Implicit a posteriori error estimation for the time-harmonic Maxwell equations

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MAFELAP Conference, Brunel University, London
14 June, 2006

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Outline of Presentation

- Time harmonic Maxwell equations
- Definition of the local error equations
- Numerical solution of the local error equations
- Theoretical results for the local error equations and implicit error estimates
- Numerical examples
Time Harmonic Maxwell Equations

- Time harmonic Maxwell equations - function spaces with perfectly conducting boundary conditions:

\[
\text{curl curl } E - k^2 E = J, \quad \text{in } \Omega \subset \mathbb{R}^3
\]
\[
E \times \nu = 0, \quad \text{on } \partial \Omega,
\]

with \( J \in [L_2(\Omega)]^3 \) a given source term and \( \nu \) the outward normal on \( \partial \Omega \).

- The Hilbert space corresponding to the Maxwell equation is:

\[
H(\text{curl}, \Omega) = \{ u \in [L_2(\Omega)]^3 : \text{curl } u \in [L_2(\Omega)]^3 \},
\]
\[
H_0(\text{curl}, \Omega) = \{ u \in H(\text{curl}, \Omega) : \nu \times u|_{\partial \Omega} = 0 \}
\]

equipped with the curl norm:

\[
\| u \|_{\text{curl}, \Omega} = (\| u \|_{[L_2(\Omega)]^3}^2 + \| \text{curl } u \|_{[L_2(\Omega)]^3}^2)^{1/2}.
\]


\textbf{Definitions}

- Define the bilinear form $B_K$ on $H(\text{curl}, K) \times H(\text{curl}, K)$ and the trace operators $\gamma_T$ and $\pi_T$ with

\[ B_K(u, v) = (\text{curl } u, \text{curl } v)_K - k^2(u, v)_K \]

\[ \gamma_T v = \nu \times v|_{\partial K} \text{ and } \pi_T v = (\nu \times v|_{\partial K}) \times \nu. \]

- Weak formulation of (1): Find an $E \in H_0(\text{curl}, \Omega)$ such that

\[ B_\Omega(E, v) = (J, v), \quad \forall v \in H_0(\text{curl}, \Omega). \]

- Discrete weak form of (1): Find an $E_h \in H_0^h(\text{curl}, \Omega)$ such that

\[ B_\Omega(E_h, v_h) = (J, v_h), \quad \forall v_h \in H_0^h(\text{curl}, \Omega), \]

where $H_0^h$ is the Nédélec edge element space (e.g. of order 1).
Error Estimation: Basic Setting

• Define the computational error on an element $K$ as:

$$e_h = (E - E_h)|_K.$$  

• Overall aim: estimate $\|e_h\|_{\text{curl}, K}$.  

• Informations at hand:
  ▶ $J$, $E_h$ with boundary conditions, the subdomain $K$.
  ▶ The element residual on $K$

$$r_K := J - \text{curl curl } E_h + k^2 E_h \text{ in } K.$$  

▶ The tangential jump of the curl at the element face $l_j$ between $K$ and $K_j$

$$R_{l_j} = \frac{1}{2}(\nu_j \times \left[ \text{curl } E_h|_K - \text{curl } E_h|_{K_j} \right]).$$
A Posteriori Error Estimates

- Objective: estimation of the error for an existing approximation.
- Main tool: weak form for the error, localization to the subdomains.

- Two types of a posteriori error estimates are frequently used:
  - **Explicit error estimates**, which use data provided by the numerical solution; practically a “simple formula” depending on known data.
  - **Implicit error estimates**, which solve local error equations with the data provided by the numerical solution.
Local Error Equation

• Variational formulation for the local error: Find an $e_h \in H(\text{curl}, K)$ such that:

$$B_K(e_h, \nu) = (\text{curl } e_h, \text{curl } \nu)_K - k^2(e_h, \nu)_K$$

$$= (\text{curl } E, \text{curl } \nu)_K - k^2(E, \nu)_K - ((\text{curl } E_h, \text{curl } \nu)_K - k^2(E_h, \nu)_K)$$

$$= (J, \nu)_K - (\gamma_{\tau} \text{curl } E, \pi_{\tau} \nu_{\partial K})_K - B_K(E_h, \nu), \quad \forall \nu \in H(\text{curl}, K).$$

• At the faces $l_j$ of element $K$ we use the approximation:

$$\gamma_{\tau} \text{curl } E|_{l_j} \approx \gamma_{\tau} \text{curl } E|_{l_j} = \frac{1}{2}(\nu_j \times [\text{curl } E_h|_K + \text{curl } E_h|_{K_j}]).$$
Numerical Solution of Local Problems

- Local error formulation:

