Multilevel block preconditioning for shifted Maxwell equations

Matthias Bollhöfer (TU Braunschweig), S. Lanteri (INRIA Sophia Antipolis)

Sparse Days and ANR SOLSTICE
Toulouse
June 15-17, 2010
Outline

1. Maxwell’s equations
2. Shifted Systems
3. Block ILU
4. Multilevel ILU
5. Numerical results
6. Conclusions
First order formulation

\[
\begin{align*}
+i\omega \varepsilon E - \text{curl}(H) &= 0, \\
-i\omega \mu H - \text{curl}(E) &= 0,
\end{align*}
\]

+ b.c.

discretization using Discontinous Galërkin

- collective treatment \( W = (E, H) \)

\[
i\omega G_0 W + G_x \partial_x W + G_y \partial_y W + G_z \partial_z W = 0
\]

discretization using tetrahedral elements, \( W \) approximated by vector with (discontinuous) polynomial components.

- integral representation over internal interfaces (divergence theorem)

- discretized system with block structure, block size depending on the degree of the polynomial (e.g. block size is 24 for linear polynomials)
Time-harmonic Maxwell equations

General problem for numerical solvers:
- 3D problem, not feasible for sparse direct solvers
- large null space of curl operator makes it extremely sensitive to approximate factorizations
- time-harmonic problem is highly indefinite
- Necessary to modify the system prior to application of numerical solvers
Second order formulation (inserting $\mathbf{H}$ into the first equation)

$$
\frac{1}{i \omega} \left( -\omega^2 \varepsilon \mathbf{E} + \text{curl} \left( \frac{1}{\mu} \text{curl}(\mathbf{E}) \right) \right) = i \omega \varepsilon \mathbf{E} + \text{curl} \left( \frac{1}{i \omega \mu} \text{curl}(\mathbf{E}) \right) = 0, \quad \text{+ b.c.}
$$

Helmholtz decomposition $\mathbf{E} = \text{grad} \varphi + \mathbf{U}$, where $\text{div} \mathbf{U} = 0$

$$
\rightarrow \begin{cases} 
-\omega^2 \text{div}(\varepsilon \text{grad}) \varphi, \\
\left( -\omega^2 \varepsilon - \text{div} \left( \frac{1}{\mu} \text{grad} \right) \right) \mathbf{U}
\end{cases}
$$

twisted scaled Laplacian operator and Helmholtz operator for $\mathbf{E}$
Consider the Helmholtz equation

\[-\Delta u - \omega^2 u = 0, + \text{b.c.}\]

→ discrete system

\[(A - \omega^2 M)x = b, \text{ where } A, M \text{ are sym. pos. def.}\]

Work by Magolu, Erlangga, Vuik, Oosterlee, van Gijzen: Introduce a complex shift, i.e., compute numerical solver for the shifted system

\[A - (1 - \beta i)\omega^2 M\]

where \(\beta\) suitably chosen (e.g. \(\beta = 1, \beta = 0.5\)) and then apply it to unshifted system

\[A - \omega^2 M\]

- \(A - (1 - \beta i)\omega^2 M\) is much easier to approximate
- eigenvalues of \((A - (1 - \beta i)\omega^2 M)^{-1}(A - \omega^2 M)\) can be easily characterized
Shifted Helmholtz Equations
Eigenvalues of the preconditioned system

M. Bollhöfer (TU BS)
Shifted Maxwell equations

- add artificial conductivity for $E$ and similar contribution for $H$ such that the reduced second order system refers to a shifted Helmholtz equation

\[
\begin{align*}
+i\omega\varepsilon E - \text{curl}(H) &= -\beta_E\omega\varepsilon E, \\
-i\omega\mu H - \text{curl}(E) &= +\beta_H\omega\mu H,
\end{align*}
\]

