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Adaptive Mesh Refinement for Time-Domain Electromagnetics Using Vector Finite Elements: A Feasibility Study

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Abstract

This report investigates the feasibility of applying Adaptive Mesh Refinement (AMR) techniques to a vector finite element formulation for the wave equation in three dimensions. Possible error estimators are considered first. Next, approaches for refining tetrahedral elements are reviewed. AMR capabilities within the Nevada framework are then evaluated. We summarize our conclusions on the feasibility of AMR for time-domain vector finite elements and identify a path forward.

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Introduction

With an implementation of a vector finite-element formulation of the wave equation within the Nevada framework, the finite-element method (FEM) has become a key tool in the analysis of weapon systems and pulsed power components at Sandia. The unconditionally stable, massively parallel implementation provides Sandia with a unique electromagnetic analysis capability. In many cases the limiting factor is now the ability to generate adequately resolved meshes. Adaptive-mesh refinement (AMR) techniques which modify the element size (h-adaptivity) as the simulation evolves address this issue by optimizing the distribution of unknowns for improved accuracy and computational efficiency. Besides facilitating the more effective utilization of computational resources, AMR provides for improved fidelity in modeling electromagnetic fields as required by many critical and coupled physics phenomena. An AMR capability reduces the dependence of our simulations on the limitations of volumetric meshing tools and expert domain knowledge. The development of error metrics will also aid in reducing uncertainty in our simulations.

The formulation of interest [25] is the wave equation for the electric field expanded using vector (Whitney one-form [26] or Nédélec edge [19]) basis functions. The current implementation employs linear (or first-order) basis function. Because the hexahedral basis function are non-divergence free for skewed elements we are primarily interested in tetrahedral elements. The formulation employs an unconditionally stable time advancement scheme allowing the arbitrary selection of a time step relative to the edge lengths present in the mesh.

The report is structured as follows. We begin with a review of error estimators and consider some possible estimators for the formulation of interest. Next, we consider approaches for refining tetrahedral elements and discuss the relative merits of the approaches for edge basis functions. We then evaluate the AMR capabilities of the Nevada framework keeping in mind the requirements for implementing error estimators and refining tetrahedral elements. We summarize our conclusions on the feasibility of AMR for time-domain vector finite elements and identify a path forward.

Error Estimators

The investigation of numerical error in finite-element calculations is a subject that has received a great deal of attention. Typically analysts are aware of such errors but tend to rely on their judgment or intuition rather than attempting to quantify the error. Such an approach can be fraught with error, even for the most experienced analysts.

The direct calculation of the numerical error, e

$$e = u - u_h \tag{1}$$

requires the exact solution, u, which in typically not available for most problems of practical interest as well as the computed approximate solution u_h.

A priori error analysis typically only provides general information on the rate of convergence of the finite-element approximation.

A posteriori error estimation develops an error estimator which the approximates the norm of numerical error using the computed solution u_h. Typically, a local (e.g., element) error indicator, η_k, a function of the locally computed solution is used to construct a global error estimator, ε. For example, one approach is to define

$$\varepsilon = \left(\sum_k \eta_k^2 \right)^{1/2} \tag{2}$$

The effectivity index of an error estimator can be defined as the ratio of the error estimator to the energy norm of the numerical error

$$\frac{\varepsilon}{||e||} \tag{3}$$

An asymptotically exact estimator is one whose effectivity index approaches unity in the limit of vanishingly small cell size.

Advances have been made in the theory of a posteriori error estimation [1], especially for one and two-dimensional elliptic partial differential equations. However, little theoretical work exists for three-dimensional hyperbolic partial differential equations. The two main categories of a posteriori error estimators are recovery and residual based. Recovery based error estimators were first introduced by Zienkiewicz and Zhu [28] and were justified through a heuristic argument. However, recovery based error estimators have since been subjected to theoretical analysis. The residual based error estimators were first introduced by Babuska and Rhienboldt [3] and have experienced continued theoretical development to this day. Residual based estimators can further be classified as being explicit or implicit. Implicit a posteriori error estimators involve the solution of an auxiliary local boundary value problem approximating the residual equation satisfied by the numerical error. The relationship between the residual and recovery based methods was examined and explained by Zhu and Zhang [27].

Recovery Error Estimator

The original recovery error estimator was defined and justified through heuristic arguments [28]. Later precise mathematical proofs were given to show the bounds on this type of error estimator for 1-D and 2-D elements [14]. In addition, superconvergent patch recovery techniques have been developed but apply only in special circumstances. In particular, superconvergence has not been investigated for vector basis functions. Recovery error estimators based on the recovery of equilibrium of patches [7],[6] have been developed to address cases were superconvergent points do not exist.

