Efficient resolution of time-harmonic Maxwell equations with high-order edge finite elements

M. Durufle, G Cohen

INRIA, project POEMS

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M. Durufle, G Cohen (INRIA, project POEMS)Efficient resolution of time-harmonic Maxwell

- Cohen, Monk, mass lumping for Maxwell's equations (hexahedra)
- S. Fauqueux, mixed spectral elements for wave and elastic equations (hexahedra)
- S. Pernet, Discontinuous Galerkin methods for Maxwell's equations (hexahedra)
- M. Durufle, Numerical integration and high order finite element method applied to time-harmonic Maxwell equations
- Apply techniques of "mass lumping" and "mixed formulation", which are efficient in temporal domain
- Efficient preconditioning technique to solve linear system ,

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Space of approximation

 $V_h = \{ \vec{u} \in H(\operatorname{curl},\Omega) \text{ so that } DF_i^t \vec{u} \circ F_i \in Q_{r-1,r,r} \times Q_{r,r-1,r} \times Q_{r,r,r-1} \}$ Basis functions

$$\begin{split} \vec{\varphi}_{i,j,k}^{1}(\hat{x}, \hat{y}, \hat{z}) &= \hat{\psi}_{i}^{G}(\hat{x}) \ \hat{\psi}_{j}^{GL}(\hat{y}) \ \hat{\psi}_{k}^{GL}(\hat{z}) \ \vec{e_{x}} \quad 1 \leq i \leq r \quad 1 \leq j, k \leq r+1 \\ \vec{\varphi}_{j,i,k}^{2}(\hat{x}, \hat{y}, \hat{z}) &= \hat{\psi}_{j}^{GL}(\hat{x}) \ \hat{\psi}_{i}^{G}(\hat{y}) \ \hat{\psi}_{k}^{GL}(\hat{z}) \ \vec{e_{y}} \quad 1 \leq i \leq r \quad 1 \leq j, k \leq r+1 \\ \vec{\varphi}_{k,j,i}^{3}(\hat{x}, \hat{y}, \hat{z}) &= \hat{\psi}_{k}^{GL}(\hat{x}) \ \hat{\psi}_{j}^{GL}(\hat{y}) \ \hat{\psi}_{i}^{G}(\hat{x}) \ \vec{e_{z}} \quad 1 \leq i \leq r \quad 1 \leq j, k \leq r+1 \end{split}$$

 ψ_i^G, ψ_i^{GL} lagragian functions linked respectively with Gauss points and Gauss-Lobatto points. See. G. Cohen, P. Monk, Gauss points mass lumping

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Nedelec's first family on hexahedra

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 $\vec{\hat{\varphi}}^3_{k,j,i}(\hat{x},\hat{y},\hat{z}) \quad = \quad \hat{\psi}^{GL}_k(\hat{x}) \; \hat{\psi}^{GL}_j(\hat{y}) \; \hat{\psi}^G_i(\hat{x}) \; \vec{\boldsymbol{e_z}} \quad 1 \leq i \leq r \quad 1 \leq j,k \leq r+1$

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See. G. Cohen, P. Monk, Gauss points mass lumping

Elementary matrices

Mass matrix :

$$(M_h)_{i,j} = \int_{\hat{K}} J_i DF_i^{-1} \varepsilon DF_i^{*-1} \hat{\varphi}_i \cdot \hat{\varphi}_k d\hat{x}$$

Stiffness matrix :

$$(K_h)_{i,j} = \int_{\hat{K}} \frac{1}{J_i} DF_i^t \mu^{-1} DF_i \hat{\nabla} \times \hat{\varphi}_i \cdot \hat{\nabla} \times \hat{\varphi}_k d\hat{x}$$

• Use of Gauss-Lobatto quadrature ($\omega_k^{GL}, \xi_k^{GL}$)

Block-diagonal matrix

$$(A_h)_{k,k} = \left[J_i DF_i^{-1} \varepsilon DF_i^{*-1}\right] (\xi_k^{GL}) \omega_k^{GL}$$