- Reduced second order system

\[
\begin{align*}
\frac{1}{i\omega} \left( -(1 - \beta_E i)\omega^2\varepsilon + \text{curl}\left( \frac{1}{(1 - i\beta_H)\mu} \text{curl} \right) \right) E &= 0, \quad + \text{b.c.} \\
\left( -(1 - \beta_E\beta_H - (\beta_E + \beta_H)i)\omega^2\varepsilon + \text{curl}\left( \frac{1}{\mu} \text{curl} \right) \right) E &= 0, \quad + \text{b.c.} \\
\rightarrow \begin{cases} \\
-(1 - \beta_E\beta_H - (\beta_E + \beta_H)i)\omega^2\varepsilon \text{div}(\varepsilon \text{grad})\varphi, \\
\left( -(1 - \beta_E\beta_H - (\beta_E + \beta_H)i)\omega^2\varepsilon - \text{div}\left( \frac{1}{\mu} \text{grad} \right) \right) U
\end{cases}
\end{align*}
\]
Discretized Maxwell equations

- Discretization by discontinuous Galerkin for \( \mathbf{W} = \begin{pmatrix} \mathbf{E} \\ \mathbf{H} \end{pmatrix} \)

\[ \mathbf{Ax} = \mathbf{b} \]

- Matrix block structure (first taking \( \mathbf{E} \), then \( \mathbf{H} \))

\[ \mathbf{A} = \mathbf{i}\omega \begin{pmatrix} \mathbf{M}_\varepsilon & 0 \\ 0 & -\mathbf{M}_\mu \end{pmatrix} - \begin{pmatrix} \mathbf{C}_{11} & \mathbf{C}_{12} \\ \mathbf{C}_{12} & \mathbf{C}_{22} \end{pmatrix} \]

- \( \mathbf{M}_\varepsilon, \mathbf{M}_\mu \) refer to discretized mass matrices w.r.t. \( \mathbf{i}\omega\varepsilon\mathbf{E}, -\mathbf{i}\omega\mu\mathbf{H} \), block diagonal, s.p.d.

- \( \mathbf{C}_{ij} = \mathbf{C}^T_{ij} \) \( i, j = 1, 2 \) refer to the discretized curl operators \( \text{curl}(\mathbf{H}), \text{curl}(\mathbf{E}) \), \( \mathbf{C}_{11}, \mathbf{C}_{22} \) are block-diagonal

\[ \Rightarrow \mathbf{A} \text{ is complex-symmetric.} \]

- Further underlying block structure of dense blocks arising from DG discretization (e.g. \( P_1 \) elements yields block size \( 4 \times 3 = 12 \) for \( \mathbf{E} \) as well as for \( \mathbf{H} \))
Discretized shifted Maxwell equations

- Original system

\[ A = \begin{pmatrix} i\omega M_\varepsilon & 0 \\ 0 & -i\omega M_\mu \end{pmatrix} - \begin{pmatrix} C_{11} & C_{12} \\ C_{12} & C_{22} \end{pmatrix} \]

- Shifted system

\[ P = \begin{pmatrix} (i + \beta_E)\omega M_\varepsilon & 0 \\ 0 & -(i + \beta_H)\omega M_\mu \end{pmatrix} - \begin{pmatrix} C_{11} & C_{12} \\ C_{12} & C_{22} \end{pmatrix} \]

- Reduced shifted system (refers to shifted Helmholtz), Schur complement of \( P \).

\[ P_S = -(i + \beta_H)\omega M_\mu - C_{22} - C_{12} ((i + \beta_E)\omega M_\varepsilon - C_{11})^{-1} C_{12} \]

- Three classes of shifted operators
  - \( P_1 \): \( P \) for \( \beta_E = \beta_H = \beta \)
  - \( P_2 \): \( P_S \) for \( \beta_E = \beta_H = \beta \)
  - \( P_3 \): \( P_S \) for \( \beta_E = 0, \beta_H = \beta \)
Discretized shifted Maxwell equations

Eigenvalues of the preconditioned system

Block structure of $\mathcal{P}$

The larger the $\beta$, the more diagonal dominant the systems will be.