On each element $K$, find $\hat{e}_h \in V_{h,K}$, the implicit error estimate such that $\forall \ w \in V_{h,K}$ the following relation is satisfied:

$$(\text{curl} \ \hat{e}_h, \text{curl} \ w)_K - k^2(\hat{e}_h, w)_K = (J, w)_K - (\text{curl} \ E_h, \text{curl} \ w)_K$$

$$+ k^2(E_h, w)_K - \frac{1}{2}(\nu_j \times (\text{curl} \ E_h|_K + \text{curl} \ E_h|_{K_j}), w)_{\partial K}.$$ 

- Chief question: how to choose $V_{h,K}$?
Basis Functions for the Local Error Equation

On the reference element $\hat{K} = (0, 1)^3$ define $V_{h,\hat{K}} = \text{span}(\{\phi^0_k\}_{k=1}^9)$, where

$\phi^0_1 = ((1 - \xi)(1 - \eta)\eta(1 - \zeta)\zeta, 0, 0)^T$, $\phi^0_2 = (\xi(1 - \eta)\eta(1 - \zeta)\zeta, 0, 0)^T$,
$\phi^0_7 = ((1 - \xi)\xi(1 - \eta)\eta(1 - \zeta)\zeta, 0, 0)^T$, $\phi^0_3 = (0, (1 - \xi)(1 - \eta)(1 - \zeta)\zeta, 0)^T$,
$\phi^0_4 = (0, (1 - \xi)\xi\eta(1 - \zeta)\zeta, 0)^T$, $\phi^0_8 = (0, (1 - \xi)\xi(1 - \eta)\eta(1 - \zeta)\zeta, 0)^T$,
$\phi^0_5 = (0, 0, (1 - \xi)\xi(1 - \eta)\eta(1 - \zeta))^T$, $\phi^0_6 = (0, 0, (1 - \xi)\xi(1 - \eta)\eta\zeta)^T$,
$\phi^0_9 = (0, 0, (1 - \xi)\xi(1 - \eta)\eta(1 - \zeta)\zeta)^T$.

The space $V_{h,K}$ is obtained with an affine transformation; $K$ is rectangular.
Well Posedness of Local Problems

- **Theorem 1** Assume that $k$ is not a Maxwell eigenvalue in the sense that the problem: Find $u \in H(\text{curl}, K)$ such that

\[ B(u, v) = 0, \quad \forall \, v \in H(\text{curl}, K) \]

has only the trivial ($u = 0$) solution. Then the variational problem: Find $\hat{e}_h \in H(\text{curl}, K)$ such that

\[ B(\hat{e}_h, v) = (\tilde{J}, v), \quad \forall \, v \in H(\text{curl}, K) \tag{2} \]

has a unique solution for all $\tilde{J} \in [L_2(K)]^3$.

- Using lifting, the variational problem for the error can be rewritten into (2).
- This is also the case for any reasonable choice of $\gamma_{\tau \text{curl} E}$.
Eigenvalues for the Local Error Equation on a Rectangular Domain

- **Theorem 2** The eigenfunctions in the Maxwell eigenvalue problem (corresponding to (2)):

  Find $\mathbf{v} \in H(\text{curl}, K)$ and $k \in \mathbb{R}$ such that

  $\text{curl curl } \mathbf{v} - k^2 \mathbf{v} = 0$ in $K,$

  $\mathbf{v} \times \text{curl } \mathbf{v} = 0$ on $\partial K$

  with $K = (0, a) \times (0, b) \times (0, c)$ are:

  $$
  \mathbf{v}(x, y, z) = \begin{pmatrix}
  C_1 \sin \frac{k_1 \pi}{a} x \cos \frac{k_2 \pi}{b} y \cos \frac{k_3 \pi}{c} z \\
  C_2 \cos \frac{k_1 \pi}{a} x \sin \frac{k_2 \pi}{b} y \cos \frac{k_3 \pi}{c} z \\
  C_3 \cos \frac{k_1 \pi}{a} x \cos \frac{k_2 \pi}{b} y \sin \frac{k_3 \pi}{c} z
  \end{pmatrix},
  $$
for any $k_1, k_2, k_3 \in \mathbb{N}$ with

$$\frac{k_1 \pi}{a} C_1 + \frac{k_2 \pi}{b} C_2 + \frac{k_3 \pi}{c} C_3 = 0 \quad \text{and} \quad C_1, C_2, C_3 \in \mathbb{R}.$$ 

The appropriate eigenvalues are $k^2 = \left(\frac{k_1 \pi}{a}\right)^2 + \left(\frac{k_2 \pi}{b}\right)^2 + \left(\frac{k_3 \pi}{c}\right)^2$ with $k_1, k_2, k_3 \in \mathbb{N}$ arbitrary.