Conceptually the recovery error estimator is easy to understand. As noted above, in general the exact solution is not known and a method to recover this solution is needed to evaluate the error - hence the name recovery error estimator. The recovered solution u_* replaces the exact solution u in equation (1) to estimate the error. Any recovery process which reduces error in the solution has been shown to produce a reasonable error estimator. If the recovered solution converges at a higher rate than the computed solution, then the error estimator will be asymptotically exact.

The following error estimator is based on the application of recovery based error estimation to magnetostatic problems solved using a vector potential. In [18] the individual element error in the magnetic energy was given by

$$e^e = \sqrt{\int_{V^e} (\bar{B}_h^e - \bar{B}_*^e) \cdot \nu (\bar{B}_h^e - \bar{B}_*^e) dV} \tag{4}$$

where the superscript e implies an elemental quantity, $\bar{B}$ is the magnetic flux density, ν is the reluctivity or the inverse of the permeability, and the subscript $*$ indicates a recovered quantity.

The magnetic flux density recovery, $\bar{B}_*$, is done in two steps. First the average magnetic flux density at an edge is calculated by averaging the magnetic flux density contributions of the n elements that share that edge

$$\bar{B}_{ave} = \frac{1}{n}\sum_{i=1}^{n} \bar{B}^{e_i} \tag{5}$$

where $\bar{B}^{e_i}$ is the magnetic flux density in element e_i. Next the magnetic flux density along an edge

$$B_j^{edge} = \hat{l}_j^{edge} \cdot \bar{B}_{ave} \tag{6}$$

is expanded using the shape function to give the spatial dependence of the recovered magnetic flux density within an element.

$$\bar{B}_*^e = \sum_j \bar{N}_j \bar{B}_j^{edge} \tag{7}$$

The element error defined in (4) can then be calculated.

The final question is how to use the error to select elements for refinement. A standard technique is normalize the elemental error (4) by the average energy per element to define an elemental error indicator

$$\eta^e = \frac{e^e}{\sqrt{\frac{1}{N_e}\sum_{e=1}^{N_e}\int_{V_e} \bar{B}^e \cdot \nu \bar{B}^e dV}} \tag{8}$$

Once this indicator exceeds a predetermined threshold the element is marked for refinement.

The problem of interest is the wave equation with the electric field described by Whitney one-forms (which automatically provide tangential continuity of these fields across the elements). When linear order elements are used to expand the electric field, the application of Maxwell's equations to find the magnetic flux density will give a constant value in an element. As a result, a recovery error estimator similar to the one described above can be applied to the problem of interest.

Residual Error Estimator

Residual error estimators make use of the approximation for the solution in form of the residual, the bilinear form for the weighted residual formulation, the equation for the error, and the orthogonality property of the error. After considerable algebra the energy norm of the numerical error can be written [1]

$$\|e\|^2 \leq C\left\{\sum h_k^2 \|r\|^2 + \sum h_k \|R\|^2\right\} \tag{9}$$

h_k is the diameter of the element, C is a (unknown) constant, r and R are the interior and boundary residual, respectively. The summations are over the elements and the boundaries of the elements. The contribution from each element to the error bound can be determined and used to identify candidate elements for refinement as a local error indicator

$$\eta_k^2 = h_k^2 \|r\|^2 + \frac{1}{2} h_k \|R\|^2 \tag{10}$$

Because the above indicator can be computed explicitly an error estimator based on (10) is referred to as an explicit estimator. Residual error estimators were used by Salazar-Palma and Garcia-Castillo in the quasi-static analysis of transmission lines [13]. For one and two-dimensional cases the constant C can be determined explicitly. The three-dimensional case using tetrahedral vector elements has not been considered.

