: Transmission coefficient



Solution of
Dispersive media in TD

Ongoing work:
Elimination of convolutions in TD

Huang et. al., SIAM J. SCI. COMPUT., Vol. 35, No. 1, pp. B248–B274, 2013



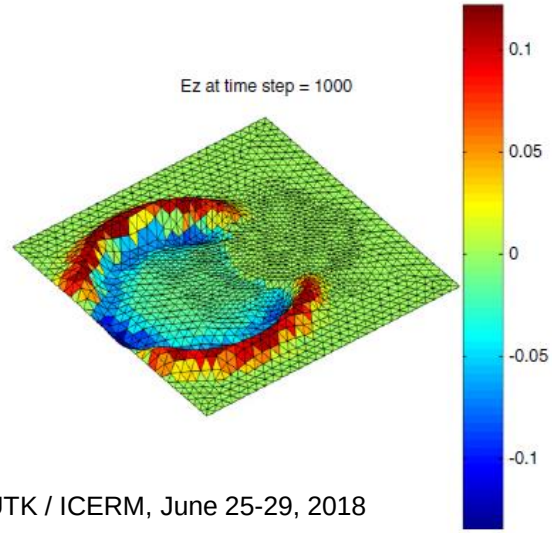
Drude material

$$\epsilon_0 \frac{\partial \boldsymbol{E}}{\partial t} = \nabla \times \boldsymbol{H} - \widetilde{\boldsymbol{J}} + \boldsymbol{f} \quad \text{in } \Omega \times (0,T),$$

$$\mu_0 \frac{\partial \boldsymbol{H}}{\partial t} = -\nabla \times \boldsymbol{E} - \widetilde{\boldsymbol{K}} \quad \text{in } \Omega \times (0,T),$$

$$\frac{\partial \widetilde{\boldsymbol{J}}}{\partial t} + \Gamma_e \widetilde{\boldsymbol{J}} = \epsilon_0 \omega_{pe}^2 \boldsymbol{E} \quad \text{in } \Omega \times (0,T),$$

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



Dispersive (metamaterial)
TD
PML

Jichun Li, Journal of Computational and Applied Mathematics 236 (2011) 950–961

Ongoing work:
Elimination of convolutions in TD

- Electromagnetic equations in FD

$$j\omega \bar{\boldsymbol{D}}^{\boldsymbol{t}} - \nabla \times \bar{\boldsymbol{H}} = 0 \quad : \quad \text{Ampère's law with Maxwell addition}$$

$$j\omega \bar{\boldsymbol{B}}^{\boldsymbol{t}} + \nabla \times \bar{\boldsymbol{E}} = 0 \quad : \quad \text{Faraday law of induction}$$

- Frequency domain constitutive relation for an **<u>isotropic</u>** media:

$$\bar{D}^t(j\omega) = \bar{\epsilon}(j\omega)\bar{E}(j\omega) \qquad \Rightarrow \qquad (j\omega)\bar{D}^t{}_k(j\omega) = \overbrace{j\omega\bar{\epsilon}(j\omega)}^{\bar{g}(j\omega)}\,\bar{E}^k(j\omega)$$

- Pull-back in time domain involves a convolution:

$$\boxed{\dot{D}^t_k(t) = \int_{-\infty}^{t} g(t-t')E^k(t')\mathrm{d}t'}$$

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,

$$\bar{\epsilon}(j\omega) = \epsilon_\infty + \frac{\epsilon_s - \epsilon_\infty}{1 + (j\omega)t_0} \qquad \Rightarrow$$

$$(j\omega)\bar{D}^t{}_k(j\omega) = (j\omega)\epsilon_\infty \bar{E}^k(j\omega) + \frac{\epsilon_s - \epsilon_\infty}{t_0}\bar{E}^k(j\omega) + \overbrace{\left\{ -\frac{\epsilon_s - \epsilon_\infty}{t_0(1 + (j\omega)t_0)}\bar{E}^k(j\omega) \right\}}^{\bar{P}_{(k)}(j\omega)}$$

- By the introduction of Auxiliary Field P we get,

$$\begin{cases} (j\omega)\bar{D}^t{}_k(j\omega) = \epsilon_\infty (j\omega)\bar{E}^k(j\omega) + \frac{\epsilon_s - \epsilon_\infty}{t_0}\bar{E}^k(j\omega) + \bar{P}_{(k)}(j\omega) \\ \bar{P}_{(k)}(j\omega) = -\frac{\epsilon_s - \epsilon_\infty}{t_0(1+(j\omega)t_0)}\bar{E}^k(j\omega) \end{cases} \quad \begin{array}{l} \Rightarrow \dot{D}^t_k(t) = \epsilon_\infty \dot{E}^k(t) + \frac{\epsilon_s - \epsilon_\infty}{t_0}E^k(t) + P_{(k)}(t) \\ \Rightarrow t_0 \dot{P}_{(k)}(t) + P_{(k)}(t) = -\frac{\epsilon_s - \epsilon_\infty}{t_0}E^k(t) \end{array}$$