◊ Example: $a = b = c = 1$ (unit cube).
Smallest eigenvalue: $\pi^2\left(1^2 + 1^2 + 1^2\right) \approx 29.6$.

**Corollary 1** (2) is well posed whenever $k$ is not a Maxwell eigenvalue in the sense of Theorem 2.
Implicit Error Estimate as Lower Bound of the Error

• Introduce $\eta_K$ as error indicator - an explicit error estimate on $K$:

$$
\eta_K = (h^2 \| r \|_{L^2(K)}^3 + h \| R \|_{L^2(\partial K)}^3)^{\frac{1}{2}}.
$$

• Theorem 3  The implicit a posteriori error estimate $\hat{e}_h$ can be used as a lower bound for the exact error with respect to the curl norm as follows:

$$
\| \hat{e}_h \|_{\text{curl}, K} \leq C \eta_K \leq \sqrt{D} C (1 + k^2) \| e_h \|_{\text{curl}, \bar{K}} + \text{Res}(r, R)
$$

with $C$, $D$ constants independent of the mesh size $h$ and frequency $k$ and

$$
\text{Res}(r, R) = (h^2 \| \bar{r} - r \|_{L^2(K)}^3 + h \| \bar{R} - R \|_{L^2(\partial K)}^3)^{1/2}
$$

arising from the interpolation errors of $r$ and $R$. 

Solution of the local problems

$K$: cubic subdomain with edge length $h$.

The bilinear form for the bubble function space $\text{span}(\{\phi_k\}_{k=1}^9)$ on $K$:

- $B_{1,K}$ - stiffness matrix of size $9 \times 9$.
- $B_{1,K} = B_{1,\text{curl}} - k^2 B_{1,0}$, where

$$B_{1,\text{curl}}[i][j] = \int_{K} \text{curl} \phi_i \cdot \text{curl} \phi_j, \quad B_{1,0}[i][j] = \int_{K} \phi_i \cdot \phi_j.$$  

- Scaling: $B_{1,K} = \frac{1}{h} B_{1,\text{curl}} - k^2 h B_{1,0}$. 

Properties of the local problems

- Ill conditioned matrices arise:

\[
\text{cond}(B_{1,K}) \sim \frac{1}{h^2}.
\]

- The solution of the local problem seems to become less precise as \( h \to 0 \).

**Theorem 4** The following inf-sup condition holds:

There is a \( C \in \mathbb{R} \) such that for any \( \mathbf{u} \in \text{span}(\{\phi_j\}_{j=1}^9) \)

\[
\sup_{\|\mathbf{v}\|_{\text{curl},K}=1} |B_{1,K}(\mathbf{u}, \mathbf{v})| \geq C \|\mathbf{u}\|_{\text{curl},K},
\]

where \( C \) does not depend on \( \mathbf{u} \) and the finiteness parameter \( h \).
Main difficulties and tasks

- Challenges in the analysis and computations
  - Non-coercive bilinear forms in 3D.
  - Non-smooth solutions arise.
  - Non-convex domains with edges, corners arise.
  - Presence of big or even small wave numbers ($k$).

- The performance of the implicit error estimator is evaluated by:
  - checking if the estimator provides the right type of error distribution
  - comparing the magnitude of the global error estimate and its convergence under mesh refinement with the exact error.
Definition of Error Contributions

- The exact error $\delta_K$ and the implicit local error estimate $\hat{\delta}_K$ on element $K$ are defined as:
  $$\delta_K = \| E - E_h \|_{\text{curl},K}, \quad \hat{\delta}_K = \| \hat{e}_h \|_{\text{curl},K}.$$ 
- The exact global error $\delta$ and the implicit global error estimate $\delta_h$ are obtained by summing the local contributions
  $$\delta = \left( \sum_{K \in T_h} \delta_K^2 \right)^{1/2}, \quad \delta_h = \left( \sum_{K \in T_h} \hat{\delta}_K^2 \right)^{1/2}.$$ 
- In all cases: comparison of
  analytic error : $\| E - E_h \|_{\text{curl},K} = \| e_h \|_{\text{curl},K}$ and implicit error : $\| \hat{e}_h \|_{\text{curl},K}$. 
Test case 1: Smooth Solution

- The Maxwell equations on $\Omega = (0, 1)^3$ with given source term

$$J(x, y, z) = (\pi^2(p^2 + m^2) - 1) \begin{pmatrix} \sin(\pi py) \sin(\pi mz) \\ \sin(\pi px) \sin(\pi my) \\ \sin(\pi pz) \sin(\pi mx) \\ \sin(\pi px) \sin(\pi my) \end{pmatrix}$$

with $p, m \in \mathbb{N}$, which has a smooth solution:

$$E(x, y, z) = \begin{pmatrix} \sin(\pi py) \sin(\pi mz) \\ \sin(\pi px) \sin(\pi my) \\ \sin(\pi px) \sin(\pi my) \end{pmatrix}.$$
Test case 1: Locations for Local Error Computations

