Multilevel block preconditioning for shifted Maxwell equations

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Outline

Time-harmonic Maxwell equations

First order formulation

$$\left\{ \begin{array}{rcl} +\mathbf{i}\omega\varepsilon\mathbf{E} - \mathrm{curl}(\mathbf{H}) & = & 0, \\ -\mathbf{i}\omega\mu\mathbf{H} - \mathrm{curl}(\mathbf{E}) & = & 0, \end{array} \right. \quad + \text{b.c.}$$

discretization using Discontinous Galërkin

- collective treatment $\mathbf{W} = (\mathbf{E}, \mathbf{H})$

$$i\omega G_0\mathbf{W} + G_x\partial_x\mathbf{W} + G_y\partial_y\mathbf{W} + G_z\partial_z\mathbf{W} = 0$$

- discretization using tetrahedral elements, **W** approximated by vector with (discontinous) 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

Time-harmonic Maxwell equations

Second order formulation (inserting **H** into the first equation)

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

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

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

twisted scaled Laplacian operator and Helmholtz operator for **E**

Shifted Helmholtz Equations

Consider the Helmholtz equation

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

$\longrightarrow$ 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

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

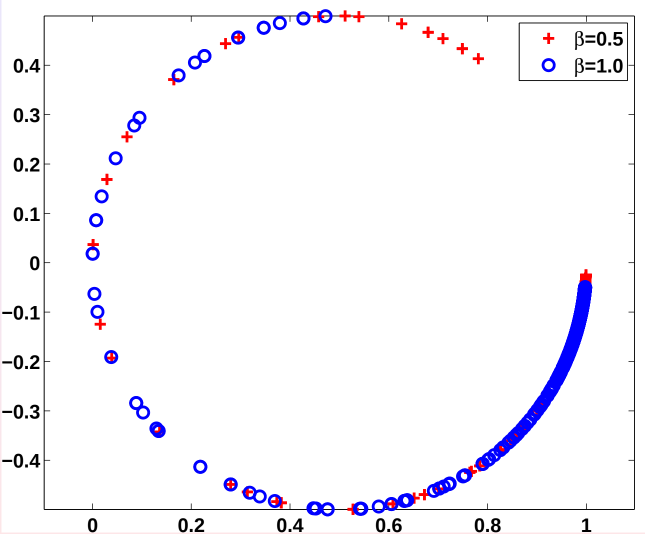
where β suitably chosen (e.g. $\beta = 1$, $\beta = 0.5$) and then apply it to unshifted system

$$A - \omega^2 M$$

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



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

$$\left\{\begin{array}{rcl} +\mathbf{i}\omega\varepsilon\mathbf{E} - \mathrm{curl}(\mathbf{H}) & = & -\beta_{\mathbf{E}}\omega\varepsilon\mathbf{E}, \\ -\mathbf{i}\omega\mu\mathbf{H} - \mathrm{curl}(\mathbf{E}) & = & +\beta_{\mathbf{H}}\omega\mu\mathbf{H}, \end{array}\right. \quad + \text{b.c.}$$

- Reduced second order system

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

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

$$\rightarrow \left\{\begin{array}{c} -(1-\beta_{\mathbf{E}}\beta_{\mathbf{H}} - (\beta_{\mathbf{E}}+\beta_{\mathbf{H}})\mathbf{i})\omega^2 \mathrm{div}(\varepsilon\,\mathrm{grad})\varphi, \\ \left(-(1-\beta_{\mathbf{E}}\beta_{\mathbf{H}} - (\beta_{\mathbf{E}}+\beta_{\mathbf{H}})\mathbf{i})\omega^2\varepsilon - \mathrm{div}(\frac{1}{\mu}\mathrm{grad})\right)\mathbf{U} \end{array}\right.$$

Discretized Maxwell equations

- Disrectization by discontinous Galërkin for $\mathbf{W} = \binom{\mathbf{E}}{\mathbf{H}}$

$$\mathcal{A}x = b$$

- Matrix block structure (first taking **E**, then **H**)

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

- M_ε, M_μ 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.
- $C_{ij} = C_{ij}^T \ i, j, = 1, 2$ refer to the discretized curl operators curl(**H**), curl(**E**), C_{11}, C_{22} are block-diagonal

$$\Rightarrow \mathcal{A} \text{ is complex-symmetric.}$$

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

Discretized shifted Maxwell equations

- Original system

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

- shifted system

$$\mathcal{P} = \begin{pmatrix} (\mathbf{i}+\beta_{\mathbf{E}})\omega M_\varepsilon & 0 \\ 0 & -(\mathbf{i}+\beta_{\mathbf{H}})\omega M_\mu \end{pmatrix} - \begin{pmatrix} C_{11} & C_{12} \\ C_{12} & C_{22} \end{pmatrix}$$

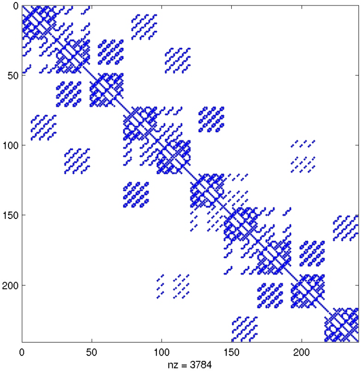
- reduced shifted system (refers to shifted Helmholtz), Schur complement of $\mathcal{P}$.