Block-diagonal matrix

$$(\boldsymbol{B}_h)_{k,k} = \left[\frac{1}{J_i} DF_i^t \mu^{-1} DF_i\right] (\xi_k^{GL}) \omega_k^{GL}$$

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$$\hat{\boldsymbol{C}}_{i,j} = \hat{\varphi}_i(\xi_i^{GL}) \qquad \hat{\boldsymbol{R}}_{i,j} = \hat{\nabla} \times \hat{\varphi}_i^{GL}(\xi_j^{GL})$$

Then, we have : $M_h = \hat{C} A_h \hat{C}^*$ $K_h = \hat{C} \hat{R} B_h \hat{R}^* \hat{C}^*$

- Complexity of $\hat{C} U$: 6 $(r + 1)^4$ operations in 3-D
- Complexity of $\hat{R} U$: 12 $(r + 1)^4$ operations in 3-D

• Complexity of $A_h U + B_h U$: 30 $(r + 1)^3$ operations Complexity of standard matrix vector product $18r^3 (r + 1)$

Matrix-vector product 67% slower by using exact integration

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Spurious free method

Computation of eigenvalues in a cubic cavity, with tetrahedra split in hexahedra



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Spurious free method

Computation of eigenvalues in a cubic cavity, with tetrahedra split in hexahedra



Numerical eigenvalues if we use Gauss-Lobatto points at right, or Gauss points for the stiffness matrix at left.

Gauss-Lobatto integration leads to a spurious-free method

Convergence of the method

Scattering by a perfectly conductor sphere $E \times n = 0$



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Convergence of the method

Convergence of Nedelec's first family on regular meshes



Optimal convergence O(h^r) in H(curl,Ω) norm

Convergence of the method

Convergence on tetrahedral meshes split in hexahedra



• Loss of one order, convergence $O(h^{r-1})$ in H(curl, Ω) norm

Is the matrix-vector product fast ?

Comparison between standard formulation and discrete factorization

Order	1	2	3	4	5
Time, standard formulation	55s	127s	224s	380s	631
Time, discrete factorization	244s	128s	106s	97s	96s
Storage, standard formulation	18 Mo	50 Mo	105 Mo	187 Mo	308 Mo
Storage, discrete factorization	23 Mo	9.9 Mo	6.9 Mo	5.7 Mo	5.0 Mo

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Is the matrix-vector product fast ?

Comparison between tetrahedral and hexahedral elements



At left, time computation for a thousand iterations of COCG At right, storage for mesh and matrices

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Preconditioning used

• Incomplete factorization with threshold on the damped Maxwell equation :

$$-k^{2}(\alpha + i\beta)\varepsilon \mathbf{E} - \nabla \times (\frac{1}{\mu}\nabla \times \mathbf{E}) = \mathbf{0}$$

• ILUT threshold \geq 0.05 in order to have a low storage

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- Use of a Q₁ subdivided mesh to compute matrix



Preconditioning used

Incomplete factorization with threshold on the damped Maxwell equation :

$$-k^{2}(\alpha + i\beta)\varepsilon \boldsymbol{E} - \nabla \times (\frac{1}{\mu}\nabla \times \boldsymbol{E}) = 0$$

- Multigrid iteration on the damped Maxwell equation
 - Use of the Hiptmair smoother
 - Low-storage algorithm even with high order
- Without damping, both preconditioners **does not lead** to convergence.
- A good choice of parameter is $\alpha = 1, \beta = 1$

Let us count the number of iterations and the memory used by the preconditioner, for different values of (α, β)

