Validating a high-order time domain hybrid implicit/explicit FEM implementation

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Abstract — **This paper discusses aspects of the verification and validation of a high-order time domain hybrid implicit/explicit FEM scheme, which also incorporates hybrid meshes. Methods to test both the spatial and temporal discretizations, as well as the hybrid mesh, are discussed.**

1 INTRODUCTION

This paper will present results from recent work on an efficient high-order time domain hybrid implicit/explicit FEM scheme, which has extended an earlier low-order implicit/explicit FETD-FDTD hybrid to high-order. In particular, aspects of the verification and validation of this scheme will be addressed.

To place this work in perspective, earlier work in this field will be briefly recounted. In [1], a provably stable FETD-FDTD hybrid was proposed, which for the first time brought these methods together without weak instability, offering the computational efficiency of the leapfrogging explicit FDTD for regular parts of the computational domain with the superior geometric modelling capability of the FETD. In this case, the FETD used an unconditionally stable implicit scheme based on the wave equation. The FDTD was shown to be equivalent to a coupled FETD scheme using mixed first order elements, with suitable reduced-order integration being uses to "mass lump" and hence produce a fully explicit scheme. In [2], an improved scheme was presented.

In [3], the present authors reviewed and compared three finite element schemes for the discretization of Maxwell's equations in the time domain; one based on the vector wave equation, and the other two on the coupled first order Maxwells curl equations. These were described as the EBHD formulation (discretizing $\vec{E}$, $\vec{B}$, $\vec{H}$ and $\vec{D}$) and the EB formulation (discretizing only $\vec{E}$, $\vec{B}$). Of the two coupled first order schemes, the former, originally proposed in [4] — but not implemented — had both previously unreported implementation issues (which were, however, successfully addressed in [3]) and serious performance limitations, so the coupled first order scheme used in the present hybrid is the EB formulation of [3]. In [5], a scheme was described to directly connect higher-order hexahedral to tetrahedral elements. With these component parts in place, and using diagonalized high-order hexahedral elements based on those of Cohen and Monk [6], an efficient high-order time domain hybrid implicit/explicit FEM scheme, incorporating hybrid hexahedral/tetrahedral meshes, was derived and described in [7, 8].

2 VERIFICATION AND VALIDATION

Verification and validation [9, Chapter 1] are essential when developing a new computational method. Not only may there be problems at formulation level, but implementation bugs are almost inevitable. For FEM implementations, checking convergence rates in h and p is a very standard method, but in the time domain, the issue is further complicated by the time-integration [3]. The literature on this topic is however limited.

Cavity eigen solutions comprise a good test of a new FEM code. Although the eigensolution can be computationally very expensive, from an implementation viewpoint (assuming a packaged eigensolver is being used) these are the simplest possible problems to solve, needing no sources, termination schemes, or time discretization, and basic boundary conditions can usually be trivially applied. The eigen problem is essentially a test of the semi-discretizations (i.e. a discretization in space only). It can be applied several ways (notation as in [3, 7]:

- As a test of 1-form ($\vec{E}$ fields in this formulation) semi-discretizations and their curls, the standard Helmholtz vector-wave eigen problem can be solved:

$$[S]\{e\} = \omega^2 [M_\epsilon]\{e\}. \tag{1}$$

- As a test of 1-form semi-discretizations, 2-form discretizations ($\vec{B}$ fields in this formulation) and the $[C]$ discrete curl operator, the following eigen problem, derived from the coupled first order system, can be solved:

$$[C]^T [M_{\mu^{-1}}][C]\{e\} = \omega^2 [M_\epsilon]\{e\}, \tag{2}$$

- As a test of 2-form discretizations and their divergence, the linearized acoustic vector wave equation [10] can be solved.

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Only the first two solutions are strictly necessary for electromagnetic wave problems, since the divergence of the basis functions is usually not needed in such codes. The last test is still useful as an independent verification of the 2-form basis functions if the second problem does not yield acceptable results. Cavity problems have smooth solutions and hence discrete p'th order bases should converge as $O(h^{2p})$ [11]. Under p refinement, exponential convergence should generally be seen.

