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# Computation of resonant modes in cavities with a Discontinuous Galerkin time domain approach

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## ABSTRACT

We present a method of obtaining frequency domain quantities of an electromagnetic resonator, such as the frequency spectrum, quality factors, resonant frequencies and the associated mode shapes, using a parallelised Discontinuous Galerkin solver with explicit time marching. The method is validated using a 2D free-space cavity with analytically known resonant frequencies. The relative error in resonant frequency is quantified and we demonstrate a faster convergence of error, using the filter diagonalisation method (FDM), than with the traditional fast Fourier transform (FFT). The implementation of material dispersion in the solver is validated using a 2D dispersive cavity with known analytical solution.

***Key Words:*** *Finite Element, Discontinuous Galerkin, Electromagnetics, Resonant Cavities, Time Domain*

## 1. Introduction

Recent advances in manufacturing techniques, such as electron beam lithography, make it possible to manufacture resonant cavities on the scale of the wavelength of light. These nanoresonators, key components in nanolasers, can have many desirable qualities such as well defined resonant frequencies and high quality factors [1]. However, the typical scale and the geometric complexity introduce several challenges for numerical simulation.

The behaviour of these resonators is described by Maxwells' equations of classical electromagnetics. For dispersive materials, an auxiliary ordinary differential equation based on the Drude models [2] is coupled to the Maxwell system. Frequency domain solvers are traditionally employed to find the resonant frequencies and associated modes, but as the scale and geometric complexity of the devices increase, the large eigenvalue system that must be solved becomes computationally prohibitive.

We propose to use the Discontinuous Galerkin (DG) method with explicit time marching, which only requires solving a block diagonal system of equations for each timestep [3]. The frequency spectrum, resonant frequencies and quality factors can then be recovered by a Fourier transform of the time domain solution.

## 2. DG solution of the transient Maxwell's equations in dispersive media

Maxwell's equations of classical electromagnetics and the auxiliary ordinary different equation required for dispersive media can be written in linear, dimensionless, conservation form as

$$\frac{\partial \mathbf{U}}{\partial t} + \sum_{k=1}^{nsd} \frac{\partial \mathbf{F}_k(\mathbf{U})}{\partial x_k} = \mathbf{S}(\mathbf{U}) \,, \tag{1}$$

where $nsd$ denotes the number of spatial dimensions. The vector of unknowns, $\mathbf{U}$, the flux vectors, $\mathbf{F}_k$, and the source $\mathbf{S}$ are given by

$$\mathbf{U}_1 = \begin{pmatrix} \epsilon E_1 \\ \epsilon E_2 \\ \epsilon E_3 \\ \mu H_1 \\ \mu H_2 \\ \mu H_3 \\ J_1 \\ J_2 \\ J_3 \end{pmatrix}, \quad \mathbf{F}_1 = \begin{pmatrix} 0 \\ H_3 \\ -H_2 \\ 0 \\ -E_3 \\ E_2 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad \mathbf{F}_2 = \begin{pmatrix} -H_3 \\ 0 \\ H_1 \\ E_3 \\ 0 \\ -E_1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad \mathbf{F}_3 = \begin{pmatrix} H_2 \\ -H_1 \\ 0 \\ -E_2 \\ E_1 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad \mathbf{S} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ \omega^2 E_1 - \gamma J_1 \\ \omega^2 E_2 - \gamma J_2 \\ \omega^2 E_3 - \gamma J_3 \end{pmatrix},$$

where $E_k$, $H_k$ and $J_k$ are the $k$th spatial components of the dimensionless intensity vectors of electric field, magnetic field and the polarisation current respectively. The material parameters $\epsilon$, $\mu$, $\omega$ and $\gamma$ are the electric permittivity, magnetic permeability, plasma frequency and electron damping coefficient respectively.

We discretise the computational domain $\Omega$ on an unstructured mesh. The DG weak formulation [4] of (1) on an element $\Omega_e$ can then be written as

$$\int_{\Omega_e} \mathbf{W} \frac{\partial \mathbf{U}_e}{\partial t} d\Omega + \int_{\Omega_e} \mathbf{W} \cdot \left( \sum_k^{nsd} \frac{\partial \mathbf{F}_k (\mathbf{U}_e)}{\partial x_k} - \mathbf{S}(\mathbf{U}_e) \right) d\Omega + \int_{\partial\Omega_e} \mathbf{W} \cdot \mathbf{A}_n^- [\![\mathbf{U}_e]\!] \, d\Gamma_e = 0 \,,$$

