Technische
Universität
Braunschweig

Institute for Computational Mathematics

Model Order Reduction for Maxwell Equations based on Moment Matching

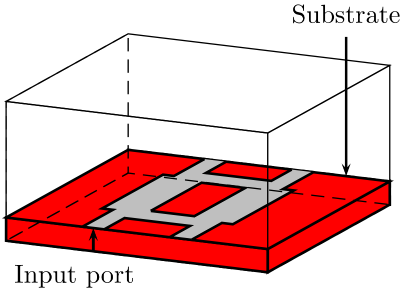
Matthias Bollhöfer (joint work with André Bodendiek)
INRIA Sophia Antipolis , July 28, 2015

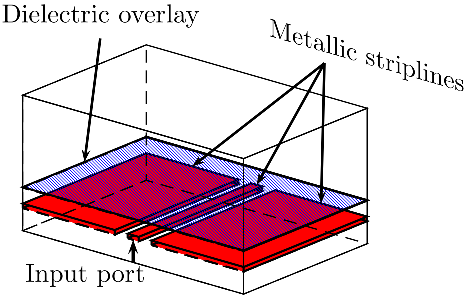
Outline

- **Maxwell's Equations**
- **Model Order Reduction**
  - MOR for Maxwell Equations
  - Model Order Reduction Based on Moment Matching
  - Numerical Results
- **Modified Adaptive-Order Rational Arnoldi Method**
  - Savings for the AORA method
  - QMR Method
  - Simplified QMR
  - QMR with Subspace Recycling
- **Numerical Results**
- **Conclusions**

Outline

Model Problems

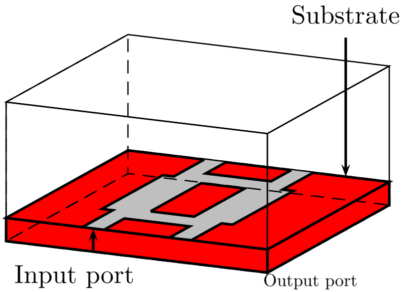


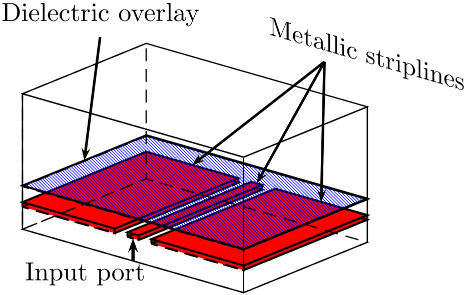


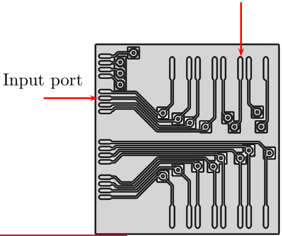
Left picture: branchline coupler on a substrate with PMC boundary conditions, two parallel microstriplines, coupled together in form of a transversal bridge, frequency range 1.0 to 10.0 GHz, $N = 73'385$.

Right picture: coplanar waveguide with a dielectric overlay, PEC boundary conditions, frequency range 0.6 to 3.0 GHz, $N = 32'924$.

Model Problems







PCB circuit on a substrate within the frequency range from 7.5 to 10.0 GHz, $N = 226'458$

PEC boundary condition for the conducting lines, PMC boundary condition for the rest

Maxwell's Equations

$$
\begin{aligned}
\frac{\partial(\varepsilon \mathbf{E})}{\partial t} &= -\sigma \mathbf{E} + \nabla \times \mathbf{H} \\
\frac{\partial(\mu \mathbf{H})}{\partial t} &= -\nabla \times \mathbf{E} \\
(0 &= \nabla \cdot (\varepsilon \mathbf{E}),\ 0 = \nabla \cdot (\mu \mathbf{H}))
\end{aligned}
$$

ε electric permittivity, μ magnetic permeability, σ electric conductivity.