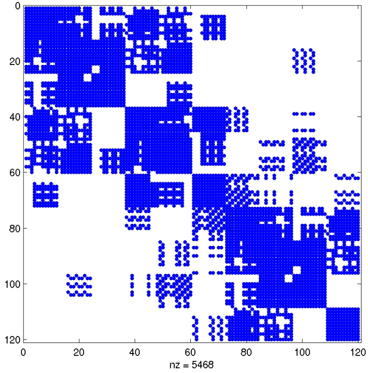
$$\mathcal{P}_S = -(\mathbf{i}+\beta_{\mathbf{H}})\omega M_\mu - C_{22} - C_{12}\left((\mathbf{i}+\beta_{\mathbf{E}})\omega M_\varepsilon - C_{11}\right)^{-1} C_{12}$$

- Three classes of shifted operators
  - $\mathcal{P}_1$: $\mathcal{P}$ for $\beta_{\mathbf{E}} = \beta_{\mathbf{H}} = \beta$
  - $\mathcal{P}_2$: $\mathcal{P}_S$ for $\beta_{\mathbf{E}} = \beta_{\mathbf{H}} = \beta$
  - $\mathcal{P}_3$: $\mathcal{P}_S$ for $\beta_{\mathbf{E}} = 0$, $\beta_{\mathbf{H}} = \beta$

Discretized shifted Maxwell equations

Eigenvalues of the preconditioned system





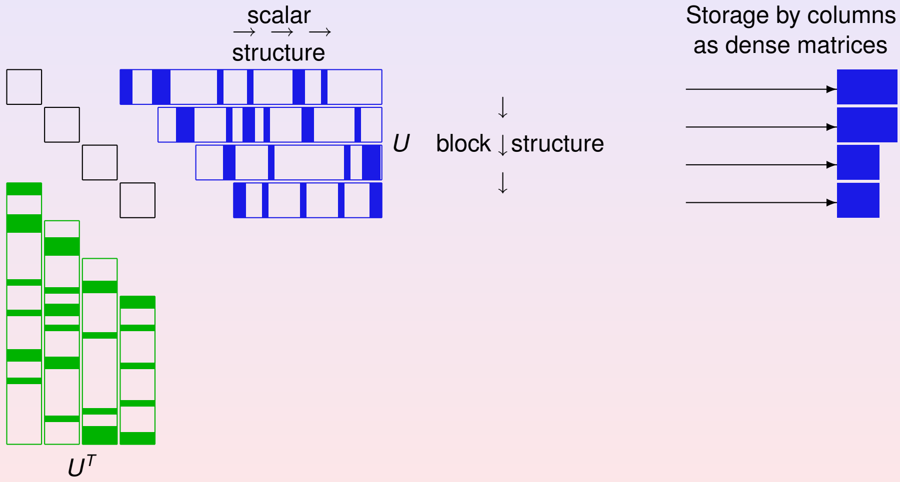
Block structure of $\mathcal{P}$

Block structure of $\mathcal{P}_S$

The larger the β, the more diagonal dominant the systems will be.

Block-structured ILUs

Left-looking block ILU (Crout version)



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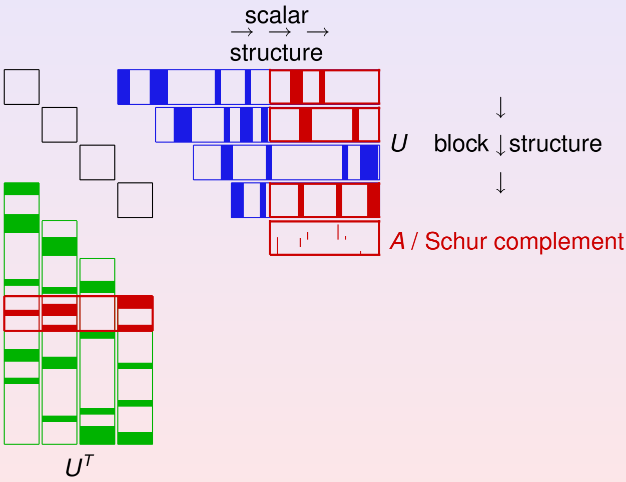
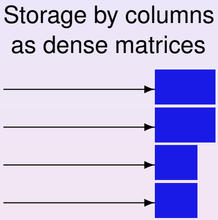
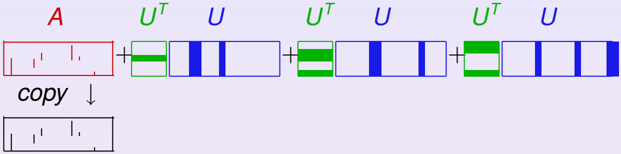