Threshold	1 <i>e</i> – 4	1 <i>e</i> – 3	0.01	0.05	0.1	
$\alpha = 1 \ \beta = 0$	30/370 <i>Mo</i>	$\infty/350Mo$	$\infty/340\mathit{Mo}$	$\infty/326Mo$	$\infty/314$ Mo	
$\alpha = 1 \ \beta = 0.5$	55/299 <i>Mo</i>	55/242 <i>Mo</i>	55/149 <i>Mo</i>	82/74 <i>Mo</i>	145/47 <i>Mo</i>	
$\alpha = 1 \beta = 1$	97/244 <i>Mo</i>	97/197 <i>Mo</i>	99/108 <i>Mo</i>	110/53 <i>Mo</i>	155/34 <i>Mo</i>	

The use of a Q1 subdivided mesh is very accurate for the scalar Helmholtz equation, but has some difficulties for Maxwell equations. Let us count the number of iterations depending the frequency. The frequency 1 corresponds to the "normal" frequency.

Order	F = 0.125	F = 0.25	F = 0.5	F = 1.0	F = 1.5
Q ₂ (110 000ddl)	NC	49	19	16	49
Q4(92000ddl)	NC	NC	42	30	123
Q ₆ (72000ddl)	NC	NC	71	47	159

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Problems in low-frequency case, because of the difference between the discrete kernels (of Q1 and high order).

The smoother of Hiptmair is based on the Helmholtz decomposition :

 $\boldsymbol{E} = \nabla \varphi + \boldsymbol{u}$

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The smoother of Hiptmair is based on the Helmholtz decomposition :

$$E = \nabla \varphi + u$$

The potential φ is solution of the "Laplacian" variationnal formulation :

$$\int_{\Omega} \nabla \varphi \nabla \psi - ik \int_{\Sigma} \nabla \varphi \times \mathbf{n} \cdot \nabla \psi \times \mathbf{n} = \int_{\Omega} f \cdot \nabla \psi$$

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 A_{ϕ} finite element matrix associated to this formulation

Caracteristics of the multigrid iteration

The smoother of Hiptmair is based on the Helmholtz decomposition :

 $\boldsymbol{E} = \nabla \varphi + \boldsymbol{u}$

Let us introduce the operator P:

$$\begin{array}{rcl} P: H_0^1(\Omega) & \leftrightarrow & H(\operatorname{curl}, \Omega) \\ \varphi & & \leftrightarrow & \nabla \varphi \end{array}$$

then $A_{\phi} = P^* A_e P$ and the smoother can be written as :

- Relaxation on edge finite element operator $A_e x = b$
- Projection on nodal finite element $b_{\phi} = P^*(b A_e x)$
- Relaxation on nodal finite element operator $A_{\phi} x_{\phi} = b_{\phi}$
- Projection on edge finite element $x = x + P x_{\phi}$

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Caracteristics of the multigrid iteration

The smoother of Hiptmair is based on the Helmholtz decomposition :

 $E = \nabla \varphi + u$

- Jacobi relaxation used, because it avoids us storing the matrices (compared to a SSOR relaxation).
- Prolongation operator is an interpolation from the coarse order to the fine order. A matrix-free implementation of the prolongation operator is used.
- Incomplete factorization for the resolution of the coarsest order
- Use of a W-cycle, and one step of pre and post-smoothing (in order to get the symmetry of the preconditioning)

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The smoother of Hiptmair is based on the Helmholtz decomposition :

 $\boldsymbol{E} = \nabla \boldsymbol{\varphi} + \boldsymbol{u}$

The use of a multigrid iteration on the Q1 subdivided mesh is not optimal

- Fail of a good preconditioning in low-frequency case, because the "Q1" discrete kernel is different from the high order discrete kernel
- Overcost in storage, because we store all the needed Q1 matrices

Scattering by a dielectric sphere



- Sphere of radius 2 with $\varepsilon = 3.5 \ \mu = 1$
- Outside boundary on a sphere of radius 3.

