Spacetime Discontinuous Galerkin FEM: Spectral Response

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Abstract. Materials in nature demonstrate certain spectral shapes in terms of their material properties. Since successful experimental demonstrations in 2000, metamaterials have provided a means to engineer materials with desired spectral shapes for their material properties. Computational tools are employed in two different aspects for metamaterial modeling: 1. Mircoscale unit cell analysis to derive and possibly optimize material's spectral response; 2. macroscale to analyze their interaction with conventional material. We compare two different approaches of Time-Domain (TD) and Frequency Domain (FD) methods for metamaterial applications. Finally, we discuss advantages of the TD method of *Spacetime Discontinuous Galerkin* finite element method (FEM) for spectral analysis of metamaterials.

1. Introduction
Since about a decade ago researchers have been able to design materials with particular repeating microstructure that demonstrate desirable spectral properties. Some notable advancements in electromagnets include materials with negative permittivity [1], permeability [2], or both [3]. Some of their applications are in electromagnetic and acoustic cloaking [4], perfect absorbers [5,6] sub diffraction imaging [7], and memory metamaterials [8]. In this paper, we discuss some approaches and challenges in numerical spectral analysis of metamaterials.

2. Numerical methods for spectral analysis and computation of metamaterials
Figure 1 shows the micro to macro transition of metamaterial properties and the use of computational tools. In Fig.1(a) we observe an electromagnetic metamaterial formed by an array of *Split Ring Resonators* (SRRs). The feature size and spacing of microstructures must be much smaller than wavelengths of interest. Computational tools are employed in two scales. At microscale, computational tools analyze a unit cell, *cf.* 1(b), with periodic boundary to obtain spectral properties of metamaterial. As shown in Fig.1(c) such forward analysis tools can be combined with an optimization scheme to enhance metamaterial properties. Once a metamaterial with desired spectral is designed, its interaction at macroscale with other material can still be model with computational tools as shown in Fig.1(d).

3. Computational challenges for metamaterials
In electromagnetics, acoustics, and electrodynamics most solvers are designed for conventional materials and are not suited for metamaterial applications. In Fig. 2 shows resonance phenomena and operation mechanism for metamaterials, for a *Split Hollow Sphere* (SHS) and
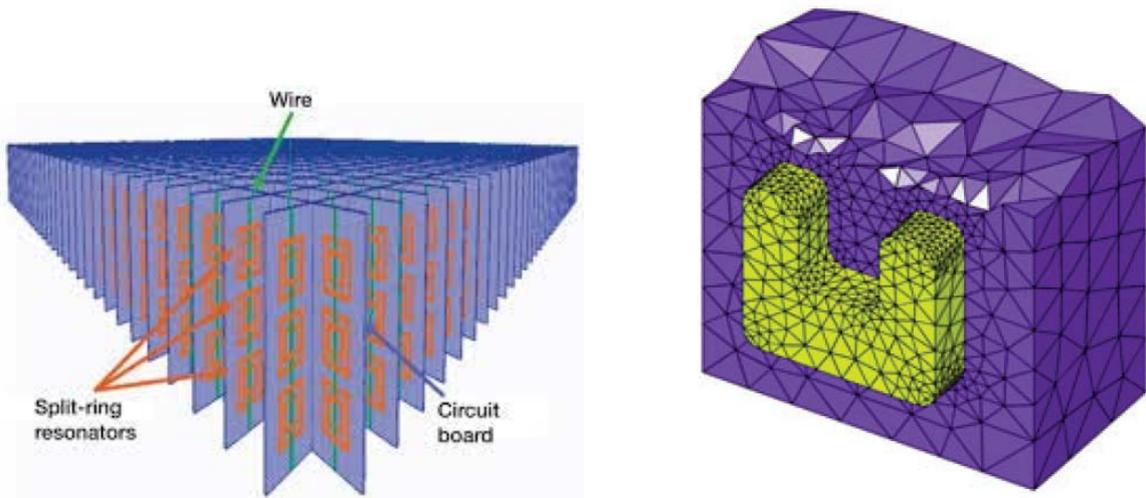
(a) A structured array of microstructures (Wikipedia).