- That is convolution term is eliminated by the addition of the field $P_{(k)}$.

$$\boxed{\begin{array}{l} \dot{D}^t_k(t) = \epsilon_\infty \dot{E}^k(t) + \frac{\epsilon_s - \epsilon_\infty}{t_0}E^k(t) + P_{(k)}(t) \\ t_0 \dot{P}_{(k)}(t) + P_{(k)}(t) = -\frac{\epsilon_s - \epsilon_\infty}{t_0}E^k(t) \\ P_{(k)}(t) \end{array}}$$

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:

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

$$\bar{\mathbf{J}}^{\mathcal{I}}_{\epsilon_d} := \sum_{\mathcal{J}=1}^{2} \{j\omega\bar{\epsilon}_d{}^{\mathcal{I}\mathcal{J}}(\omega)\}\bar{\mathbf{U}}_{\mathcal{J}}$$

- The pull-back to time domain is:

$$\bar{L}(j\omega) = \bar{P}_0(j\omega) + D\bar{X}(j\omega) \quad \Rightarrow \quad \boxed{L(t) = P_0(t) + DX(t) \quad \text{time domain representation of } L}$$

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

$$R_{iP} = \frac{B_{\bar{b}-i-1}}{B_{\bar{b}}}P_0(t) - P_{i+1}(t) + \frac{1}{B_{\bar{b}}}\left\{DB_{\bar{b}-i-1} - \sum_{a+c=\bar{b}-i-1} A_a C_c\right\}X(t) = 0, i_{\max}, \quad \text{Source terms}$$

$$i_{\max} = \max(i^b_{\max}, i^{ac}_{\max}) = \max(\bar{b} - \underline{b} - 1, \bar{b} - (\underline{a} + \underline{c}) - 1) \quad \text{and the number of ADEs } n_P = i_{\max} + 1$$

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.

TDDG, PML, dispersive media: - **Tiao Lu, Pingwen Zhang, Wei Cai**, DG methods for dispersive and lossy Maxwell's equations and PML boundary conditions, JCP 200 (2004) 549–580
- Jichun Li, Development of discontinuous Galerkin methods for Maxwell's equations in metamaterials and perfectly matched layers, Journal of Computational and Applied Mathematics 236 (2011) 950–961
- Busch, Konig 2011, etc

Time Domain Electromagnetics SDG: Formulation of PML for dispersive media

- Perfectly matched layer for bi-anisotropic dispersive media

$$\overline{\overline{\epsilon}}_{\mathrm{PML}} = (\det \overline{\overline{S}})^{-1}[\overline{\overline{S}} \cdot \overline{\overline{\epsilon}}(\omega) \cdot \overline{\overline{S}}]$$
$$\overline{\overline{\mu}}_{\mathrm{PML}} = (\det \overline{\overline{S}})^{-1}[\overline{\overline{S}} \cdot \overline{\overline{\mu}}(\omega) \cdot \overline{\overline{S}}]$$
$$\overline{\overline{\zeta}}_{\mathrm{PML}} = (\det \overline{\overline{S}})^{-1}[\overline{\overline{S}} \cdot \overline{\overline{\zeta}}(\omega) \cdot \overline{\overline{S}}]$$
$$\overline{\overline{\xi}}_{\mathrm{PML}} = (\det \overline{\overline{S}})^{-1}[\overline{\overline{S}} \cdot \overline{\overline{\xi}}(\omega) \cdot \overline{\overline{S}}].$$

PML stretching ⇨ dispersive relations

Teixeira, Chew, General closed-form PML constitutive tensors to match arbitrary bianisotropic and dispersive linear media, IEEE Microw. Guid. Wave Lett., 1998