where $\mathbf{U}_e$ denotes the solution vector restricted to the element $\Omega_e$, $\mathbf{W}$ is a vector of test functions and $[\![\mathbf{U}_e]\!] = \mathbf{U}_e - \mathbf{U}_{out}$ denotes the jump of the solution across the element boundary $\Gamma_e$. The boundary term, derived after introducing the numerical flux on the boundary and using a flux-splitting technique, results in

$$\mathbf{A}_n^- [\![\mathbf{U}_e]\!] = \frac{1}{2} \begin{pmatrix} -\mathbf{n} \times [\![\mathbf{H}]\!] + \mathbf{n} \times (\mathbf{n} \times [\![\mathbf{E}]\!]) \\ \mathbf{n} \times [\![\mathbf{E}]\!] + \mathbf{n} \times (\mathbf{n} \times [\![\mathbf{H}]\!]) \\ \mathbf{0}_3 \end{pmatrix} ,$$

where $\mathbf{n}$ is the outward unit normal of the element and $\mathbf{0}_3$ is a zero vector of length 3. After introducing the approximation of the solution and using a Galerkin formulation, the following system of ordinary differential equations is obtained,

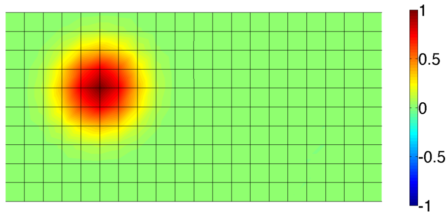
$$\mathbf{M} \frac{d\boldsymbol{U}}{dt} + \mathbf{R}(\boldsymbol{U}) = \mathbf{0} \,,$$

where $\boldsymbol{U}$ is the vector of nodal values, $\mathbf{M}$ is the block diagonal mass matrix and $\mathbf{R}(\boldsymbol{U})$ is the residual vector. The system of ordinary differential equations is advanced in time using a fourth-order explicit Runge-Kutta method.

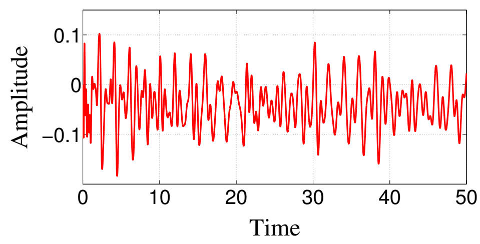
## 3. Computation of resonant frequencies

The engineering quantities of interest in cavities are usually the resonant frequencies, associated modes and quality factors. In order to obtain these quantities using a time domain solver, the electromagnetic field is first excited by introducing an initial condition or a source in the domain (Figure 1(a)). As the solution is advanced in time, its value is monitored at each timestep for a given period of time, $T$ (Figure 1(b)). Using the fast Fourier transform, or more sophisticated techniques, we can then obtain the frequency spectrum (Figure 1(c)) from the monitored solution. The resonant frequencies of the cavity can be obtained from the locations of peaks in the frequency spectrum by curve-fitting and the quality factors from the width of the peaks. Mode shapes can be obtained by running the time domain simulation with the resonant frequency as an input.

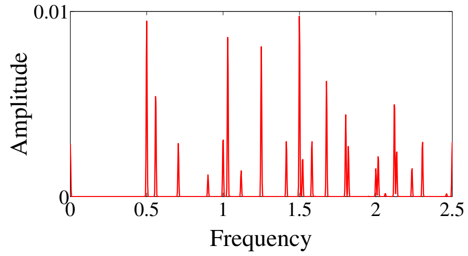
The error in frequency is inversely proportional to $T$, and the highest frequency is inversely proportional to the simulation timestep. The main limitation of the proposed approach is therefore the need for longer periods in order to minimise the error in the obtained resonant frequencies. To overcome this issue we considered the filter diagonalisation method [5] (FDM) which gives a much better accuracy than FFT in a significantly shorter time period.




(a) Gaussian initial condition




(b) Solution monitored at a point



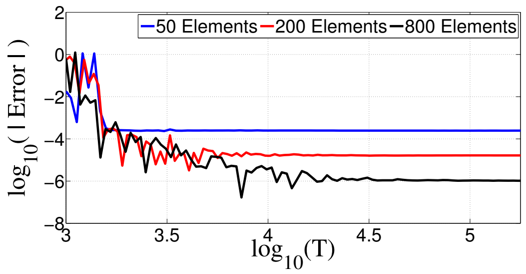

(c) Eigenspectrum obtained by FFT

Figure 1: Steps required to find the frequency spectrum and resonant frequencies shown for a 2D rectangular cavity.