The formal application of (9) in what is known as the classical element residual method involves solving an auxiliary problem over local subdomains for the error with the residual as the forcing function. Such approaches have been successfully applied to one and two-dimensional elliptical systems. For the three-dimensional time-dependent of interest, the bilinear form for the initial value problem can be extracted from [25] as

$$\begin{aligned} B(\bar{E},\bar{W}) = \int_\Omega \nabla \times \bar{W} \cdot \nabla \times \bar{E} dv + \frac{\varepsilon_r}{c^2} \int_\Omega \bar{W} \cdot \frac{\partial^2 \bar{E}}{\partial t^2} dv + \mu_0 \int_\Omega \bar{W} \cdot \frac{\partial \bar{J}}{\partial t} dv \\ + \oint_S \frac{1}{c\mu_r} \hat{n} \times \frac{\partial \bar{E}}{\partial t} \cdot \hat{n} \times \bar{W} ds = 0 \end{aligned} \tag{11}$$

While the application of residual based estimators has not been performed for this particular formulation, strides have been made to formulate an error estimator under simplifying assumptions. Consider the steady-state case for three-dimensional microwave devices and two-dimensional waveguides with a port excitation [24].

$$B(\bar{E},\bar{W}) = \int_\Omega \nabla \times \bar{W} \cdot \nabla \times \bar{E} dv - k^2 \int_\Omega \bar{W} \cdot \varepsilon_r \bar{E} dv + j\omega\mu_0 \oint_S \bar{W} \cdot \bar{J} ds = 0 \tag{12}$$

In this case the impressed current $\bar{J}$ is over the port of the device. A reflection coefficient can be defined as the scattering parameter

$$S_{11} = 1 - \oint_{port} \bar{E} \cdot \bar{J} ds \tag{13}$$

An error functional can then be defined as the error in reflection coefficient

$$F = S_{11}(\bar{E}) - S_{11}(\bar{E}_h) = \oint_{port} \bar{e} \cdot \bar{J} ds \tag{14}$$

Using the bilinear form and the standard orthogonality condition for the error in the Galerkin projection, the error functional can written as

$$F = \frac{1}{-j\omega\mu_0}\left[\int_\Omega \nabla\times\bar{e}\cdot\nabla\times\bar{e}dv - k^2\int_\Omega \bar{e}\cdot\varepsilon_r\bar{e}dv\right] \tag{15}$$

Noting that the terms in (15) can be recast in terms of volume and surface residual currents, an element error indicator is defined as

$$\eta^e = \int_{\Omega^e} \bar{e}^e\cdot\bar{j}_v^e dv \tag{16}$$

To evaluate η^e only from local sources an approximation is made. The error $\bar{e}^e$ evaluated in each element is expressed in terms of an approximate Green's function. This can be interpreted as solving the implicit residual system in an approximate sense. As a result the element error indicator can be computed explicitly solely from the approximate solution $\bar{E}_h$. The contributing terms have the convenient physical interpretation of the residual change and current in the element. It has not been investigated whether a similar port-based approach can be adapted for use with a time-domain formulation.

Finally, a popular, intuitively appealing heuristic error estimator notes the prominent role the jump in inter-element flux plays in (10). For example, consider the technique applied to the normal electric flux density for two-dimensional elements [9]. Extending to three dimensions, an error indicator at interior faces can be defined as the difference in flux continuity between adjacent elements

$$\eta^{face_{i,j}} = |\hat{n}\cdot(\varepsilon_i\bar{E}_i^e - \varepsilon_j\bar{E}_j^e)| \tag{17}$$

A measure of the error is

$$\|\eta^{face}\|^2 = \int_{face}\left(\eta^{face}\right)^2 ds \tag{18}$$

A global error estimator is obtained as the root-mean-square over the interior faces

$$\varepsilon = \left[\sum \|\eta^{face}\|^2\right]^{1/2} \tag{19}$$

Refinement of Tetrahedral Elements

In this section we consider approaches for refining tetrahedral elements. We begin by reviewing some definitions that are commonly used to characterize the refinement algorithm and the resulting mesh. Next we highlight some previous work in this area. We conclude by discussing the relative merits of each of the approaches for vector finite elements.

A mesh is called compatible, consistent, closed, or conforming if the intersection between any two elements is either empty, a common face, a common edge, or a common node. A mesh is referred to as stable if the refined element quality is bounded from below. Typically the interior angles of an element are used as the quality metric but this is not always the case. When the interior angle quality metric is used, a stable mesh may also be referred to as being non-degenerate. The refinement algorithm is called finite or bounded if it can be shown that a finite number of steps produce a conforming mesh. A sequence of meshes may be called nested if there is a clearly defined element parent/child hierarchy in either a topological or logical sense.

Spatial Subdivision

Although not the focus of this section, the creation of the original mesh can be closely related to the refinement approach. Popular approaches for unstructured tetrahedral mesh generation include advancing front methods which fill empty regions and spatial subdivision approaches like octree and Delaunay based techniques that place additional elements/nodes in an existing grid [17], [10]. The latter approaches are particularly relevant because the issue of adding additional degrees of freedom is central to mesh refinement. Likewise the issue of mesh quality is a closely related topic because approaches for improving quality include node insertion/deletion, local topology changes like face/edge swapping, and mesh smoothing to relocate nodes [11].