2 Levels of ADEs needed in TD

Constitutive model ⇨

	Level	Inductive	Conductive	Dispersive
PML	Base			✓
	L1	✓	✓	✓
	L2	✓	✓	✓

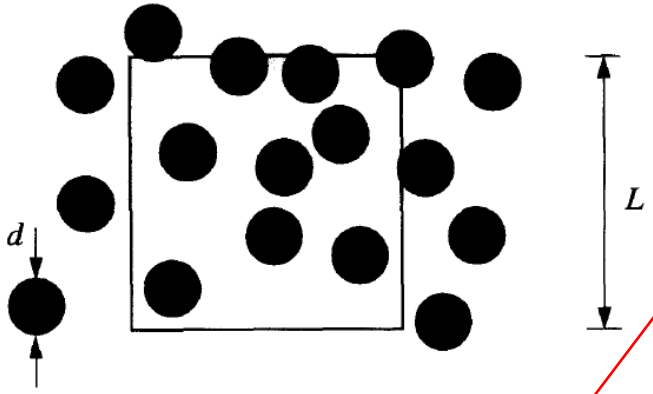
- 3 levels for linear PML (2 additional levels to the base material) $s_i = 1 + \sigma_i / j\omega$
- **5 levels** for CFS-PML. $s_i = \kappa_i + \omega_i / (\alpha_i + j\omega)$
- Even more levels for second order PML.

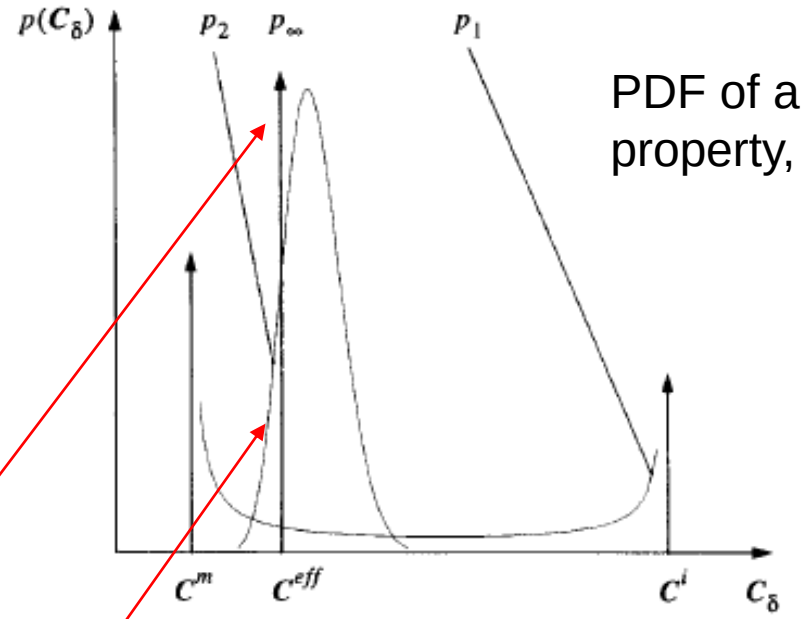
Recursive formulation of ADEs automatically formulates PML equations.

Random media:
Solution of stochastic PDEs

Representative Volume Elements (RVEs) versus Statistical Volume Elements (SVEs)

$$d \ll l \ll L$$





PDF of a material property, e.g. stiffness

RVE limit: l is very large

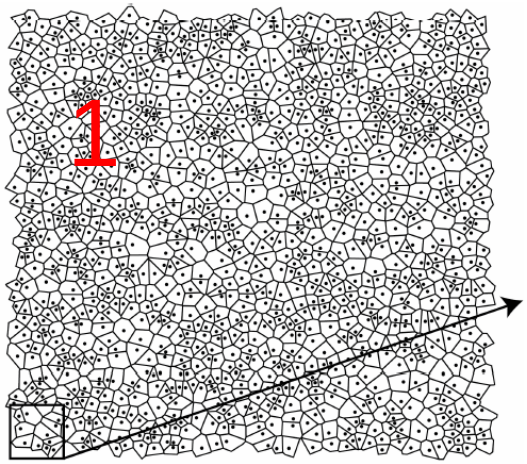
Ostoja-Starzewski 1998

SVE sizes: Material property is probabilistic

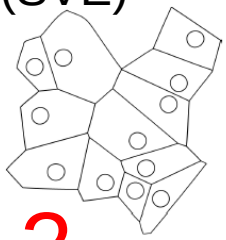
- RVEs are good for many elastic regime problems
- For **fracture** modeling (particularly quasi-brittle material):
  - Need to preserve **spatial inhomogeneity**
  - **Randomness** (sample to sample variations)

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

Stochastic PDEs: Elastodynamics



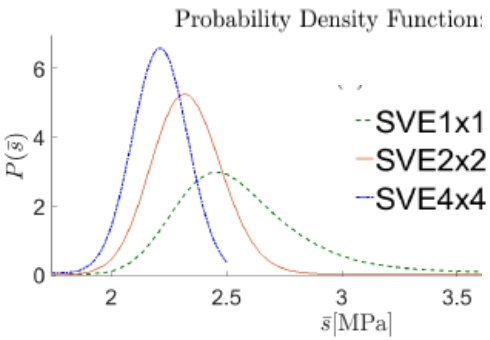
Statistical Volume Element (SVE)



