Spacetime Discontinuous Galerkin FEM: Spectral Response Reza Abedi, Omid Omidi, and Philip L. Clarke

Dept. of Mechanical, Aerospace & Biomedical Engineering, University of Tennessee Space 22nd Conference on Spectral Line Shapes, June 1-6 2004, Tullahoma, TN, USA

We present the novel spectral properties of metamaterials, discuss their highly multiscale and rich solution features, followed by challenges in their computational modeling. After elaborating on the advantages of time domain schemes, we elaborate on unique features of TD method of Spacetime Discontinuous Galerkin method for metamaterial and spectral analyses.

Metamaterials and photonic crystals

- Feature sizes of the system are:
 - comparable to (Photonic crystals) or
 - much smaller (metamaterials) than the wavelength of incident waves
- Metamaterials can be considered as effective media whose frequency-dependent properties are determined by building blocks

Properties and applications of metamaterials

- Negative permittivity (Schurig et al 2006a), permeability (Shelby et al 2001), ulletor both (negative index of refraction: Smith et al 2000) for electromagnetics
- Electromagnetic (Schurig et al 2006b) & acoustic cloaking
- Negative mass density and/or density for acoustics
- Unusually high refractive indices (Choi et al 2011)
- Perfect absorbers (Landy et al 2008, Tao et al 2008)
- Sub diffraction imaging (Fang et al 2005)
- Memory metamaterials (Driscoll et al 2009)



Caveats with TD methods

1. Frequency-dependent material properties: In TD method, frequency dependent properties that are more easily handles in FD are pulled back to a convolution; e.g. for acoustic equations:

$$\int_{-\infty}^{\infty} \rho_{0(x,t-t')} \cdot \frac{\partial v}{\partial t'} dt' + \nabla p = 0$$

2. Global coupling: Most TDs, e.g. implicit method pose a global coupling. 3. Time integration problems from multiscale domains:



- Explicit methods eliminate the global coupling of implicit methods
- For multiscale meshes time step is limited by minimum element size
- **IMEX** and subcycling method



Numerical methods for spectral analysis

- Provide all spectral information
- **Optimization (geometry & material)**
- Information not available by experiments

a)

E 0.06

% 0.04

0.02





0.006 0.004

0.002

for acoustic metamaterial

Split hollow sphere (SHS); microstructure

Scattering by metallic sphere (Stannigel et al 2009) Mie theor ∃, 0.012 × DGTD DGTD 0.0 0.008

Double negative acoustic metamaterial: strong vibration of the sound medium at the resonant frequency (top); transmission results (bottom): (Ding et al 2010)

Computational topology and material optimization

Wavelength [nm]



Topology optimization to minimize permeability (Otomori et al 2012) using plasmas (Sakai & Tachibana 2012)

Computational challenges for metamaterials

Most of literature on Maxwell solvers for free & dispersive media but not for metamaterials. Same applies to acoustic & electromagnetic metamaterial.



Mie theory

Wavelength [nm]

partially alleviate the problem and are generally limited to low orders

Х

Multiscale explicit methods

Frequency-dependent properties in TD

There can be two approaches to eliminate the convolution op. in item 1: 1. Auxiliary Differential Equations (ADE): By "auxiliary fields" (cf. Rodriguez 2005 for treatment of Debye & plasma materials in EM) ω is eliminated from acoustic equation) $m_i^{eff} = m_1 + \frac{m_2(\omega_0)_i^2}{(\omega_0)_i^2 - \omega^2}$ (i = 1, 2)Matrix material 2. Multi-field (e.g. displacement) continuum formulation: $\bar{\rho}_m \frac{\partial^2 U_i}{\partial t^2} + \frac{\Sigma'_{\underline{i}\underline{i}}}{R} - \frac{\partial \Sigma_{ij}}{\partial X_j} = 0 \text{ (macro)}$ Huang & Sun 2012 $\frac{m_2}{A}\frac{\partial^2 U_{2i}}{\partial t^2} - \frac{\Sigma'_{\underline{i}\underline{i}}}{R}$ = 0 (micro) displacements

Spacetime Discontinuous Galerkin method

Direct discretizion of spacetime, enforcing causality property in discrete setting, and discontinuous basis functions yields these distinct advantages:

- 1. Local solution property
- 2. O(N) cost vs. number of elements
- 3. Excellent resolution of high gradient fields and discontinuities
- 4. Arbitrary element size and (h) polynomial order (p) adjustment (below)
- 5. Arbitrary high order in time (below)



- Computation of metamaterials is much more challenging:
 - High gradient fields and sharp discontinuities • Jumps in material properties and very strong fields at air/metamaterial interface call for highly dense and high order meshes
 - Multiscale domains: Very small grid spacing

Two waveguides coupled to a slotted microresonator (Busch 2011)

Time Domain (TD) vs. Frequency Domain (FD)

- Quasi-static FD solution may be sufficient (Ding et al 2010):
 - How can the field get to its stable state?
 - In there any strong scattering in the process?
 - How long is the relaxation process?
 - What is the system response to a pulse?
 - TD needed for dynamic topics such as temporal coherence, change in propagation, tuning of cavity frequency, and the nonlinear response
- Obtaining the entire spectra with one simulation: FD requires one simulation per point in spectra while in TD response and subsequent Fourier transformation to a broad-band signal is sufficient (Stannigel et al 2009)
- Nonlinearity: nonlinear phenomena cannot easily be treated in FD
- Efficiency, scaling: Unlike FD domains that entail a global coupling, some TD solution scales linearly versus number of unknowns/elements.

Intensity distribution for a silver V shape excited at resonance (Stannigel et al 2009)





- Excellent for multiscale domains; local 6. time step not affected by smallest size
- 7. Local & asynchronous features ideal for adaptive & parallel simulations



Front tracking & adaptive operations ; more than 95% scaling for adaptive simulations

Refernces

(Abedi el. al. 2006) Comput Method Appl M, 195 (25), 3247-3273. (Busch et al 2011) Laser Photonics Rev. 5, No. 6, 773-809. (Choi et al 2011), Nature 470, 369. (Ding et al 2010) J. of Applied Physics 108, 074911. (Driscoll et al 2009) Science 325, 1518. (Fang et al 2005) Science 308, 534. (Huang & Sun 2012) Mech. Mater. 46, 1–10. (Huang et al 2013) SIAM J. Sci. Comput., 35, B248-B274. (Landy et al 2008) Phys. Rev. Lett. 100, 207402. (Li 2011) J COMPUT APPL MATH, 236, 950–961.

(Otomori et al 2012) Comput Method Appl M, 237, 192-211.

(Sakai & Tachibana 2012) Plasma Sources Sci. Technol. 21. (Schurig et al 2006a) Science 314, 977. (Schurig et al 2006b) Appl. Phys. Lett. 88, 041109. (Shelby et al 2001) Science 292, 77. (Smith et al 2000) Phys. Rev. Lett. 84, 4184-4187. Stannigel et al 2009) Optics Express, 17 14934. (Tao et al 2008) Phys. Rev. B 78, 241103.