Block-structured ILUs

Computation based on Level-3 BLAS



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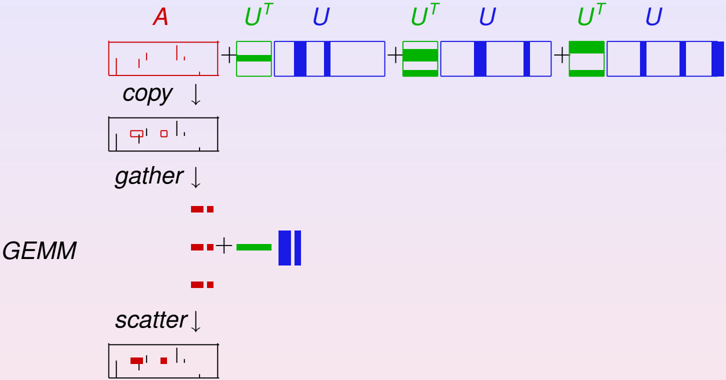

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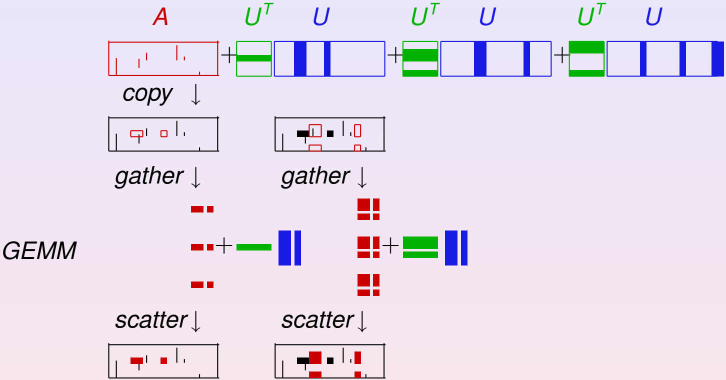

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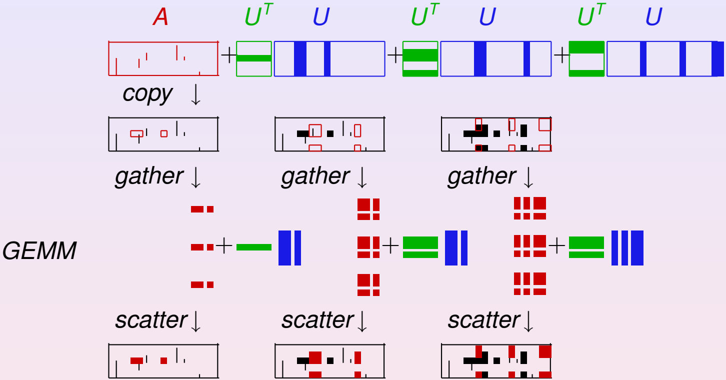

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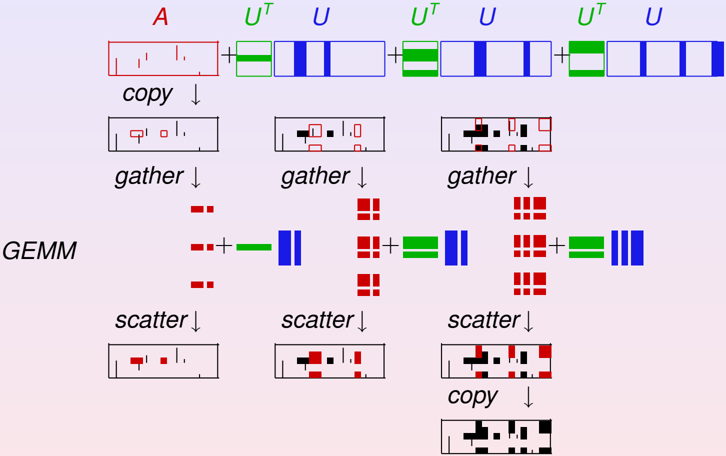