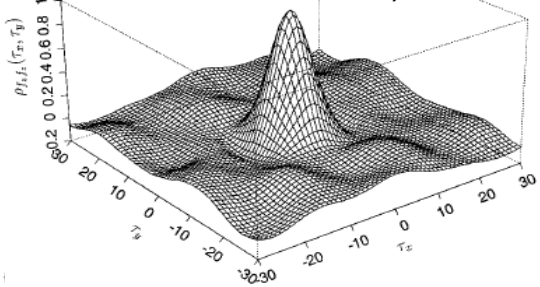
2

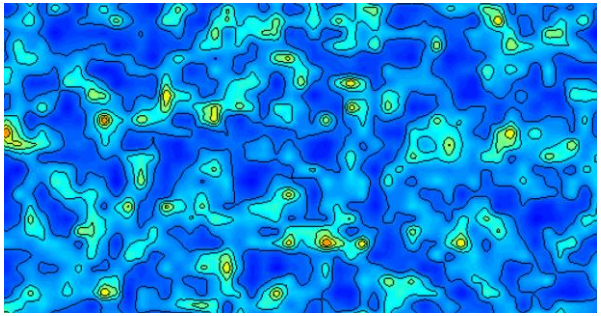
Random field statistics

3



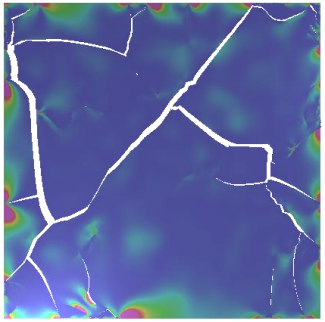
Baxter, 2000

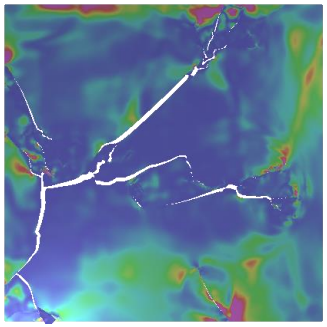


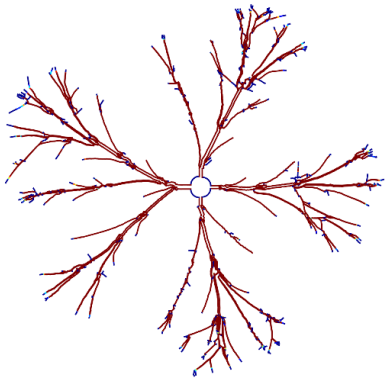


4 Random field realizations

5 Macroscopic Simulations







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

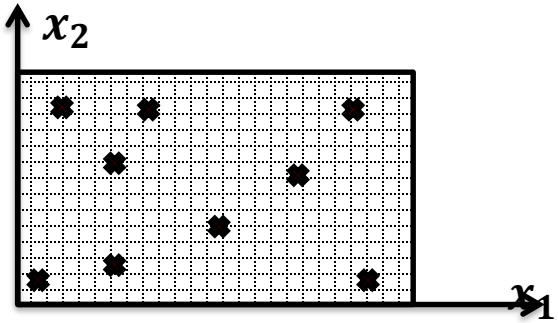
→ A very efficient and accurate model for fracture modeling

Stochastic Decomposition:
Karhunen-Loeve expansion

Gaussian random field $\eta(\boldsymbol{x})$:

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

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



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

$$\int_{\bar{D}} COV_\eta(\boldsymbol{x}^1, \boldsymbol{x}^2) b(\boldsymbol{x}^2) d\boldsymbol{x}^2 = \lambda b(\boldsymbol{x}^1)$$

$$COV\big(\bar{s}(\boldsymbol{X}), \bar{s}(\boldsymbol{Y})\big) = e^{-\left(\frac{|\boldsymbol{X}-\boldsymbol{Y}|}{d_c}\right)^2}$$

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

Non- Gaussian random field:

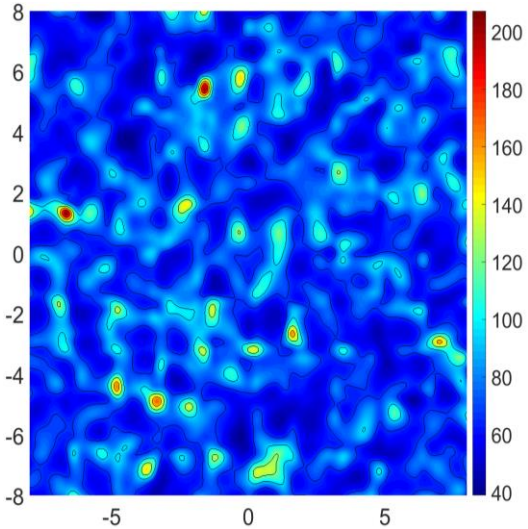
$$\xi(\boldsymbol{x}) = F_\xi^{-1}\Big(F_\eta\big(\eta(\boldsymbol{x})\big)\Big)$$

$$\eta(\boldsymbol{x}) \sim N(0,1)$$

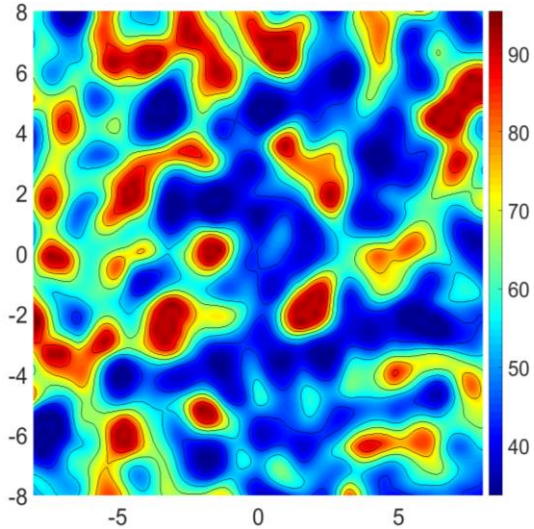
$$\bar{s}(\boldsymbol{x}) = \xi(\boldsymbol{x}) = F_\xi^{-1}\left(\frac{1}{2}\left\{1 + Erf\left(\frac{\eta(\boldsymbol{x})}{\sqrt{2}}\right)\right\}\right)$$

(Inverse Transform Method)