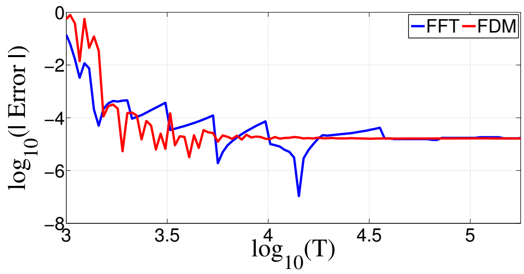
To further improve the performance of the proposed approach, the relative ease of parallelisation of the DG method is exploited to achieve the long periods required in reasonable computational time. The solver has been parallelised using MPI and the implementation and performance has been validated using two- and three-dimensional test cases.

## 4. Numerical Results

The first example presented is a rectangular 2D non-dispersive free-space cavity ($\epsilon = \mu = 1, \omega = \gamma = 0$) surrounded by a perfect electric conductor (PEC) with a width twice its length. Analytical expressions for the resonant frequencies of this cavity are known [6]. Figure 2(a) shows the relative error in the resonant frequencies converging as expected with $T$. The final value is the error due to the spatial discretisation of the domain, which decreases with mesh refinement. The error using FDM can be seen to converge almost an order of magnitude quicker than FFT, as Figure 2(b) shows.




(a)




(b)

Figure 2: (a) Convergence of the relative error in calculated resonant frequencies with increasing period T for three different meshes in a free space cavity. (b) Comparison of convergence with period obtained with FDM and FFT.

The second example presented is a dispersive cavity with an additional source term added to the right hand side of Maxwell's equations ((1)) to ensure that the problem has an exact known solution. The same 2D rectangular cavity as the previous example was considered filled with a gold medium ($\epsilon = 1, \sigma = 1, \omega = 6.7433, \gamma = 0.0799$). Snapshots in time of the solutions obtained for the electric intensity vectors are shown in Figure 3.

Optimal convergence (i.e. a rate of $p + 1$ ) was achieved in the $\mathcal{L}^2(\Omega)$ norm of the relative error in the solution as shown in Figure 4 for component $E_1$.

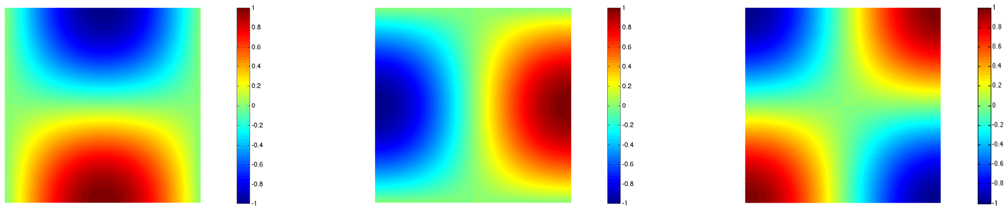


Figure 3: Left to right: Components $E_1$, $E_2$ and $E_3$ of the solution obtained for a rectangular cavity with a dispersive material and a volumetric source.

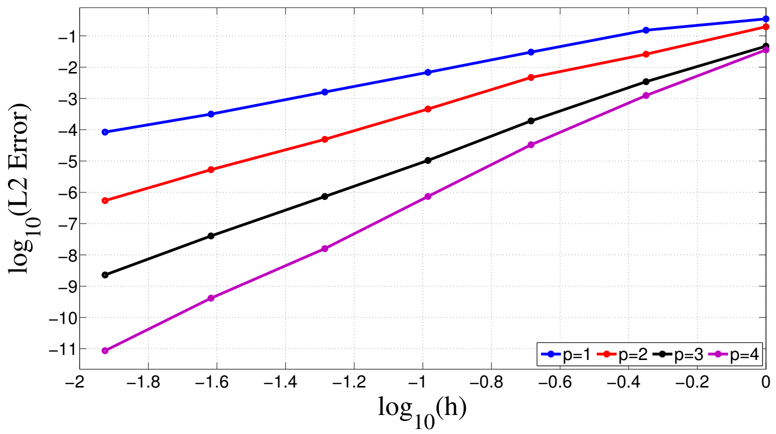



Figure 4: $h$-convergence of the $\mathcal{L}^2(\Omega)$ norm of the relative error in $E_1$ for a cavity filled with dispersive material with an additional source term.

## 5. Conclusions

A method has been presented for obtaining frequency spectrum, resonant frequencies, mode shapes and quality factors for resonant cavities using a parallelised Discontinuous Galerkin time domain electromagnetic solver. Excellent agreement with analytical values has been observed for the resonant frequencies of a 2D free-space resonant cavity, and the convergence of the solution with the time period has been presented. The dispersive media implementation has been validated with the expected $h$-convergence of the $\mathcal{L}^2(\Omega)$ norm of the relative error.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