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Discrete equations:

$$\left.\begin{aligned} M_\varepsilon\dot{E} &= -M_\sigma E + GH + B_E u \\ M_\mu\dot{H} &= -G^T E \qquad\quad + B_H u \end{aligned}\right. + \text{b.c.}$$

$$\begin{aligned} (0 &= D_E M_\varepsilon E, \quad 0 = D_H M_\mu H) \\ y &= C_E E + C_H H \end{aligned}$$

- u input, y output
- M_ε, M_μ are sym. pos. def., M_σ sym. pos. semidef. (mass matrices)
- G highly singular! (curl operator)

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Model Order Reduction

$$
\begin{aligned}
\mathcal{M}\dot{x} &= \mathcal{A}x + \mathcal{B}u \\
(0 &= \mathcal{D}x) \\
y &= \mathcal{C}x
\end{aligned}
$$

$$
\mathcal{M} = \begin{pmatrix} M_\varepsilon & 0 \\ 0 & M_\mu \end{pmatrix},\ \mathcal{A} = \begin{pmatrix} -M_\sigma & G \\ -G^T & 0 \end{pmatrix}, x = \begin{pmatrix} E \\ H \end{pmatrix}.
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Model Order Reduction: find full rank $S, T \in \mathbb{R}^{2n,r}$ such that $r \ll 2n$ and use instead

$$\begin{aligned} (S^*\mathcal{M}T)\,\dot{\tilde{x}} &= (S^*\mathcal{A}T)\,\tilde{x} + (S^*\mathcal{B})\,u \\ (0 &= (\mathcal{D}T)\,\tilde{x}) \\ \tilde{y} &= (\mathcal{C}T)\,\tilde{x} \end{aligned}$$

$$\|y - \tilde{y}\| \text{ small}$$

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Structure-Preserving MOR for Maxwell's Equations

$$\text{Here use } S = T = \begin{pmatrix} V & 0 \\ 0 & W \end{pmatrix}$$

Structured MOR: find full rank $V, W \in \mathbb{R}^{n,r}$ such that $r \ll n$ and use instead

$$\begin{aligned}
(V^* M_\varepsilon V)\ \dot{e} &= -(V^* M_\sigma V)\ e + (V^* G W)\ h + (V^* B_E)\ u \\
(W^* M_\mu W)\ \dot{h} &= -\left(W^* G^T V\right)\ e \qquad\qquad + (W^* B_H)\ u \\
(0 &= (D_E M_\varepsilon V)\, e, \quad 0 = (D_H M_\mu W)\, h) \\
\tilde{y} &= (C_E V)\ \ e + \ (C_H W)\ \ h
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\tilde{M}_\varepsilon \, \dot{e} &= -\tilde{M}_\sigma \, e + \tilde{G} \, h + \tilde{B}_E \, u \\
\tilde{M}_\mu \, \dot{h} &= -\tilde{G}^T \, e \qquad + \tilde{B}_H \, u \\
(0 &= \tilde{D}_E e, \quad 0 = \tilde{D}_H h) \\
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Moment-Matching — Basic Idea

$$\mathcal{M} = \begin{pmatrix} M_\varepsilon & 0 \\ 0 & M_\mu \end{pmatrix}, \ \mathcal{A} = \begin{pmatrix} -M_\sigma & G \\ -G^T & 0 \end{pmatrix}, \ \mathcal{B} = \begin{pmatrix} B_E \\ B_H \end{pmatrix}. \ \mathcal{C} = \begin{pmatrix} C_E & C_H \end{pmatrix}.$$

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Transfer function

$$\mathcal{H}(s) = \mathcal{C}\mathcal{P}\left(s\mathcal{M} - \mathcal{A}\right)^{-1}\mathcal{B} \qquad (\mathcal{P} \text{ projector to divergence-free part })$$

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Taylor/Laurent expansion at some expansion point s_j:

$$\mathcal{A}_j := \left(s_j\mathcal{M} - \mathcal{A}\right)^{-1}\mathcal{M},\; \mathcal{B}_j := \left(s_j\mathcal{M} - \mathcal{A}\right)^{-1}\mathcal{B},\; \mathcal{C}_j := \mathcal{C}\mathcal{P}\left(s_j\mathcal{M} - \mathcal{A}\right)^{-1}.$$

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$$\Rightarrow \mathcal{H}(s) = \sum_{p=0}^{\infty} \mathcal{C}\mathcal{P}\overbrace{[-\mathcal{A}_j]^p\mathcal{B}_j}^{X_j^{(p)}}(s - s_j)^p = \sum_{p=0}^{\infty} \underbrace{\mathcal{C}_j[-\mathcal{A}_j]^p}_{Y_j^{(p)}}\mathcal{B}(s - s_j)^p$$

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$X_j^{(p)}$ input moments, Taylor coefficients $Z_j^{(p)} = \mathcal{C}\mathcal{P}X_j^{(p)} = Y_j^{(p)}\mathcal{B}$ output moments.