Scattering by a dielectric sphere

How many dofs/time to reach an error less than 0.5 dB



Finite Element	Q ₂	Q_4	Q_6
Nb dofs	940 000	88 000	230 000
No preconditioning	19486 s	894 s	4401 s
ILUT(0.05)	-	189 s	1 035 s
Two-grid	5814s	280 s	1379s
Multi-grid	5814s	499 s	2515s
Q1 Two-grid	4 4344 s	488 s	1095s

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Scattering by a dielectric sphere

How many dofs/time to reach an error less than 0.5 dB



No preconditioning	171 Mo	10 Mo	24 Mo
ILUT(0.05)	-	99 Mo	271 Mo
Two-grid	402 Mo	34 Mo	132 Mo
Multi-grid	402 Mo	12 Mo	28 Mo
Q1 Two-grid	947 Mo	67 Mo	180 Mo

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Scattering by a cobra cavity



- Cobra cavity of length 10, and depth 2
- Outside boundary at a distance of 1

Scattering by a cobra cavity

How many dofs/time to reach an error less than 0.5 dB



Finite Element	Q_4	Q_6
Nb dofs	412000	187 000
No preconditioning	14039 s (47 Mo)	12 096 s (22 Mo)
ILUT(0.05)	2 247 s (391 Mo)	<mark>846 s</mark> (161 Mo)
Two-grid	2 355 s (91 Mo)	2319 s (65 Mo)
Multigrid	4 519 s (59 Mo)	-
Q1 Two-grid	9 294 s (260 Mo)	10 500 s (130 Mo)

Local refinement for the Fichera corner



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Local refinement for the Fichera corner



- Q4 approximation on a local refined mesh
- Incomplete factorization fails on this case
- Multigrid preconditioning needs SSOR smoother to be efficient
- 480 000 dofs and cells 256 times smaller than other ones

Local refinement for the Fichera corner



Algorithm	Iterations	Time	Memory
No preconditioning	> 1 000 000	∞	33 Mo
Multigrid with Jacobi smoother	30 560	35h	63 Mo
Multigrid with SSOR smoother	579	1h	790 Mo

Eigenmodes with the second family

The second family uses Q_r^3 instead of $Q_{r-1,r,r} \times Q_{r,r-1,r} \times Q_{r,r,r-1}$ Mesh used for the simulations (**Q**₃)



Eigenmodes with the second family

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Two types of penalization

Mixed formulation of Maxwell equations

$$-\omega \int_{\Omega} \mathbf{E} \cdot \varphi + \int_{\Omega} \mathbf{H} \cdot \operatorname{rot}(\varphi) - i\alpha \sum_{e \text{ face}} \int_{\Gamma_{e}} [\mathbf{E} \cdot n][\varphi \cdot n] = \int_{\Omega} f \cdot \varphi$$
$$-\omega \int_{\Omega} \mathbf{H} \cdot \varphi + \int_{\Omega} \operatorname{rot}(\mathbf{E}) \cdot \varphi - i\delta \sum_{e \text{ face}} \int_{\Gamma_{e}} [\mathbf{H} \times n] \cdot [\varphi \times n] = 0$$

Approximation space for H

$$W_h = \{ \vec{u} \in L^2(\Omega) \text{ so that } DF_i^* \vec{u} \circ F_i \in (Q_r)^3 \}$$

• Equivalence with second-order formulation ($\alpha = \delta = 0$)

- Dissipative terms of penalization
- Penalization in α does not need of a mixed formulation

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$$-\omega \int_{\Omega} \mathbf{H} \cdot \varphi + \int_{\Omega} \operatorname{rot}(\mathbf{E}) \cdot \varphi - i\delta \sum_{e \text{ face}} \int_{\Gamma_{e}} [\mathbf{H} \times n] \cdot [\varphi \times n] = 0$$

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Effects of penalization



- Case of the cubic cavity meshed with split tetrahedrals
- At left $\alpha = 0.1$, at right $\alpha = 0.5$

Effects of penalization



Four modes of the Fichera corner

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Effects of penalization



- Case of the Fichera corner
- At left $\alpha = 0.5$, at right $\delta = 0.5$
- Both penalizations efficient for regular domains
- Delta-penalization more robust for singular domains

Why choosing first family compared to second family or DG method ?

- All the methods are spectrally correct
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