Because the octree mesh generation method has a strong theoretical element quality guaranty it has also been considered as an approach for mesh refinement. Since octasection rapidly subdivides volumes it is attractive in cases where the initial mesh is coarse. The sequence of meshes produced by octree subdivision is nested. Bey [5] presented an octree based regular refinement algorithm that defines new nodes at the midpoints of all element edges. However, a set of irregular refinement rules based on adding nodes to mid-points of edges for four specific element configurations must be used when applying the technique to a subset of the elements in a mesh in order to close the grid. Proofs show that the algorithm produces consistent and stable meshes. Liu and Joe [16] described a similar subdivision approach that uses the subset of elements with either one, two, or three split edges to produce a conforming mesh with a provable bound on element quality.

Because the Delaunay criteria leads to a prescription for defining elements as nodes are added to a mesh it is a popular approach for mesh refinement. Nehl and Field [20] presented a technique which added nodes at the midpoints of selected edges to produce a compatible mesh. Edges were selected by identifying base nodes with excessive nodal error. Locally applied Delaunay tessellation was used to individually subdivide the elements with added nodes. Golias and Tsiboukis [12] used a similar approach but included node relaxation to improve the quality of the refined elements. Olszewski *et al.* [21] also applied local Delaunay tessellation to elements selected similarly to Nehl and Field but explicitly defined an algorithm based on using edge lengths to order nodes to insure a compatible mesh.

Edge Bisection

Algorithms based on bisection have been a popular for refining tetrahedral elements because by themselves they can produce a locally refined conforming mesh. Bänsch [4] presented a reversible algorithm for bisecting elements that produces a conforming mesh and proved the finiteness of the algorithm and stability of the resulting mesh. The algorithm works by marking a refinement edge on each element face. The global refinement edge shared by two faces is bisected and the algorithm prescribes how to mark refinement edges on the new faces. Elements with nonconforming nodes are iteratively bisected until a conforming mesh is obtained. Rivara [23] developed an algorithm based on generalized or longest edge bisection which produces a conforming mesh. However, the finiteness of the algorithm and the stability of the resulting mesh has not been proved for tetrahedral elements. One issue with the bisection approach is the quality of the elements resulting from bisection. Liu and Joe [15] describe a bisection algorithm which is conforming, finite, guarantees the quality of refined tetrahedral elements, and allows local refinements on elements to be smoothly extended to their neighbors. Their algorithm is similar to Bänsch's but classifies marked elements as one of four types instead of red, black, or other. Arnold, Mukherjee, and Pouly [2] presented a bisection algorithm and provided a bound on its finiteness that is an alternate but complete version of Bänsch's algorithm. Their algorithm also classified marked elements as one of four types. Plaza and Carey [22] described a bisection based finite algorithm that subdivides faces then elements in a compatible manner. Because the algorithm uses the faces of the mesh it is called skeleton based refinement.

Choi, Byun and Hwang [8] described an algorithm which switches between octasection and longest edge bisection on selected elements followed by iteratively applied face swapping and node relaxation to improve element quality. Proofs show that the algorithm is bounded and produces a compatible mesh. The algorithm has characteristics of both Bänsch's bisection and skeleton based refinement.

For the application of refining a course initial mesh, an octasection based approach seems appropriate. However, because the formulation of interest employs edge basis functions, the edge bisection based algorithms would be more suitable. By bisection edges, the location of the degrees of freedom in the formulation of interest, additional unknowns can be added where the error is the largest. The algorithm presented by Liu and Joe [15] is particularly attractive because it guarantees the quality of the generated tetrahedral elements.

Adaptivity in the Nevada Framework

The Nevada framework provides support for adaptive mesh refinement by dividing elements into uniformly smaller sub-elements. The three-dimensional AMR support presently in place is only applicable to hexahedral elements, where each element is divided into eight uniformly smaller hexahedral elements. Support exists for refinement to occur at the beginning of the simulation (initial refinement) or dynamically based on an error metric. The error metric can be used to trigger either element refinement or unrefinement. The maximum number of levels of refinement can be controlled by element block and an element budget can be specified to refine elements with the largest error first if space is at a premium. Several controls specific to unrefinement are also available. A dynamic load balance capability is supported to keep the work load balanced in parallel.