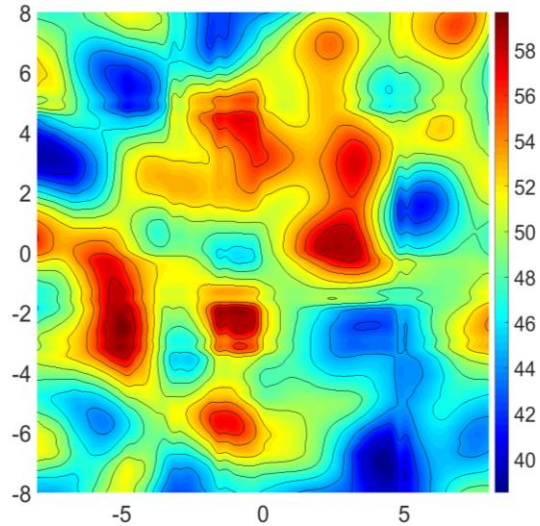
Sample KL Random Fields



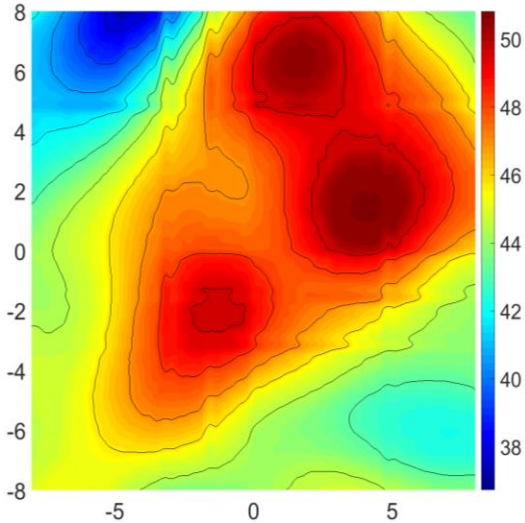
SVE1x1



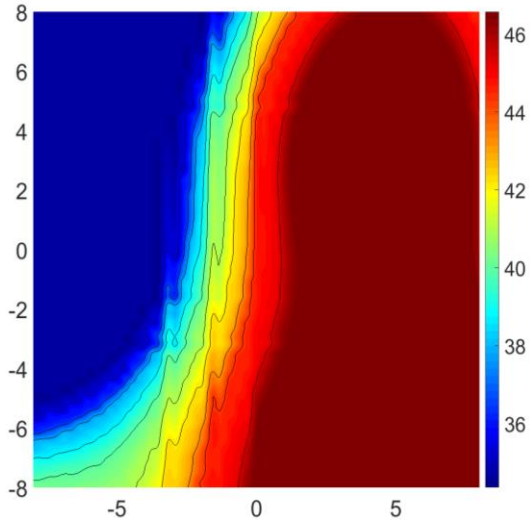
SVE2x2



SVE4x4



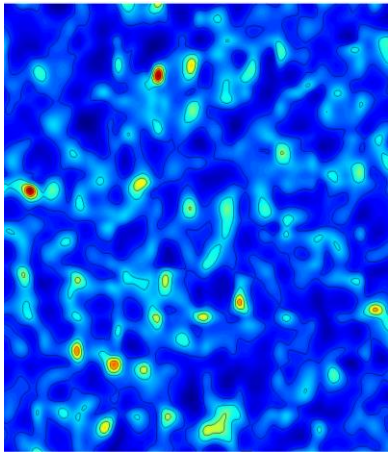
SVE8x8



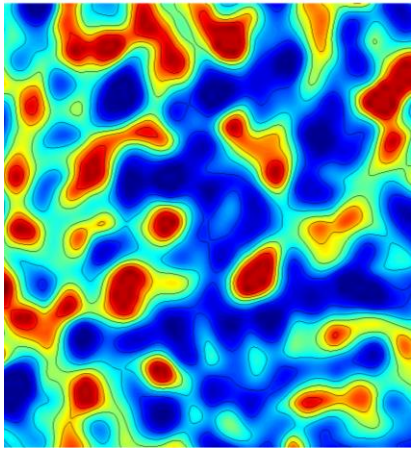
SVE16x16

Sample stochastic fracture results

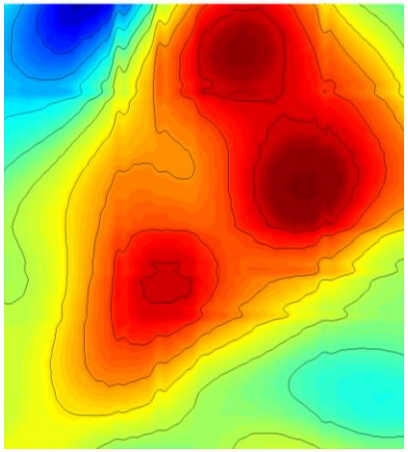
Realizations for fracture strength based on



