OpenSEMBA/DGTD: An Open-Source Full-Wave Maxwell's Equations Solver

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***Abstract*—Numerical solvers have been essential tools in the industry, R&D and other similar fields in the last two decades. While it is important to understand the advantages and limitations of most common methods and look for the best candidates in terms of simplicity, accuracy, and computational performance; the capacity to be able to simulate, with relative simplicity, complex physical problems and obtain results which can serve as validations or preliminary testing has increased efforts towards obtaining more efficient and stable methods. In this work, we will discuss our choice to utilize the discontinuous Galerkin in the time domain (DGTD) method by extending an available finite element method library, MFEM, which allows us to introduce a Maxwell's equations solver in all dimensions without having to implement the basic framework a numerical method would require. A basic form of a DGTD solver has been successfully implemented, with further development planned in the future.**

Keywords—Discontinuous Galerkin, Time-domain analysis, Numerical Methods, Maxwell Equations

I. Introduction

The usage of numerical methodology to evaluate ordinary differential equations (ODE) and partial differential equations (PDE) has been one of the key areas of computational research in the latest decades [1][2]. Popular methods such as Finite Differences (FD) [3], Finite Volume (FV) [4] and Finite Element (FE) [5] have grown and become more capable of solving multitude of problems. Although their usefulness is not questioned, these methods are without their own shortcomings when studying wave problems in the time domain [6].

The continuous Galerkin (CG) method would have been a great candidate to be used in our studies of the Maxwell's equations, but its expensive to invert mass matrix (unless lumped) and potential instabilities in heavy directional stationary flow problems (i.e. advection-diffusion) are key critical weaknesses [7], invalidating the CG method as the best candidate for our problems. Thus, we require to look for another method which is more adaptable to the problem we aim to solve. Thankfully, by performing some modifications to the formulation, we can arrive at a candidate that satisfy our requirements.

In this work we introduce our open-source Maxwell's equations solver which uses the discontinuous Galerkin in the time domain (DGTD) method, a tool that has the aim to offer a powerful simulation framework to be used in conjunction with OpenSEMBA [8]. Thanks to the finite element library MFEM, we can ease the implementation of some of the basic functionalities one would expect from an electromagnetic equation's solver.

II. Discontinuous Galerkin in the Time Domain

The Galerkin approach is a combination of the formulation used in the Finite Volume and Finite Element methods where the space for the trial and test functions is chosen to be the same for both, a space of piecewise polynomial functions. Unlike the continuous Galerkin method, and as its name implies, one of the key features of the discontinuous Galerkin method is the discontinuous nature between the elements in the computational domain. The discontinuous nature is achieved through the duplication of degrees of freedom in the interfaces between elements which also ensures the locality of the scheme.

The weak and strong formulations can be recovered through an expansion of the discretized equations, which allow us to utilize a numerical flux employed in a similar form to that used in the Finite Volume method, which will be used to solve the duality issue on the interfaces between elements to recover a unique solution. The flux also offers the advantage of allowing upwinding, which contributes to enhance the stability of the method and helps with avoiding the appearance of spurious modes in the solution. In our specific case, the choice of flux is the Lax-Friedrichs flux along the normal on the faces between elements.

Starting from the basic form of Maxwell's three-dimensional equations,

$$\mu \frac{\partial \boldsymbol{H}}{\partial t} = -\nabla \times \boldsymbol{E}, \quad \varepsilon \frac{\partial \boldsymbol{E}}{\partial t} = \nabla \times \boldsymbol{H} \qquad (1)$$

rewriting this expression in the conservation law form yields

$$\boldsymbol{Q}\frac{\partial \boldsymbol{u}}{\partial t} + \nabla \cdot \boldsymbol{f}(\boldsymbol{u}) = 0 \quad (2)$$