Block structure of $\mathcal{P}_S$
Block-structured ILUs

Left-looking block ILU (Crout version)

Scalar structure

→ → →

Block structure

Storage by columns as dense matrices

U

U^T
Block-structured ILUs

Left-looking block ILU (Crout version)

$U^T \rightarrow \rightarrow \rightarrow$ scalar structure

$U$ block structure

$A /$ Schur complement

Storage by columns as dense matrices
Block-structured ILUs

Computation based on Level-3 BLAS

\[ A \quad U^T \quad U \quad U^T \quad U \quad U^T \quad U \]

\[ \text{copy} \quad \downarrow \quad \text{gather} \quad \downarrow \quad \text{GEMM} \quad \downarrow \quad \text{scatter} \quad \downarrow \quad \text{gather} \quad \downarrow \quad \text{scatter} \quad \downarrow \quad \text{gather} \quad \downarrow \quad \text{scatter} \quad \downarrow \quad \text{copy} \quad \downarrow \]

Associated forward/backward solve only needs Level-2-BLAS
Block-structured ILUs

Computation based on Level-3 BLAS

\[
A \quad U^T \quad U \quad U^T \quad U \quad U^T \quad U
\]

\[
\text{copy} \downarrow
\]

\[
\text{gather} \downarrow
\]

\[
\text{GEMM}
\]

\[
\text{scatter} \downarrow
\]
Block-structured ILUs

Computation based on Level-3 BLAS

\[ \begin{array}{cccc}
A & U^T & U & U^T \\
\end{array} \]

copy ↓

gather ↓

GEMM

scatter ↓

Associated forward/backward solve only needs Level-2 BLAS
Block-structured ILUs

Computation based on Level-3 BLAS

\[ A + U^T U + U^T U + U^T U \]

- **copy**
- **gather**
- **GEMM**
- **scatter**
Block-structured ILUs

Computation based on Level-3 BLAS

\[ A \rightarrow U^T \rightarrow U \rightarrow U^T \rightarrow U \rightarrow U^T \rightarrow U \]

-copy\-↓

gather\-↓

GEMM

-scanter\-↓

copy\-↓

Associated forward/backward solve only needs Level-2-BLAS

M. Bollhöfer (TU BS)
Block-structured ILUs

Computation based on Level-3 BLAS

\[
A \quad U^T \quad U \quad U^T \quad U \quad U^T \quad U
\]

Associated forward/backward solve only needs Level-2-BLAS
Inverse-based pivoting: keep $\|L^{-1}\| \leq \kappa$ for some prescribed $\kappa$ (e.g. $\kappa = 5$).
Multilevel ILU
Inverse-Based Pivoting

\[
A \rightarrow \begin{pmatrix} B & F \\ F^T & C \end{pmatrix} = \begin{pmatrix} L_B & 0 \\ L_F & I \end{pmatrix} \begin{pmatrix} D_B & 0 \\ 0 & S_C \end{pmatrix} \begin{pmatrix} L_B^T & L_F^T \\ 0 & I \end{pmatrix} + E
\]

Inverse-based pivoting: keep \( \|L^{-1}\| \leq \kappa \) for some prescribed \( \kappa \) (e.g. \( \kappa = 5 \)).
block diagonal dominance yields bounded inverse triangular factors:

\[
A = (A_{ij})_{i,j} \quad \text{block partitioning}
\]

Suppose that

\[
\sum_{i:i \neq j} \left\| A_{ij} A_{jj}^{-1} \right\| \leq \frac{\kappa - 1}{\kappa}, \quad \sum_{j:j \neq i} \left\| A_{jj}^{-1} A_{ij} \right\| \leq \frac{\kappa - 1}{\kappa}.
\]

\[
\Rightarrow \| L^{-1} \|_1 \leq \kappa, \quad \| U^{-1} \|_{\infty} \leq \kappa \quad \text{(induced block norms)}.
\]
Inverse-based Coarsening
A generalized block diagonal dominance

- block diagonal dominance yields bounded inverse triangular factors:
  \[ A = (A_{ij})_{i,j} \text{ block partitioning} \]

  Suppose that
  \[
  \sum_{i:i \neq j} \left| A_{ij} A_{jj}^{-1} \right| \leq \frac{\kappa - 1}{\kappa}, \quad \sum_{j:j \neq i} \left| A_{ij}^{-1} A_{jj} \right| \leq \frac{\kappa - 1}{\kappa}.
  \]

  \[ \Rightarrow \left\| L^{-1} \right\|_1 \leq \kappa, \quad \left\| U^{-1} \right\|_\infty \leq \kappa \] (induced block norms).