Another very important characteristic of eigen solutions is that they expose spurious modes that are present in the semi-discretization. Driven problems can sometimes mask the presence of spurious modes, see e.g. the EBHD waveguide result in [3]. Eigen solutions were also fruitful in discovering the presence of spurious modes in higher order pyramidal elements, which were originally intended for use to connect the hexahedral and tetrahedral meshes; this is discussed in detail in the next section. (As mentioned, the present hybrid uses the new scheme in [5] to directly connect high-order hexahedral and tetrahedral meshes).

By applying the eigentests to the various semi-discretization and hybrid mesh combination permutations, correct operation of a code can be ascertained.

3 AN EXAMPLE: THE EIGENPROBLEM FOR HEXAHEDRAL, TETRAHEDRAL AND PYRAMYIDAL MESHES

To verify the proposed hybrid mesh in [5], the eigensolution of the vector Helmholtz equation,

$$\nabla \times \nabla \times \vec{E} - k^2 \vec{E} = 0, \tag{3}$$

in a 19x23x29 m PEC cavity (speed of light normalised to 1 m/s) is obtained, yielding the cavity mode wavenumbers. (Normalising c to unity is quite frequently encountered in physics, see for example [12]). Numerical results using hexahedral, hybrid hexahedral-tetrahedral and two different sets of pyramidal elements are compared in Table 1. The hexahedral mesh has a cell-size of $29/4$ m. The pyramidal mesh is formed by splitting each hex-element into six pyramids. The hybrid mesh utilises half of the hexahedral mesh; the other half is meshed with unstructured tetrahedrons that conform to the hex faces on the mesh interface Γ. The hexahedral elements apply Gauss-Lobatto mass lumping as described in [7, 8], making them suitable for explicit time-domain FEM methods.

Both pyramidal element sets are identical at mixed 1st order, and show no spurious modes. For mixed 2nd order, the Coulomb elements [13] ("Pyramids 1" in Table 1) suffer from spurious modes throughout the spectrum, while the Graglia [14] pyramids exhibit a limited number of spurious modes at frequencies ranging from about $\frac{1}{50}$ to $\frac{1}{4}$ of the lowest physical cavity mode eigenvalue. In Table 1, "Pyramids 2" show the first four spurious eigenvalues of the Graglia elements. "Pyramids 3" show the physical eigenvalues calculated using Graglia's elements after discarding the spurious values. In light of the spurious modes exhibited by the pyramids, a hybrid mesh using hexahedra, tetrahedra and pyramids was not constructed. (The spurious mode issue is not as closed a book as many have indicated — in particular on non-simplicial elements — and the work in [15] may offer an explanation for the issues encountered with these pyramidal elements.) The hybrid mesh developed here does not suffer from spurious modes, and delivers accurate results.

The convergence of the hexahedral and hybrid solution eigenvalues as the total number of DOFs increases is compared in Fig. 1.

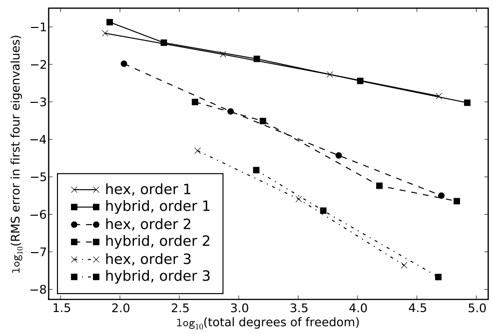

Figure 1: Convergence of hexahedral and hybrid mesh eigenvalues for mixed order 1 through 3 discretization.

The rate of convergence observed for the hybrid mesh discretization is the same as that of the individual hexahedral and tetrahedral discretization. The accuracy per degree of freedom of the pure hexahedral and hybrid meshes are also similar.