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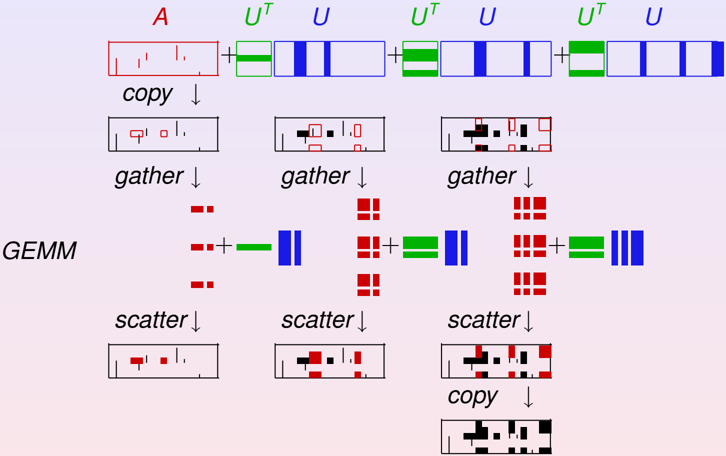

Associated forward/backward solve only needs Level-2-BLAS

$$A \rightarrow \begin{pmatrix} B & F \\ F^T & C \end{pmatrix} = \underbrace{\begin{pmatrix} L_B & 0 \\ L_F & I \end{pmatrix}}_{L} \underbrace{\begin{pmatrix} D_B & 0 \\ 0 & S_C \end{pmatrix}}_{D} \underbrace{\begin{pmatrix} L_B^T & L_F^T \\ 0 & I \end{pmatrix}}_{L^T} + E$$

Inverse-based pivoting: keep $\|L^{-1}\| \leqslant \kappa$ for some prescribed κ (e.g. $\kappa = 5$).

Multilevel ILU

Inverse-Based Pivoting

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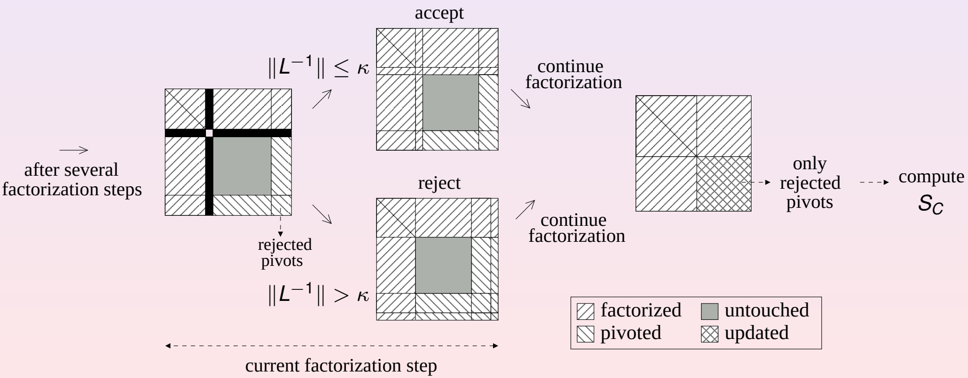

Inverse-based Coarsening

A generalized block diagonal dominance

- block diagonal dominance yields bounded inverse triangular factors:

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

Suppose that

$$\sum_{i:i\neq j} \left\| A_{ij} A_{jj}^{-1} \right\| \leqslant \frac{\kappa - 1}{\kappa}, \ \sum_{j:j\neq i} \left\| A_{ii}^{-1} A_{ij} \right\| \leqslant \frac{\kappa - 1}{\kappa}.$$

$$\Rightarrow |||L^{-1}|||_1 \leqslant \kappa, \ |||U^{-1}|||_\infty \leqslant \kappa \text{ (induced block norms).}$$

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- Inverse–based coarsening directly yields

$$|||L^{-1}|||, |||U^{-1}||| \leqslant \kappa$$

for partial decomposition.

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for partial decomposition.

- If $\begin{pmatrix} A_{\mathcal{F}\mathcal{F}} & A_{\mathcal{F}\mathcal{C}} \\ A_{\mathcal{C}\mathcal{F}} & A_{\mathcal{C}\mathcal{C}} \end{pmatrix}$ has a large size block diagonal dominant block $A_{\mathcal{F}\mathcal{F}}$, then $|||L^{-1}|||$, $|||U^{-1}|||$ are small and a large portion of the system can be reduced.