- Inverse–based coarsening directly yields
  \[ \left\| L^{-1} \right\|, \left\| U^{-1} \right\| \leq \kappa \]
  for partial decomposition.
block diagonal dominance yields bounded inverse triangular factors:

\[ A = (A_{ij})_{i,j} \text{ block partitioning} \]

Suppose that

\[
\begin{align*}
\sum_{i:i\neq j} \| A_{ij} A_{jj}^{-1} \| &\leq \frac{\kappa - 1}{\kappa}, \\
\sum_{j:j\neq i} \| A_{ii}^{-1} A_{ij} \| &\leq \frac{\kappa - 1}{\kappa}.
\end{align*}
\]

\[ \Rightarrow \| L^{-1} \|_1 \leq \kappa, \quad \| U^{-1} \|_\infty \leq \kappa \text{ (induced block norms)}. \]

Inverse–based coarsening directly yields

\[ \| L^{-1} \|, \| U^{-1} \| \leq \kappa \]

for partial decomposition.

If \[
\begin{pmatrix}
A_{FF} & A_{FC} \\
A_{CF} & A_{CC}
\end{pmatrix}
\]
has a large size block diagonal dominant block \( A_{FF} \), then

\[ \| L^{-1} \|, \| U^{-1} \| \]
are small and a large portion of the system can be reduced.
Bounded Interpolation

\[
A^{-1} \approx L^{-T} D^{-1} L^{-1} \approx \kappa
\]

\[
\|I_h\| \leq \kappa
\]

M. Bollhöfer (TU BS)  Block ILU for Maxwell  Sparse Days 2010
Bounded Interpolation

\[ A^{-1} \approx \begin{pmatrix} L^{-T} & D^{-1} & L^{-1} \\ \approx \kappa & \approx \kappa & \end{pmatrix} \]

\[ = \begin{pmatrix} (L_{FF}D_{FF}L_{TFF})^{-1} & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} -L_{FF}^{-T}L_{TFF}^{T} \\ -L_{FF}L_{TFF}^{-1} \end{pmatrix} S_{CC}^{-1} \begin{pmatrix} -L_{FF}L_{FF}^{-1} \\ I \\ I_{h}^{T} \end{pmatrix} \]
Bounded Interpolation

\[
A^{-1} \approx \begin{pmatrix} L^{-T} D^{-1} L^{-1} \end{pmatrix} \approx \kappa
\]

\[
= \begin{pmatrix} (L_{\mathcal{F}} D_{\mathcal{F}} L_{\mathcal{F}}^T)^{-1} & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} -L_{\mathcal{F}}^{-T} L_{\mathcal{C}}^T \\ I \end{pmatrix} S_{CC}^{-1} \begin{pmatrix} -L_{\mathcal{C}} L_{\mathcal{F}}^{-1} \end{pmatrix} \begin{pmatrix} I \end{pmatrix}
\]

\[
\Rightarrow \text{Bounded interpolation } \| l_h \| \leq \kappa
\]
A^{-1} \approx \begin{pmatrix} L^{-T} D^{-1} L^{-1} \end{pmatrix}
\approx \kappa

= \begin{pmatrix} \left( L_{FF} D_{FF} L_{FF}^T \right)^{-1} & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} -L_{FF}^{-T} L_{CC}^T \\ I \end{pmatrix} S_{CC}^{-1} \begin{pmatrix} -L_{CC} \end{pmatrix} L_{CC}^{-1} I
\approx \kappa