with the new variables being defined as

$$\boldsymbol{Q} = \begin{pmatrix} \mu & 0 \\ 0 & \varepsilon \end{pmatrix}, \boldsymbol{u} = \begin{bmatrix} \boldsymbol{H} \\ \boldsymbol{E} \end{bmatrix}, \boldsymbol{f}(\boldsymbol{u}) = \begin{bmatrix} -\hat{n} \times \boldsymbol{H} \\ \hat{n} \times \boldsymbol{E} \end{bmatrix} = \begin{bmatrix} \boldsymbol{F_H} \\ \boldsymbol{F_E} \end{bmatrix} \quad (3)$$

where $\boldsymbol{E}$ and $\boldsymbol{H}$ are time-dependent electric and magnetic field vectors with their three spatial components on the *x*, *y* and *z* directions. μ and ε are the magnetic permeability and the electric permittivity, respectively, depending too on the spatial components, and $\hat{n}$ is the outward normal on the faces of the elements.

By applying Gauss' law twice to (2) and Lax-Friedrichs flux, we can obtain the semi-discrete scheme for all six components H_h^x, H_h^y, H_h^z and E_h^x, E_h^y, E_h^z . This is the strong form of Maxwell's equations. We can then rewrite the expressions in a way we can utilize later, as an example for H_h^x

$$\frac{dH_h^x}{dt} = -\mathcal{D}_y E_h^x + \mathcal{D}_z E_h^y + \frac{\mathcal{M}^{-1}}{2J} \cdot \int_{\partial D^k} (-\widehat{n_y}[E_h^z] + +\widehat{n_z}[E_h^y] + \alpha([H_h^x] - (\widehat{\boldsymbol{n}} \cdot [\boldsymbol{H_h}])\widehat{n_x}) \boldsymbol{l}(\boldsymbol{x}) d\boldsymbol{x} \quad (4)$$

where $\boldsymbol{l}(\boldsymbol{x})$ is the test function. The rest of the terms are defined as our operators, $\mathcal{D}_i$, the product of the inverse mass matrix and the stiffness matrix in the *i*-direction. $\widehat{n_\iota}[A_h^i]$, the jump matrix assembled on the interface between elements, multiplied by the normal in the *i*-direction and applied over the field vector A in the *j*-direction. $(\widehat{\boldsymbol{n}} \cdot [\boldsymbol{A_h}])\widehat{n_j}$, where $\widehat{\boldsymbol{n}} \cdot [\boldsymbol{A_h}] = \sum_{i = x,y,z} \widehat{n_\iota} \cdot [A_h^i]$, is similar to the previous operator, with the exception that we obtain three operators in the three different spatial directions and then they are multiplied by the normal in the j-direction, which is always the same as the direction of the field which is being time discretized. Lastly, $[A_h^i]$, the jump matrix assembled on the interface between elements applied on the field vector A in the *i*-direction.

The operators that are dependent on the α coefficient, the upwind coefficient, will be referred to as 'upwind' operators, which only appear if $\alpha \neq 0$, whereas the rest of the operators that are still inside the boundary integral are referred to as the centered operators. It is also worth noting that if we found ourselves in the case of a lower dimensional problem, the six equations would still be applicable as some of the operators would evaluate to zero.

III. OPENSEMBA/DGTD

OpenSEMBA/DGTD allows for the definition of a problem through a mesh with defined attributes on its elements, which can be domain or boundary conditions, materials or special regions; it also allows to define the desired problem solution parameters such as time stepping, centered or upwind schemes; sources, be initial or time dependent illuminations and also data retrieval into some of the previously mentioned visualization programs or into data sets through the use of exporter or point probes, respectively. The code uses the MFEM library as its base, which stands for Modular Finite Element Methods library. It is an open-source library initially developed in C++ by the Lawrence Livermore National Laboratory (LLNL). Thanks to this library, the solver natively counts with up-to-date functionalities such as easy-to-implement parallelization, support for hardware devices (CUDA, HIP, …), Paraview or GLVIS exporting for visualization, and more features.