Bounded Interpolation

$$A^{-1} \approx \underbrace{L^{-T}}_{\approx\kappa} D^{-1} \underbrace{L^{-1}}_{\approx\kappa}$$

Bounded Interpolation

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\begin{aligned}
A^{-1} &\approx \underbrace{L^{-T}}_{\approx\kappa} D^{-1} \underbrace{L^{-1}}_{\approx\kappa} \\
&= \begin{pmatrix} (L_{\mathcal{F}\mathcal{F}} D_{\mathcal{F}\mathcal{F}} L_{\mathcal{F}\mathcal{F}}^T)^{-1} & 0 \\ 0 & 0 \end{pmatrix} + \underbrace{\begin{pmatrix} -L_{\mathcal{F}\mathcal{F}}^{-T} L_{\mathcal{C}\mathcal{F}}^T \\ I \end{pmatrix}}_{I_h} S_{\mathcal{C}\mathcal{C}}^{-1} \underbrace{\begin{pmatrix} -L_{\mathcal{C}\mathcal{F}} L_{\mathcal{F}\mathcal{F}}^{-1} & I \end{pmatrix}}_{I_h^T}
\end{aligned}
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$$
Ax = \varepsilon x
$$

$$
\underbrace{\frac{1}{\varepsilon} x}_{LARGE} = A^{-1} x \approx \begin{pmatrix} \underbrace{(L_{\mathcal{F}\mathcal{F}} D_{\mathcal{F}\mathcal{F}} L_{\mathcal{F}\mathcal{F}}^T)^{-1}}_{\approx C} & 0 \\ 0 & 0 \end{pmatrix} x + \underbrace{I_h}_{\approx\kappa} S_{\mathcal{C}\mathcal{C}}^{-1} \underbrace{I_h^T}_{\approx\kappa} x
$$

Bounded Interpolation

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$\Rightarrow$ by inverse-based coarsening $S_{\mathcal{C}\mathcal{C}}$ captures the eigenvalues with small modulus

Time-harmonic Maxwell equations

- 3D scattering problem discretized by a DG-$\mathbb{P}_1$ method using a mesh with 46704 tetrahedral elements
- For an incident plane wave of frequency F =900MHz 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 $20 \times nnz(A)/n \approx 200$
- Inverse bound set to $\kappa = 10$.
- Iterative solver SQMR until $\|b - Ax_k\| \leqslant 10^{-8}(\|b\| + \|A\|\|x_k\|)$

Maxwell equations

Three different shifted Systems

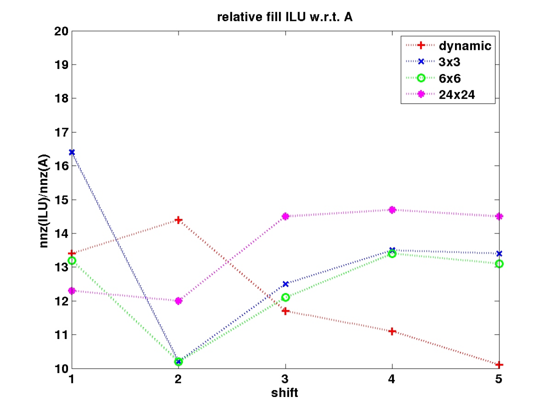
- $\mathcal{P}_1$: Original system $\mathcal{A}$ shifted by $\beta\omega \begin{pmatrix} M_\varepsilon & 0 \\ 0 & -M_\mu \end{pmatrix}$
- $\mathcal{P}_2$: Schur complement of $\mathcal{P}_1$ after elimination of **E** part
- $\mathcal{P}_3$: Schur complement of $\mathcal{A}$ after elimination of **E** part and then shifted by $\beta\omega M_\mu$ (discrete shifted curl curl operator)
- $\mathcal{P}_{2,3}$ are much denser then $\mathcal{P}_1$, approx. 40 nonzeros per row. Therefore, maximum fill is also limited to $10 \times nnz(\mathcal{P}_{1,2}) \approx 400$.
- Use shifts $\beta = 1, 2, 3, 4, 5$
- natural block sizes for $\mathcal{P}_1$:
  - 3, taking **E**, **H** separately
  - 6, taking $\mathbf{W} = (\mathbf{E}, \mathbf{H})$ 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

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

$\mathcal{P}_1$

rel. fill



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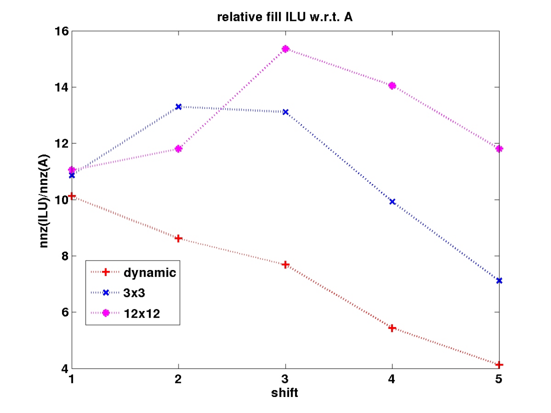
$\mathcal{P}_2$