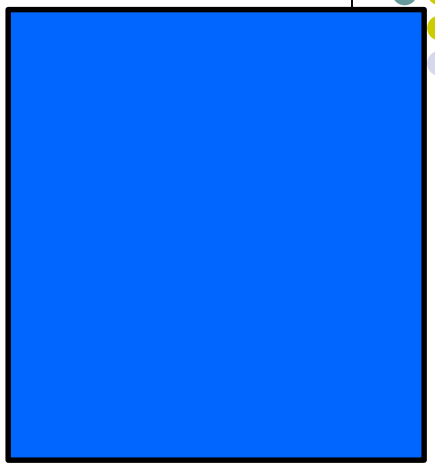
SVE1x1



SVE2x2

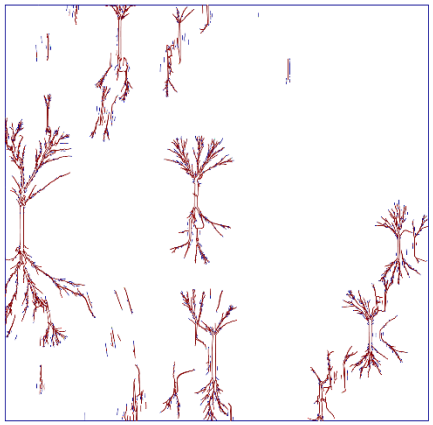


SVE8x8

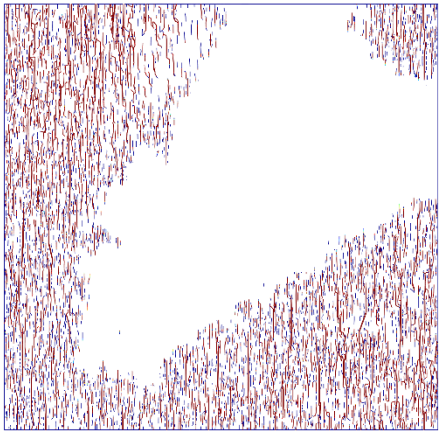


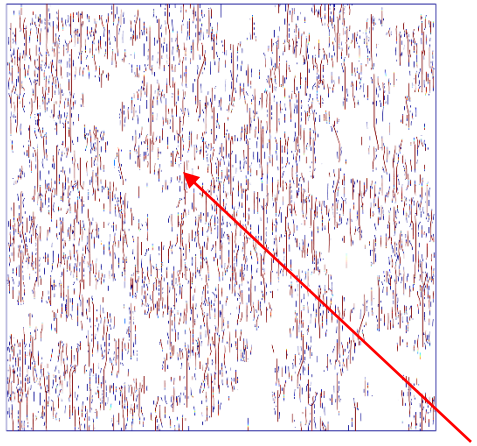
Uniform fracture strength

Window sizes uses for statistical volume elements



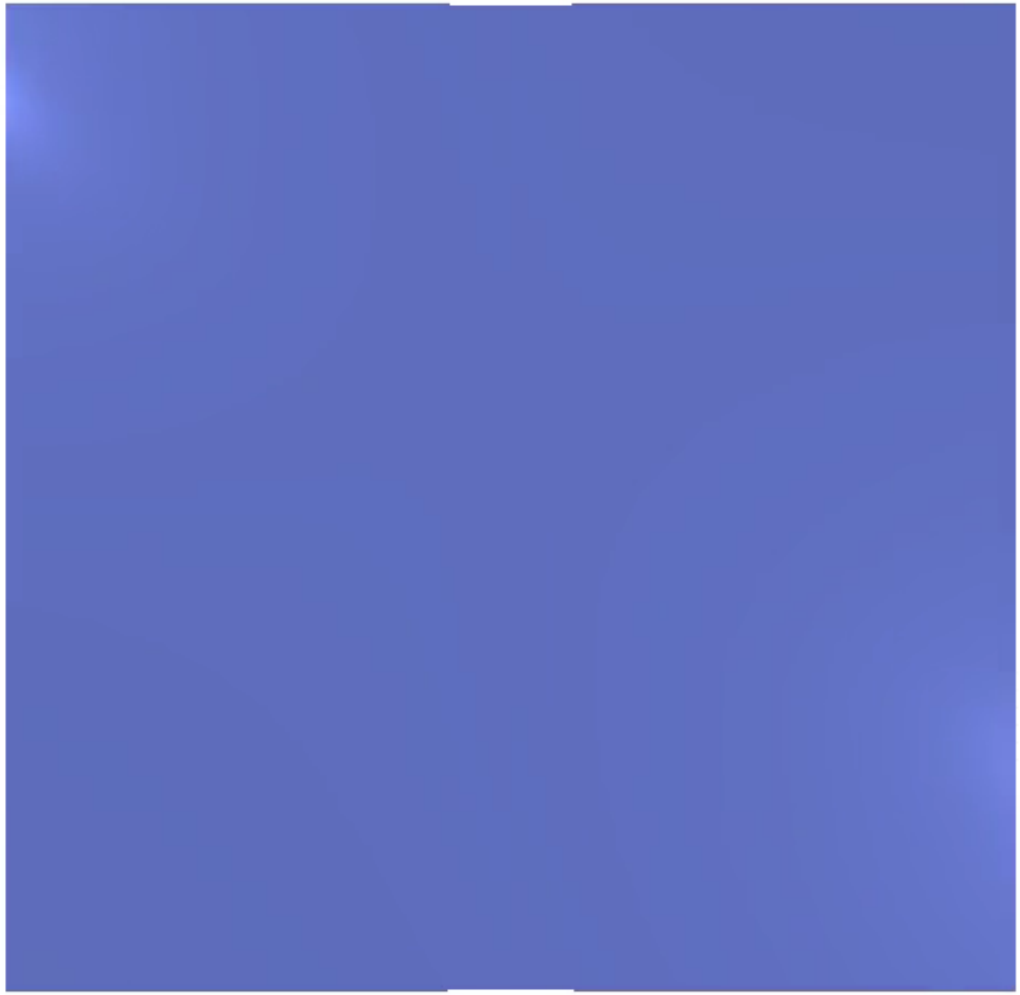
Fracture patterns under uniform load in horizontal direction

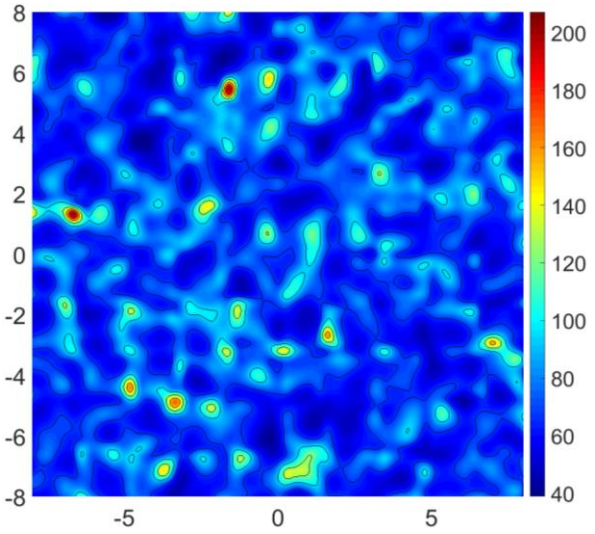




Very unrealistic fracture pattern with uniform fracture strength model

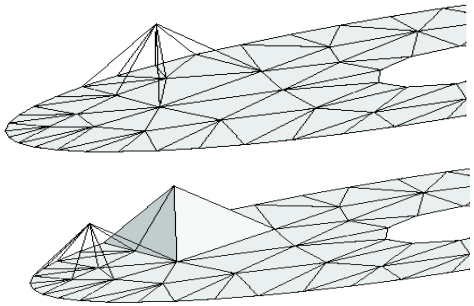
Effect of fracture strength randomness:
e.g., SVE1x1