4 PULSED CAVITY

A related test is the pulsed cavity test, where a time-domain pulse is injected into a cavity [5], [16]. Although not a complete test of the full formulation, it is a useful intermediate step between the eigenproblem test and the short-duration waveguide pulse test described in the next section. The excitation is designed to excite every mode in the cavity. A measurement is made at a point in the cavity that will pick up all the modes. After performing an FFT on the logged data, resonant peaks centered around the cavity eigen-mode frequencies should appear. This is a good test to perform when a new time-integration

Solution type	Mode eigen-value k_0^2 $(\mathrm{rad.s}^{-1})^2$				RMS error %	total DOFs
	I	II	III	IV		
Analytic	0.030393	0.039075	0.045997	0.057732	—	—
Mixed 1st order discrete						
Hexahedra	0.028862	0.036075	0.042648	0.053793	6.78	75
Pyramids	0.030821	0.040152	0.046792	0.058448	1.88	459
Hybrid	0.029659	0.037784	0.043875	0.055175	3.80	234
Mixed 2nd order discrete						
Hexahedra	0.030384	0.039048	0.045968	0.057700	0.056	854
Pyramids 1	0.007825	0.007877	0.007970	0.010426	—	2774
Pyramids 2	0.000619	0.000679	0.000683	0.000779	—	3062
Pyramids 3	0.030402	0.039100	0.046025	0.057765	0.055	3062
Hybrid	0.030394	0.039078	0.046002	0.057767	0.031	1596

Table 1: First four eigenvalues for a rectangular cavity

scheme is applied to a semi-discretization that has previously been verified by the eigen-solution. Getting extremely high-resolution frequency-domain information requires careful signal-processing. This, along with the initial verification of the formulations developed in the course of the current research was presented in [3]. The pulsed cavity test is also a good test of stability and conservation; since the cavity is lossless, the resonances should never die down. Furthermore, if a given fully discrete scheme suffers from weak instabilities it shows up clearly over an extended cavity run. It also allows the convergence of the time integration to be studied in isolation, since in the limit the resonant peaks should converge to the eigen-frequencies of the semi-discretization.

5 SHORT-TIME WAVEGUIDE PULSE

To test the full discretization is not straightforward, in particular when reduced integration is also being employed for mass-lumping. Obtaining time domain solutions with analytical solutions that are not trivial, but at the same time do not depend on the implementation of peripheral formulations such as domain termination schemes, can be a challenge. (An example of an unsuitable case for such initial testing would be scattering from a PEC sphere; clearly, an operational boundary termination scheme is essential for such a problem). Using the analytical time-domain transient response derived for waveguide modes in [17], a wide-band (short temporal duration) waveguide pulse simulation can be compared to an analytical solution. Since the field evolution only needs to be measured for a short time, a length of empty waveguide after the measurement port prevents any reflections from reaching the measurement port within the evolution time frame; since only the length dimension need be of any significant electrical size, such a problem can be run without excessive memory and runtime requirements. Actually implementing a sensible numerical experiment is somewhat involved, and was described in [3]. That same experiment was repeated with a large number of the possible formulation permutations arising out research reported here. Some permutations included:

- All tetrahedral mesh with implicit time integration and various basis orders
- All hexahedral, using consistent $[M]$ matrix integration and various basis orders
- All hexahedral, using diagonalization
- Implicit/Explicit hybrid using only hexahedral elements
- Implicit/Explicit hybrid with tetrahedra in the implicit region and the waveguide mode launched in the implicit region
- Implicit/Explicit hybrid with tetrahedra in the implicit region and the waveguide mode launched in the explicit region.
- Implicit/Explicit hybrid with tetrahdra in the implicit region and the waveguide mode launched in the implicit region with a PML termination directly after the measurement port.

The results confirmed correct operation of both the formulation and the code which implemented it in all cases and will not be presented here.

6 CONCLUSION

Verifying and validating the implementation of complex formulation such as the hybrid implicit/explicit time domain FEM scheme, complicated further by using hybrid elements, is not a trivial undertaking, but there is little published literature on this. In the present paper, some of the methods which were found useful in this present application have been outlined.

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