rel. fill



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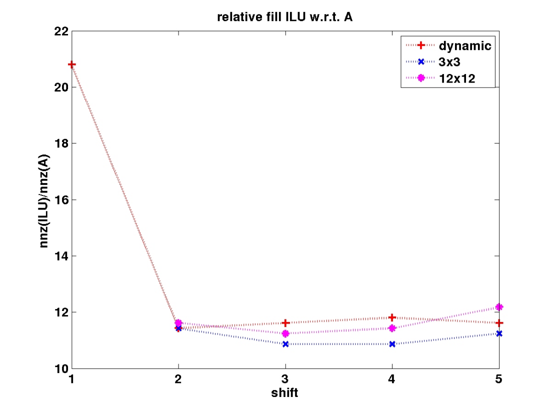
$\mathcal{P}_3$

rel. fill



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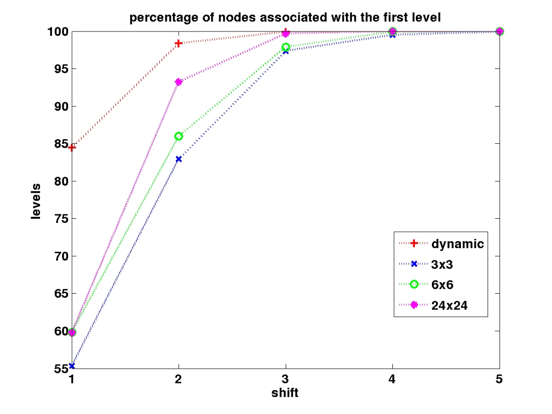
$\mathcal{P}_1$

size 1st level



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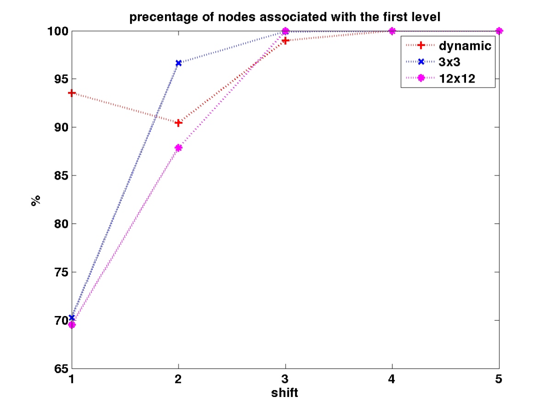
size 1st level



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$\mathcal{P}_3$

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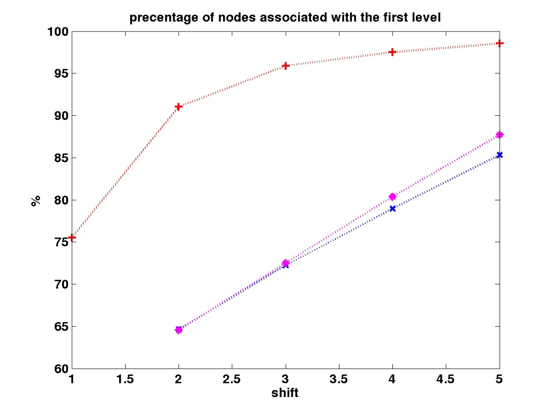

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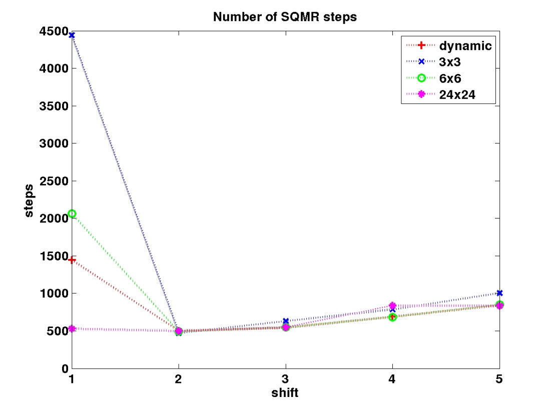
$\mathcal{P}_1$

iteration



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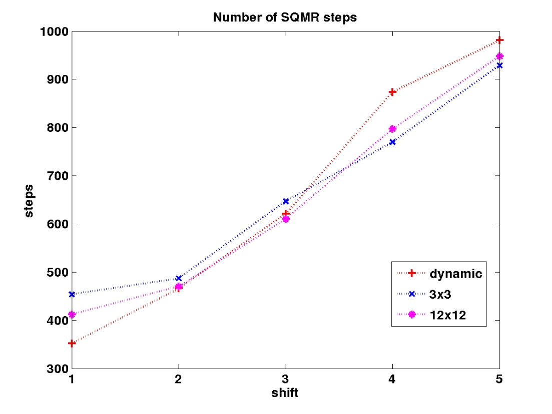
$\mathcal{P}_2$