⇒ Bounded interpolation \| l_h \| \leq \kappa

Ax = \varepsilon x
Bounded Interpolation

\[ A^{-1} \approx L^{-T} D^{-1} L^{-1} \]

\[ = \begin{pmatrix}
(L_{TF} D_{TF} L_{TF}^T)^{-1} & 0 \\
0 & 0 
\end{pmatrix} + 
\begin{pmatrix}
-L_{TF}^{-T} L_{CF}^T \\
L_{CF} 
\end{pmatrix}
\begin{pmatrix}
S_{CC}^{-1} & \begin{pmatrix}
-L_{CF} L_{TF}^{-1} & I 
\end{pmatrix}
\end{pmatrix}
\]

\[ \Rightarrow \text{Bounded interpolation } \| l_h \| \leq \kappa \]

\[ Ax = \varepsilon x \]

\[ \frac{1}{\varepsilon} x = A^{-1} x \approx \begin{pmatrix}
(L_{TF} D_{TF} L_{TF}^T)^{-1} & 0 \\
0 & 0 
\end{pmatrix} x + 
\begin{pmatrix}
I_h \\
S_{CC}^{-1} \end{pmatrix}
\begin{pmatrix}
I_h^T \\
\varepsilon
\end{pmatrix} x \]
Bounded Interpolation

\[ A^{-1} \approx (L^{-T} D^{-1} L^{-1}) \approx \kappa \]

\[ = \begin{pmatrix} (L_F D_F L_T)^{-1} & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} -L^{-T}_F L^T_C \\ I \end{pmatrix} \begin{pmatrix} -L C_F L^{-1}_F \\ I \end{pmatrix} \]

\[ \Rightarrow \text{Bounded interpolation } \| l_h \| \leq \kappa \]

\[ Ax = \varepsilon x \]

\[ \frac{1}{\varepsilon} x = A^{-1} x \approx \begin{pmatrix} (L_F D_F L_T)^{-1} & 0 \\ \approx \kappa \end{pmatrix} \begin{pmatrix} \approx C \\ \kappa \end{pmatrix} \begin{pmatrix} x \\ \text{LARGE} \end{pmatrix} + \begin{pmatrix} I_h \\ \text{LARGE} \end{pmatrix} \begin{pmatrix} S^{-1}_{CC} \\ \approx \kappa \end{pmatrix} \begin{pmatrix} I_h^T \\ \kappa \end{pmatrix} x \]

\[ \Rightarrow \text{by inverse-based coarsening } S_{CC} \text{ captures the eigenvalues with small modulus} \]
Numerical Results

Experiment Setup

Time-harmonic Maxwell equations

- 3D scattering problem discretized by a DG-\( P_1 \) method using a mesh with 46704 tetrahedral elements
- For an incident plane wave of frequency \( F = 900 \text{MHz} \) we have \( \omega = 18.84 \)
- Complex symmetric system of size \( n = 1120896 \), approx. 10 entries per row

Platform

- Platform INTEL XEON MP CPU with frequency 3.66 GHz and 16 GB of memory

Setup for the numerical solver

- drop tolerance for ILU set to \( \tau = 10^{-2} \) and \( \tau = 10^{-3} \) for the Schur complement.
- Fill per column/row limited to \( 20 \times \text{nnz}(A)/n \approx 200 \)
- Inverse bound set to \( \kappa = 10 \).
- Iterative solver SQMR until \( \|b - Ax_k\| \leq 10^{-8}(\|b\| + \|A\|\|x_k\|) \)
Maxwell equations

Three different shifted Systems

- $\mathcal{P}_1$: Original system $A$ shifted by $\beta \omega \begin{pmatrix} M_\varepsilon & 0 \\ 0 & -M_\mu \end{pmatrix}$

- $\mathcal{P}_2$: Schur complement of $\mathcal{P}_1$ after elimination of $E$ part

- $\mathcal{P}_3$: Schur complement of $A$ after elimination of $E$ part and then shifted by $\beta \omega M_\mu$ (discrete shifted curl curl operator)

$\mathcal{P}_{2,3}$ are much denser than $\mathcal{P}_1$, approx. 40 nonzeros per row. Therefore, maximum fill is also limited to $10 \times \text{nnz}(\mathcal{P}_{1,2}) \approx 400$.