Our first test was to verify that the UTDEM implementation would function properly when initial refinement was applied to a purely hexahedral mesh. To test initial refinement on a hexahedral mesh, a parallel-plate transmission line featuring a port launcher on one end and a reflector on the other end was meshed with hexahedral elements. One reason for selecting this test problem was that it has a simple analytical solution. The test case was run with up to two levels of refinement. Each refinement level increases the number of hexahedral elements by eight. The theoretical voltage pulse at an observer midway down the line show in Figure 1 was progressively improved by increasing levels of refinement as indicated in Figure 2.

Next the UTDEM implementation was modified to work with dynamic refinement by allowing complete re-initialization of the system matrix and boundary conditions after detection of a change in the topology. The modification was tested by triggering the topology change without actually having one and testing the results against those of the normal code path. The results were identical, both serial and parallel. During this testing it was observed that the performance cost of re-initialization was notable and will require performance tuning for a production implementation.

The next step was to add the methods necessary to refine a tetrahedral element. The simplest possible element refinement was chosen for testing which adds a single center node and splits the original element (parent) into four new tetrahedral elements (children). We denote this type of refinement as 1:4. The necessary interpolation method to place parent fields onto child edges was added. We discovered that the accurate interpolation of the fields to new edges was critical. Initial testing included refining only one element,

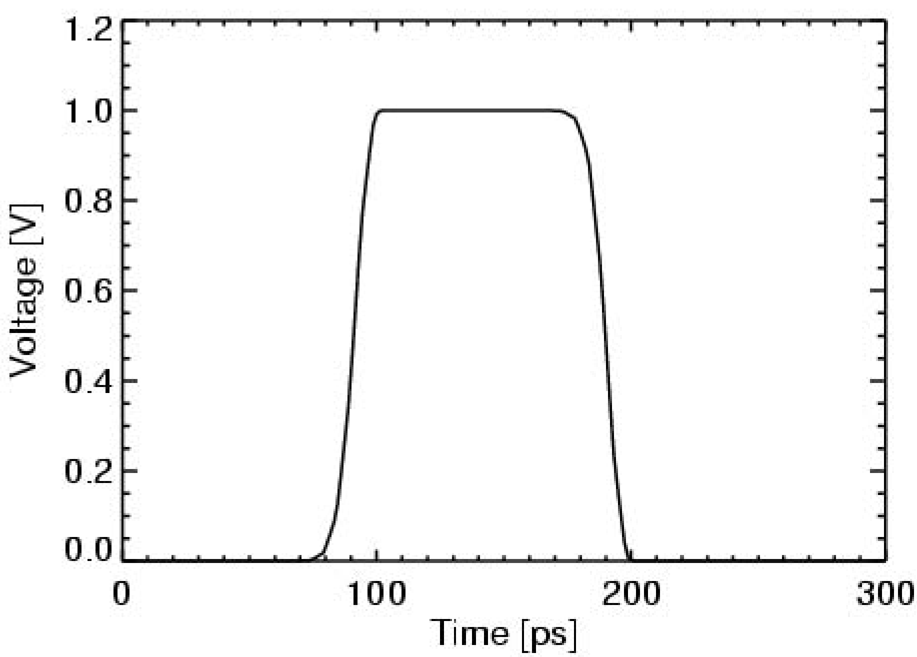

Figure 1. Theoretical voltage pulse at an observer midway down the line.