(b) Unit cell computational spectral analysis [9].
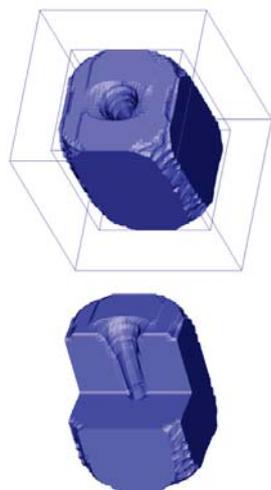
(c) Microstructure optimization [10].
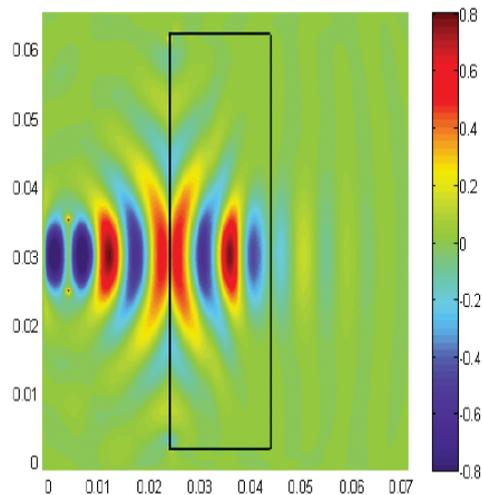
(d) Macro interaction of metamaterial with other materials [11].

Figure 1. Computational tools for analysis of metamaterials: (a) A sample array of microstructures, SRRs, in metamaterials ; (b) A unit cell computational domain to determine spectral properties of a SRR; (c) Topology optimization of microstructure to minimize effective dielecric permeability; (d) Backward wave propagation in metamaterial region (enclosed in a rectangle) using a time domain finite element method.

the corresponding acoustic transmission spectrum. Figure 3 shows intensity distribution for a silver V shape. Jumps in material properties and very strong fields both at microscale (figs. 2-3) and macroscale at material/metamaterial interface (Fig. 1(d)) call for numerical fields that can efficiently and robustly resolve these fields. In addition, metamaterial microstructure designs are inherently multiscale, *cf.* Fig. 4, a major computational challenge; *cf.* sec. 5.

## 4. Time Domain (TD) vs. Frequency Domain (FD)
Spectral lines and material response are obtained differently in Time Domain (TD) and Frequency Domain (FD) methods. FD analyze the problem in FD for various frequencies while in TD a Fourier transform of the response is employed. While FD may be more appropriate for small computational domains [9], TD has the following advantages: 1) Material nonlinearities, as
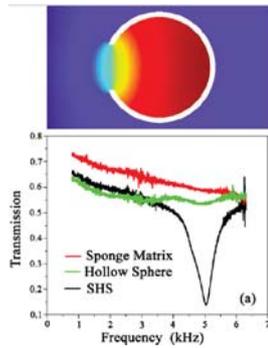
Figure 2. Resonance & transmission spectrum (SHS; [12]).
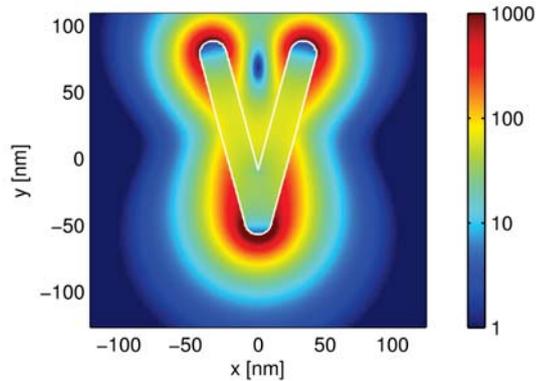
Figure 3. High gradient solutions in microscale [13].
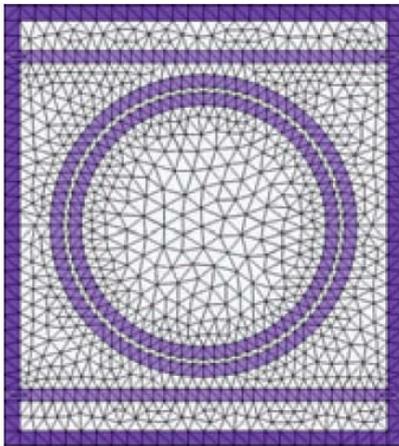