- Use shifts $\beta = 1, 2, 3, 4, 5$
- natural block sizes for $\mathcal{P}_1$:
  - 3, taking $E, H$ separately
  - 6, taking $W = (E, H)$ together
  - 24, taking the matrix element by element

- natural block sizes $\mathcal{P}_{2,3}$:
  - 3, taking $H$ separately
  - 12, taking the matrix element by element
The larger the shift, the more diagonal dominant the system.

LARGE shifts lead to:
- less fill
- less levels
- larger leading level

For smaller shifts the limit w.r.t. the fill per row/column is effective.
The larger the shift, the more diagonal dominant the system.
LARGE shifts lead to:
- less fill
- less levels
- larger leading level

For smaller shifts the limit w.r.t. the fill per row/column is effective.
The larger the shift, the more diagonal dominant the system.

LARGE shifts lead to:
- Less fill
- Less levels
- Larger leading level

For smaller shifts the limit w.r.t. the fill per row/column is effective.

\[ \mathcal{P}_3 \]

Relative fill
The larger the shift, the more diagonal dominant the system.

- LARGE shifts lead to:
  - less fill
  - less levels
  - larger leading level

For smaller shifts the limit w.r.t. the fill per row/column is effective.
The larger the shift, the more diagonal dominant the system.

LARGE shifts lead to:
- less fill
- less levels
- larger leading level

For smaller shifts the limit w.r.t. the fill per row/column is effective.

$P_2$

Size 1st level
- The larger the shift, the more diagonal dominant the system.
- LARGE shifts lead to:
  - less fill
  - less levels
  - larger leading level
- For smaller shifts the limit w.r.t. the fill per row/column is effective.
The larger the shift, the more diagonal dominant the system.

LARGE shifts lead to
- less fill
- less levels
- larger leading level

For smaller shifts the limit w.r.t. the fill per row/column is effective.
Shifted Systems versus levels and diagonal dominance

- The larger the shift, the more diagonal dominant the system
- LARGE shifts lead to
  - less fill
  - less levels
  - larger leading level
- For smaller shifts the limit w.r.t. the fill per row/column is effective
The larger the shift, the more diagonal dominant the system
LARGE shifts lead to
- less fill
- less levels
- larger leading level
For smaller shifts the limit w.r.t. the fill per row/column is effective
Computation time Multilevel Block ILU

\[ P_2 \]

\[ \text{time ILU} \]

- dynamic
- 3x3
- 12x12

- sec
- \(10^2\)
- \(10^3\)
- \(10^4\)

- shift
- 1
- 2
- 3
- 4
- 5

M. Bollhöfer (TU BS)

Block ILU for Maxwell

Sparse Days 2010 20 / 22
Computation time Multilevel Block ILU

\( P_3 \)

- dynamic
- 3x3
- 12x12

\( \text{time ILU} \)

\( \text{sec} \)

\( \text{shift} \)

1 2 3 4 5
Computation time SQMR

\[ p_1 \]

\[ \text{time SQMR} \]

- Dynamic
- 3x3
- 6x6
- 24x24

\[ \text{sec} \]

\[ \text{shift} \]
Computation time SQMR
Computation time SQMR

\[ P_3 \]

![Graph showing computation time SQMR vs. shift for different grid sizes (dynamic, 3x3, 12x12).](image)
Conclusions

- Multilevel Block ILU based on three major ingredients
  - Block-structured given system (here Maxwell equations)
  - System shifted by blocks
  - Level-3-BLAS updates resp. Level-2-BLAS forward/backward solve

- Efficient method for solving large scale complex symmetric systems arising from time-harmonic Maxwell equations

- For larger elements (e.g. $P_2$ elements) larger blocks will occur (e.g. block size 60 for $P_2$) and even more benefits are expected