OpenSEMBA/DGTD currently includes six Maxwell solvers, one for each dimensional case, with each one having Operator-By-Operator and Global Matrix schemes. The Operator-By-Operator scheme keeps each of the previously mentioned operators as individual sparse operators, which are multiplied by the correspondent direction field vector, then all solutions are added; the Global Matrix scheme assembles the operators in a global sparse matrix which is then multiplied in a single step with a global field vector. The Global Matrix scheme allows for a spectral study of the eigenvalues of the problem for stability purposes and the calculation of an optimal time stepping value through the use of the Power Method. These two schemes offer identical results.

The user can choose between Centered and Upwind fluxes in all solvers, and they all can define PEC, PMC and SMA conditions on their boundaries, although SMA requires the use of Upwind flux globally to be utilized. The setups can be illuminated with an initial Gaussian in all dimensions. Additionally, a time dependent travelling wave can be also used for illumination thanks to an extension of Total-Field Scattered-Field conditions which allows for illumination through the use of 'interior' boundaries. The previously mentioned characteristics are summarized in Fig. 1.

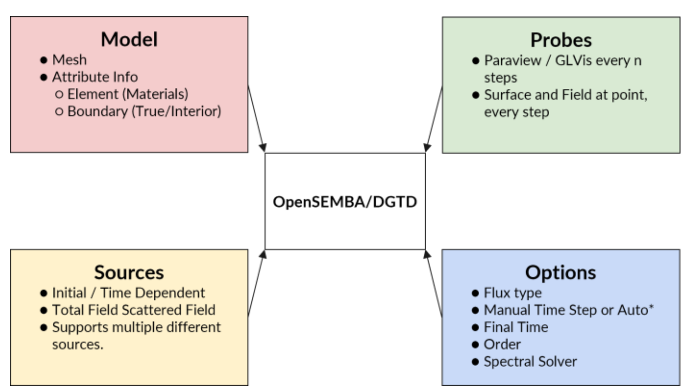
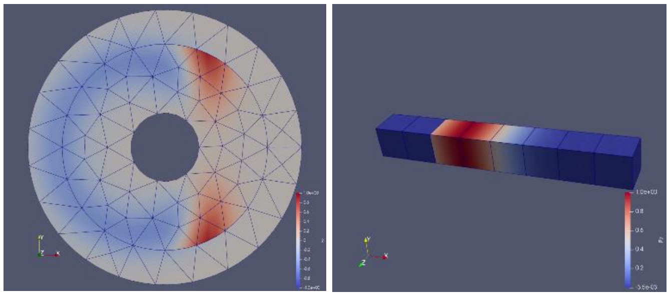


Figure 1. OpenSEMBA/DGTD problem definition.

In order to validate our implementations, multiple tests were added with the purpose of verifying the assembly of the different required operators, which must match the expected analytical results or those obtained through other code. These tests include matrix-to-matrix element checks for Mass, Stiffness, Flux and Penalty matrices, the two latter ones also include verifications for zero, one or two normal directions.



(a) (b)

Figure 2. Paraview visualization of simulated examples. (a) 2D Radar Cross Section with order 3 elements to adapt to curves. (b) Single element Total-Field Scattered-Field source load on a 3D 8x1x1 grid.

Additionally, the validation of the PEC, PMC and SMA boundaries has been performed through the solution analysis of 1D, 2D and 3D metallic resonant boxes. All validations can be verified by running the different test suites upon code compilation. The code and tests have been designed with the Unit Testing philosophy in mind, to allow for stable code refactorizations. More complex setups can be simulated as seen in Figure 2.

IV. Conclusions

OpenSEMBA/DGTD is a work-in-progress Maxwell's Equations solver and the simulations performed through the use of the previously mentioned tests verify the behavior of the simulation against analytical results or through the use of energy and boundary analysis.

At the time this work is being developed, a feature which aimed to implement Interior Boundary Face Integrators for general use has been implemented by the Dept. of Electromagnetism of the University of Granada, further improving the functionalities of the MFEM library.

Ultimately, OpenSEMBA/DGTD offers a free, open-source alternative for students and researchers alike, based on the discontinuous Galerkin in the time domain scheme.

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