Figure 4. Multiscale geometries [9].
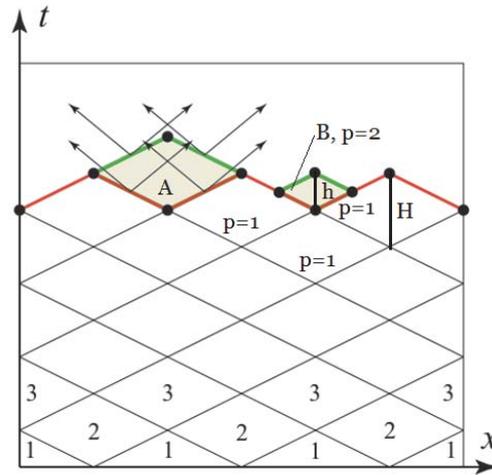
Figure 5. Schematic of SDG method (*cf.* sec. 5)

commonly encountered in metamaterials, are more naturally handled in TD; 2) Instead of several FD analyses, Fourier transformation to only one broad-band signal is sufficient in TD [13]; 3) Unlike the global spatial coupling in FD methods, in some TD methods the problem is local and solution scales linearly versus number of unknowns/elements; 4) Quasi-static FD analysis of stable state is not be sufficient when the early unsteady relaxation process is important [12].

5. Spacetime Discontinuous Galerkin (SDG) Finite Element Method

As mentioned, many TD approaches such as *Discontinuous Galerkin* (DG) methods [9] have a linear solution scaling versus number of elements, a major advantage over FD methods. However, there are still two concerns with TD methods. First, in linear scaling an explicit time integration method is needed. However, as shown in Fig. 6(a) for multiscale domains which are common in these applications, small elements severely limit the performance of these methods. While IMEX methods and subcycling in figs. 6(b-c) alleviate the problem, explicit time marching methods still perform poorly for multiscale domains. Second, frequency-dependent material properties induce a convolution term in TD. For example, $\int_{-\infty}^{\infty} \rho_0(x, t - t_0) \frac{\partial v}{\partial t'} \mathrm{d}t' + \nabla p = 0$ is the acoustic equation for frequency dependent density. The convolution term poses severe difficulties in TD.

Two approaches are used to eliminate the convolution term. First as in [14] by *Auxiliary Differential Equations* (ADE) additional fields are added to the system. Second, we maintain micro and macro fields in the formulation as opposed to homogenization to frequency-dependent metamaterials. For example in [15] convolution term is eliminated by preserving both microscale
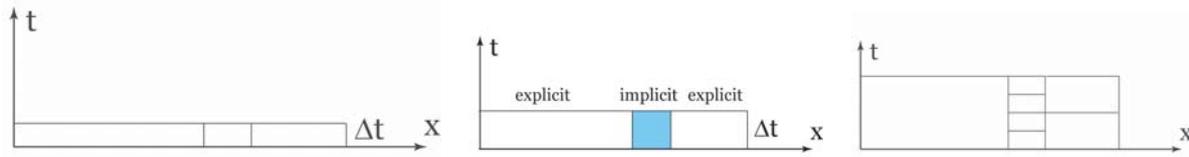
(a) Small time step for Multiscale domains.   (b) Implicit-Explicit method.   (c) Multistep time marching.

Figure 6. Multiscale domains, limitations (a) & remedies (b-c) for explicit Time Domain analyses: a) Smallest elements limit global time step; (b) Using Implicit time integration for small elements and explicit elsewhere (c) Time steps are adjusted based on element size.

(solid domain, undecorated) and microscale:

$$\bar{\rho}_m \frac{\partial^2 U_i}{\partial t^2} + \frac{\Sigma'_{ii}}{R} - \frac{\partial \Sigma_{ij}}{\partial X_j} = 0 \tag{1a}$$

$$\frac{m_2}{A} \frac{\partial^2 U_{2i}}{\partial t^2} - \frac{\Sigma'_{ii}}{R} = 0 \tag{1b}$$

Finally, the SDG method not only gracefully addresses the multiscale domain problem but also has several other advantages. In the SDG method, finiteness of the wave speed for hyperbolic problems, use of unstructured causal meshes, an use of discontinuous basis functions (a DG method) yields a local solution scheme [16, 17]. For example in figure 5, when the two inflows of element A are solved, it can be solved locally. The solution starts from any of the elements labeled 1 and continues to completion. Element B in Fig. 5 shows how element size and polynomial order can suddenly change. Some of distinct advantages of SDG over other TD methods are: 1) Linear cost vs. number of elements; 2) Excellent resolution of high gradient fields and discontinuities; 3) Arbitrary element size h and polynomial order p (element B); 4) Arbitrary high order in time as spacetime is directly interpolated instead of a separate finite difference integration in time (*cf.* element B); 5) Excellent for multiscale domains; local time step not affected by smallest size (*cf.* element B). While items 1-2 are common for DG methods, 3-5 are particular advantages of SDG over other DG methods.

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