iteration



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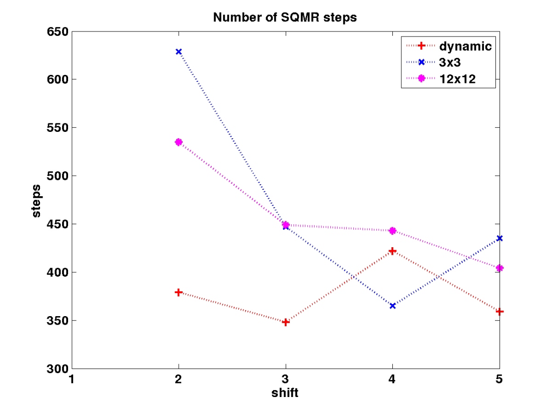
- LARGE shifts lead to
  - less fill
  - less levels
  - larger leading level
- For smaller shifts the limit w.r.t. the fill per row/column is effective

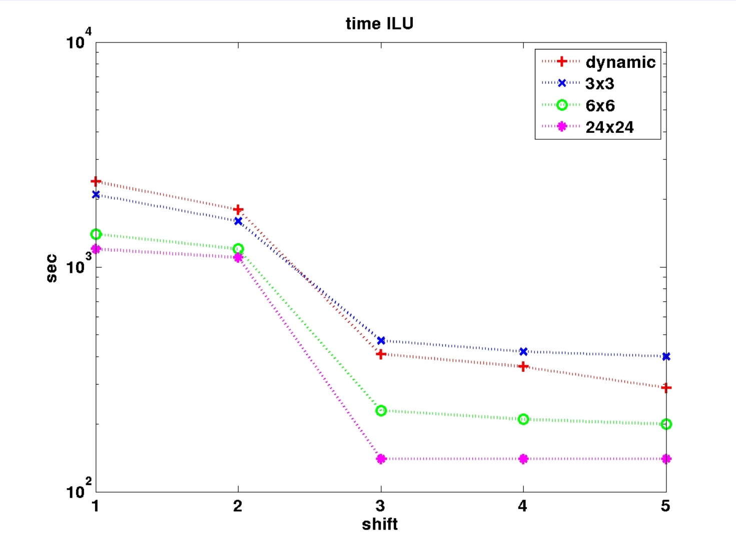
$\mathcal{P}_3$

iteration



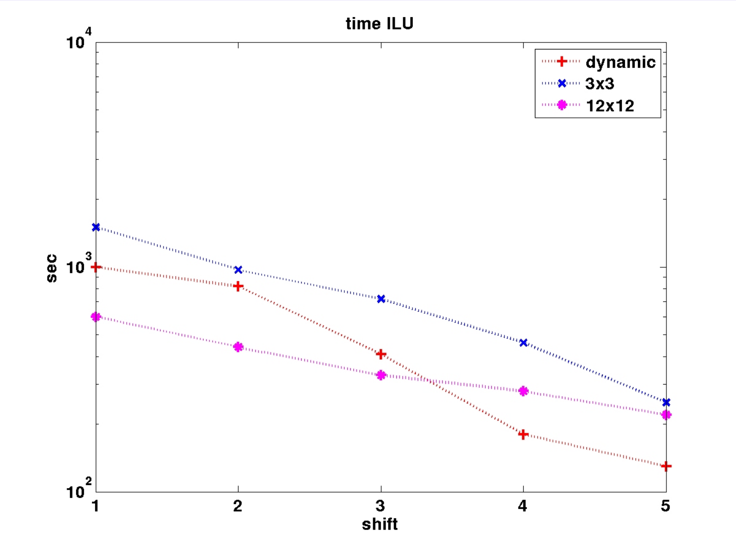
Computation time Multilevel Block ILU

$\mathcal{P}_1$



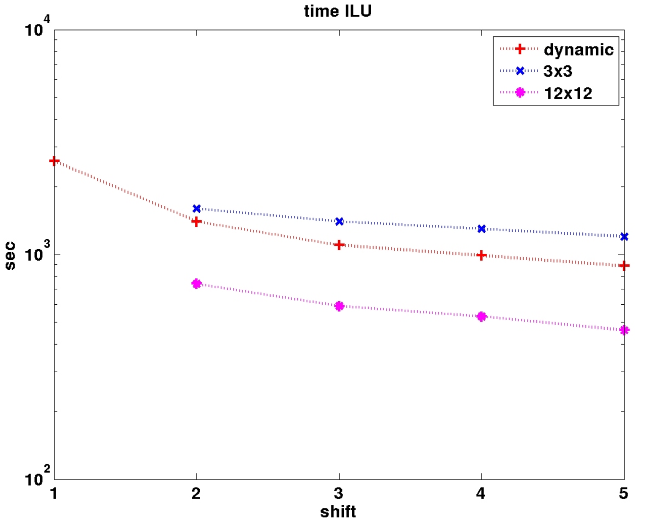
Computation time Multilevel Block ILU