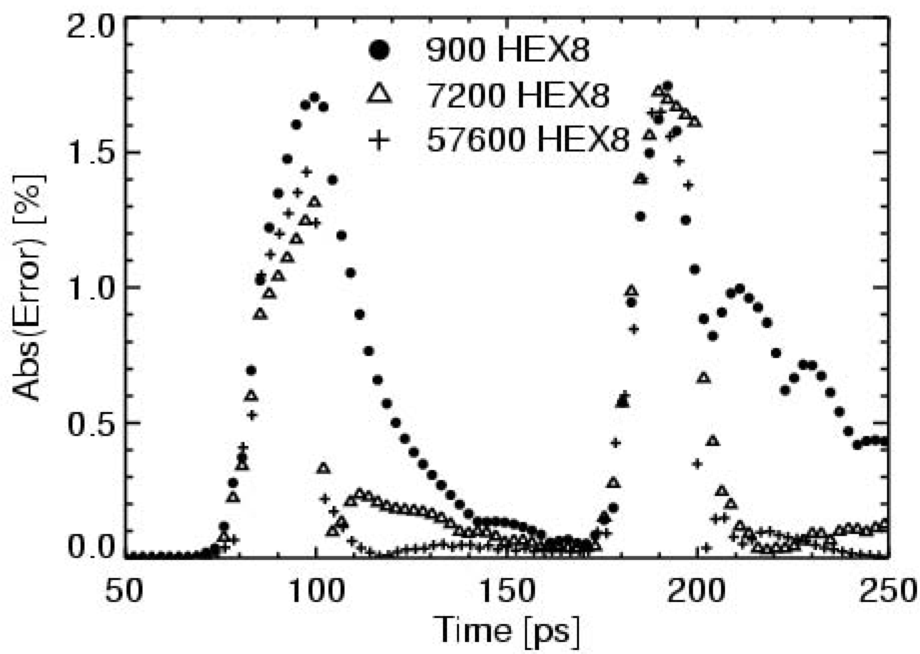

Figure 2. Percent difference from theoretical in an observer voltage for progressively refined meshes.

then two, then half the elements at a given time cycle. Once this was determined to be functional, a simplistic error metric based on the jump in the normal electric flux density between elements was added and the code was allowed to refine as necessary. Results from the various levels of refinement compared favorably with those from the original simulation.

A matching 4:1 unrefinement method was also added. This too appeared to work well based on the agreement of results with and without refinement/unrefinement.

Finally, a more realistic method to refine tetrahedral elements was implemented. The scheme involved marking an edge to bisect based on the largest face error and splitting the element into two tetrahedral elements (1:2 refinement). This was a more realistic test of the AMR support provided by the framework for our application as it represents the simplest form of edge bisection. Even this simplistic form of bisection required a special algorithm to produce a conformal mesh. This test identified some potential framework issues for our application. Firstly, some applications may require support for different initial refinement and dynamic refinement algorithms and/or a more advanced algorithm for initial refinement element marking. For example, our requirement of a conformal mesh precludes simply marking all elements for initial refinement. Secondly, current framework applications allow for the possibility of a non-conformal mesh during dynamic refinement (resulting in so-called "hanging nodes"). While not a significant obstacle, some design refactoring will be required to allow applications to override the current adaptivity controller algorithms so that applications that require a conformal mesh can implement such an algorithm. Thirdly, to implement a general recursive bisection algorithm some design refactoring may be required to allow for the possibility of multiple element marking and refinement passes within a single time step.

Time constraints did not allow for significant investigation of parallel issues such as load balancing. However, the simple 4:1 tetrahedral refinement scheme was demonstrated to work in parallel.

Path Forward

It is quite clear from this brief investigation, that the key components required to implement AMR for tetrahedral vector finite-elements exist. While little theoretical investigation into a posteriori error estimators for three-dimensional hyperbolic systems has been published, the Zienkiewicz and Zhu [28] recovery-based error estimator has achieved significant success in a broad range of applications. Several algorithms with provable characteristics for subdividing tetrahedral elements exist. Some simplistic prototyping in the Nevada framework has demonstrated that there is significant, useful leveraging to be obtained from the Nevada framework AMR capabilities.

A mix of software development and theoretical investigation tasks remain as the next step in a path forward. The next logical step is the implementation of a prototype capability to allow simultaneous numerical/analytic investigation of issues specific to transient electromagnetics.

- Identify appropriate test cases to use to validate the prototype AMR capability. Cases need to address the following issues:
  - Contain representative features of applications of interest.
  - Consider the effect of non-local errors (dispersion) in wave propagation applications on error estimators and error reduction resulting from AMR.
  - Investigate the effect of reducing the average edge length on accuracy of the unconditionally stable formulation.
  - Allow numerical verification of the error estimator effectivity by having a well known solution.
- Implement the magnetic flux density recovery based and normal electric flux density jump heuristic error estimators. Additionally we
  - Need a more formal theoretical understanding of these error estimators.
  - Need to investigate methods for identifying appropriate refinement thresholds from these local error indicators.
  - Need to numerically validate the effectivity of these error estimators.
- Implement a recursive bisection algorithm for subdividing tetrahedral elements. Primary interest is in refinement but the implementation should not preclude the addition of an unrefinement capability if time permits.
- A more quantitative investigation of parallel and performance issues needs to be performed.
  - The cost of reinitialization needs be quantified.
  - The parallel load imbalance needs to be quantified.
  - The framework provided dynamic load balancing capabilities need to be investigated.

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