Location of some elements where the implicit error estimation was conducted.
Test case 1: Error Distribution for Smooth Solution

Error distribution in $H(\text{curl})$-norm ($p = m = 1$, $h = \frac{1}{16}$).
Test case 1: Error distribution for Smooth Solution

Error distribution in $H(\text{curl})$ norm ($p = 5$, $m = 1$, $h = \frac{1}{16}$).
Test case 1: Global Error for Smooth Solution

Variation of the global error estimate and exact error in the $H(\text{curl})$-norm ($p = m = 1$).
Test case 2: Non-Smooth Solution

- Consider the domain $\Omega = (-1, 1)^3$ and the function:

  $$f : \Omega \to \mathbb{R} \text{ with } f = \max\{|x|, |y|, |z|\}.$$ 

- Define $E : \Omega \to \mathbb{R}$ as $E := -\nabla f(x, y, z)$. Then $E$ solves the following Maxwell problem:

  \[
  \text{curl curl } E - E = \nabla f \quad \text{in } \Omega,
  \]

  \[
  E \times \nu = 0 \quad \text{on } \partial \Omega.
  \]

- The right hand side is in $[L_2(\Omega)]^3$, but the exact solution is not smooth, $E \not\in [H^{1/2}(\Omega)]^3$, but $E \in [H^{1/2-\epsilon}(\Omega)]^3$ for any $\epsilon \in \mathbb{R}^+$. 

Test case 2: Locations for Local Error Computations

Location of some elements where the implicit error estimation was conducted.
Test case 2: Error Distribution for Non-Smooth Solution

Error distribution in $H(\text{curl})$-norm ($h = \frac{1}{16}$).
Test case 2: Global Error for Non-Smooth Solution

Variation of the global error estimate and exact error in the $H(\text{curl})$-norm.
Test case 3: Fichera Cube

- Consider a Fichera cube $\Omega = (-1, 1)^3 \setminus [-1, 0]^3$.

- The solution on this domain has corner and edge singularities and can serve as an interesting test case.

- Boundary conditions and source term in the Maxwell equations are chosen such that the exact solution is $E = \nabla \left( r^{2/3} \sin \left( \frac{2}{3} \phi \right) \right)$ in spherical coordinates, with $r = \sqrt{x^2 + y^2 + z^2}$, $\phi = \arccos \frac{z}{r}$.

- Note, $E$ does not belong to $[H^1(\Omega)]^3$. 
Test case 3: Locations for Local Error Computations

Location of some elements where the implicit error estimation was conducted.
Test case 3: Error Distribution for Fichera Cube Solution

Error distribution in $H(\text{curl})$-norm ($h = \frac{1}{8}$)
Test case 3: Fichera Cube

Variation of the global error estimate and exact error in the $H(\text{curl})$-norm.
Comparisons with some existing schemes

• Beck, Hiptmair et al. (*M2AN 2000*) consider the following elliptic boundary value problem

\[
\text{curl} \ (\text{curl } \mathbf{E}) + \beta \mathbf{E} = \mathbf{J} \quad \text{in } \Omega = (0, 1)^3,
\]
\[
\mathbf{E} \times \mathbf{\nu} = 0 \quad \text{on } \partial \Omega,
\]

where \( \beta \) is a given positive function on \( \Omega \).

• The exact solution is given by \( \mathbf{E} = (0, 0, \sin(\pi x)) \).

• Note, the bilinear form for this problem is coercive, contrary to the bilinear form discussed for the Maxwell equations.

• We make comparisons in terms of the effectivity index \( \varepsilon_h := \frac{\delta_h}{\delta} \). This quantity merely reflects the quality of the global estimate.
Effectivity Index

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Effectivity index $\varepsilon_h$ for the error estimator given by Beck et. al.
**Effectivity Index**

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Effectivity index $\varepsilon_h$ for the new implicit error estimator.
Conclusions

• We have developed and analyzed an implicit a posteriori error estimation technique for the time harmonic Maxwell equations.

• The algorithm is well suited both for cases where the bilinear form is coercive and the more complicated indefinite case.

• The algorithm is tested on a number of increasingly complicated test cases and the results show that it gives an accurate prediction of the error distribution and also the local and global error.

• Also, in comparison with other a posteriori estimation techniques, it gives for the cases considered a sharper estimate of the error and the error distribution.
Further works

- The same procedure on a tetrahedral mesh (in progress).

- Chief question: how to use the local basis?
  The choice \( \text{span}\left(\{\Phi_j\}_{j=1}^{9}\right) \) does the job, but what else could be chosen?

- A meaningful adaptation strategy using the error estimates.