$\mathcal{P}_2$



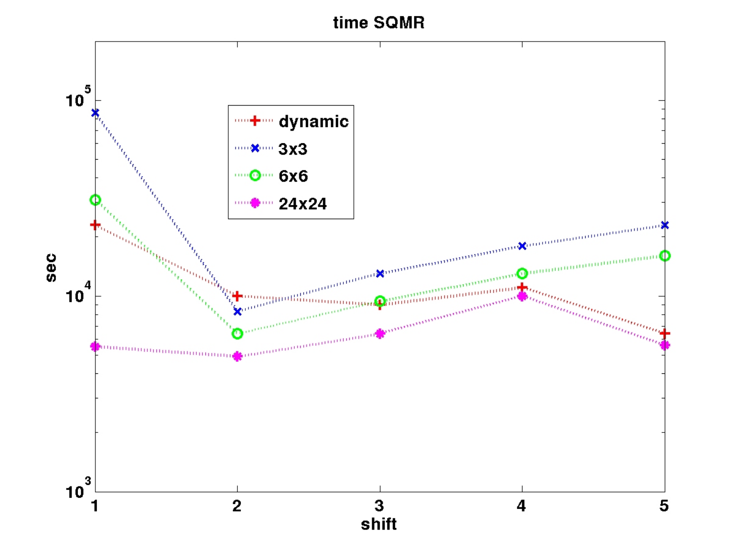
Computation time Multilevel Block ILU

$\mathcal{P}_3$



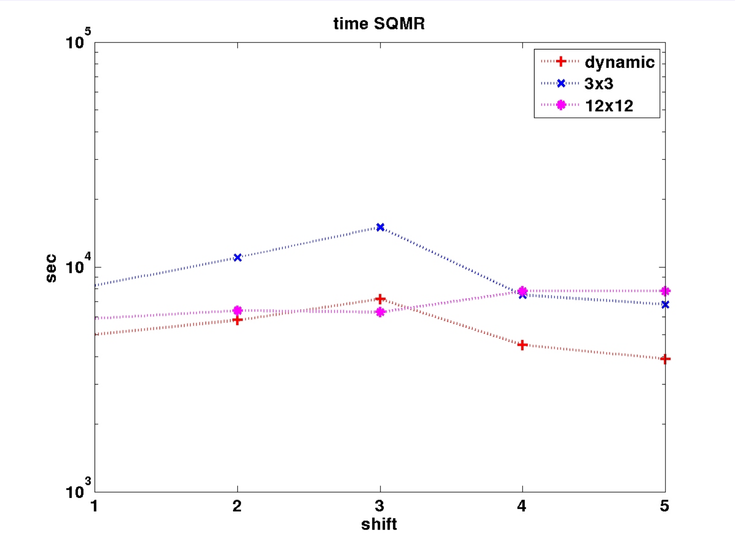
Computation time SQMR

$\mathcal{P}_1$

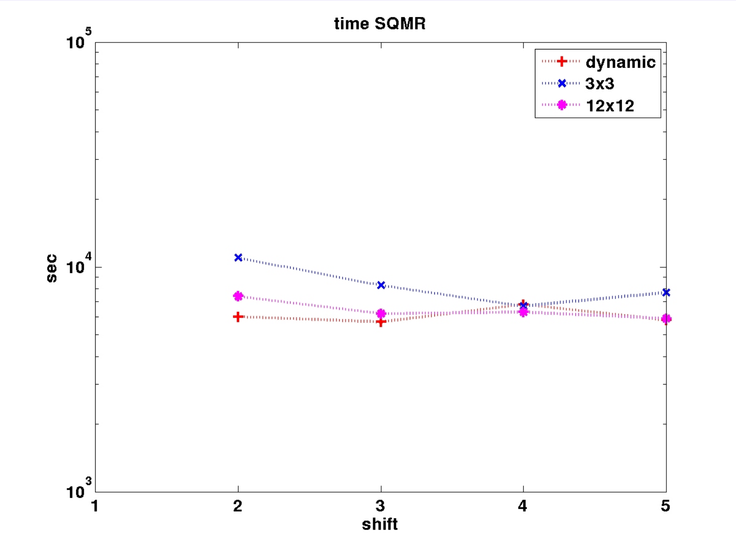


Computation time SQMR

$\mathcal{P}_2$



Computation time SQMR



$\mathcal{P}_3$

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. $\mathbb{P}_2$ elements) larger blocks will occur (e.g. block size 60 for $\mathbb{P}_2$) and even more benefits are expected