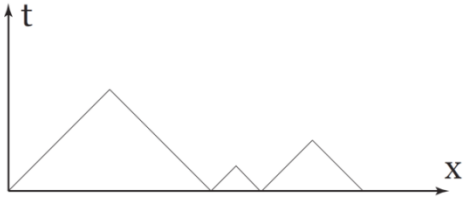


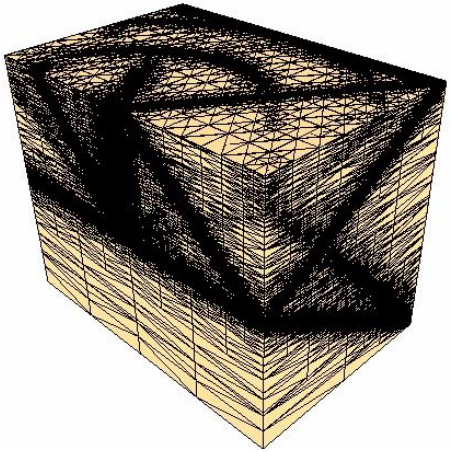
KL random fracture strength $\bar{s}(x)$

Conclusions

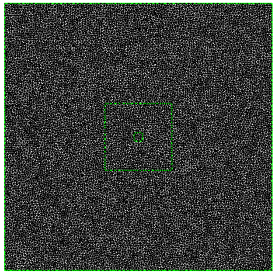


- Space time directly discretized ⇒ O(N) patch-by-patch scheme.
- Asynchronous solution scheme is ideal for the solution of grids with disparate length scales.
- It provides a powerful *h*-adaptive scheme in spacetime.
- Energy dissipation of all elements is non negative.
  - Convergence rate p + 1.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

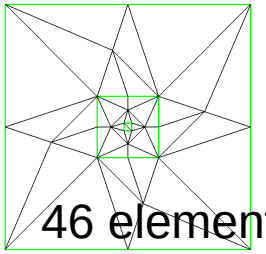




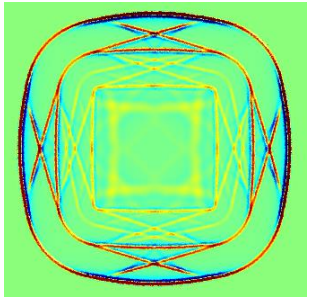
Nonadaptive



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
  - (Collocation method) for the solution of macroscopic SPDEs (in progress)

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  - Students:
    Past students:
    Scott Miller, Boris Petrakovici, Alex Mont, Aaron Becker, Shuo-Heng Chung, Yong Fan, Morgan Hawker, Jayandran Palaniappan, Brent Kraczek, Shripad Thite, Yuan Zhou, Kartik Marwah, Ian McNamara, Raj Kumar Pal, Christian Howard, Amit Madhukar.
  - NCSA Staff Member:
    Valodymyr Kindratenko

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Relevant Publications

- R. Abedi, S.H. Chung, J. Erickson, Y. Fan, M. Garland, D. Guoy, R.B. Haber, J. Sullivan, S. Thite, and Y. Zhou, “Space–time meshing with adaptive refinement and coarsening”, In Proceedings of the Twentieth Annual Symposium on Computational Geometry, SCG ’04, pages 300-309, New York, NY, USA, June 9-11 2004. ACM.
- R. Abedi, B. Petracovici, and R.B. Haber, “A spacetime discontinuous Galerkin method for linearized elastodynamics with element–wise momentum balance”, Computer Methods in Applied Mechanics and Engineering, 195:3247–3273, 2006.
- R. Abedi, R.B. Haber, S. Thite, and J. Erickson, “An h–adaptive spacetime discontinuous Galerkin method for linearized elastodynamics”, Revue Européenne de Mécanique Numérique, special issue on adaptive analysis (ed.), 15(6):619–642, 2006 (Invited paper).
- R. Abedi and S. Mudaliar, "An asynchronous spacetime discontinuous Galerkin finite element method for time domain electromagnetics. Journal of Computational Physics, 351:121--144, 2017.