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$$\mathcal{K}_r(\mathcal{A}_j, \mathcal{B}_j) \text{ and } \mathcal{K}_r(\mathcal{A}_j^*, \mathcal{C}_j^*)$$

such that $S^*T = I \rightarrow$ matches $2r$ moments $Z_j^{(0)}, \ldots, Z_j^{(2r-1)}$

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- Arnoldi-type methods [PRIMA,Odabasioglu et al.'96,'97], [SPRIM,Freund'04,'08] compute one orthonormal basis $S = T = Q \equiv Q_r \in \mathbb{R}^{2n,r}$, say, from

$$\mathcal{K}_r(\mathcal{A}_j, \mathcal{B}_j)$$

  using modified Gram-Schmidt $\rightarrow$ matches r moments $Z_j^{(0)}, \ldots, Z_j^{(r-1)}$

Structure-Preserving Moment Matching Methods

Structure Preservation for Maxwell Equations

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$$Q = \begin{bmatrix} V \\ W \end{bmatrix} \rightarrow \begin{bmatrix} V & 0 \\ 0 & W \end{bmatrix}$$

  - twice as big, but ...
  - block-structure preserved, still r moments matched
  - if we are lucky, up to $2r$ moments could be matched

Structure-Preserving Moment Matching Methods

Problems

- (How to) select $s_j \in [f_{\min}, f_{\max}]$
- (No) error bounds!? Choice of r, l, accuracy of the reduced model

$$\mathcal{H}(s) = \mathcal{C}\,(s\mathcal{M} - \mathcal{A})^{-1}\,\mathcal{B}, \quad \mathcal{H}_r(s) = \hat{\mathcal{C}}\left(s\hat{\mathcal{M}} - \hat{\mathcal{A}}\right)^{-1}\hat{\mathcal{B}}$$

$$\|\mathcal{H}(i\omega) - \mathcal{H}_r(i\omega)\| \leqslant \dots$$

- multiple expansion points $s_1, \dots s_l \in [f_{\min}, f_{\max}]$
- Restarting Arnoldi and increasing r or l whenever the “error estimate” is not accurate enough

Rational Arnoldi Methods

- multiple expansion points $s_1, \ldots, s_l$
- multiple associated Taylor expansions

$$\mathcal{H}(s) = \sum_{p=0}^{\infty} Z_j^{(p)} (s - s_j)^p, \; j = 1, \ldots, l$$

- Rational Krylov method: Compute basis Q_r for the Krylov subspaces

$$\sum_{j=1}^{l} \mathcal{K}_{r_j}(\mathcal{A}_j, \mathcal{B}_j).$$

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Lemma (Key-Lemma, Grimme,Gallivan'98)

If $s_j \neq s_k$ then

$$\mathcal{A}_k \cdot \mathcal{A}_j^{p-1} \mathcal{B}_j \in \mathcal{K}_p(\mathcal{A}_j, \mathcal{B}_j) + \mathcal{K}_1(\mathcal{A}_k, \mathcal{B}_k)$$

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$\Rightarrow$ mixing inverses with different shifts leads to a separate sum of Krylov subspaces, no "mixed powers of inverses"

Rational Arnoldi Methods

- Traditional Rational Arnoldi methods build Q_r w.r.t. $\mathcal{K}_{r_j}(\mathcal{A}_j, \mathcal{B}_j)$, $j = 1, \ldots, l$ **one after another** using modified Gram-Schmidt.

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$$\mathcal{K}_{\mathbf{r_1}}(\mathcal{A}_1, \mathcal{B}_1)$$

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$$\mathcal{K}_{r_1}(\mathcal{A}_1, \mathcal{B}_1) + \mathcal{K}_{\mathbf{r_2}}(\mathcal{A}_2, \mathcal{B}_2)$$

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- [Ruhe'94], [Gallivan,Grimme,van Dooren'95], [Grimme'99], [Bai'02], [Gugercin,Antoulas'06], [Lee,Chu,Feng'06],. . . and many others

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- At each step s_j is selected w.r.t. the largest output moment error $Z_j^{(r)} - \tilde{Z}_j^{(r)}$ which can be computed cheaply

Expansion Point Selection

- AORA called repeatedly $l = 1, 2, 3, \ldots$ with increasing number of expansion points

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$$s_1 = 2\pi i f_{\text{min}}, \; s_2 = 2\pi i \sqrt{f_{\text{min}} f_{\text{max}}}, \; s_3 = 2\pi i f_{\text{max}}$$

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$$s_1,\ s_2,\ s_3,\ s_4,\ s_5,\ \mathbf{s_6}$$

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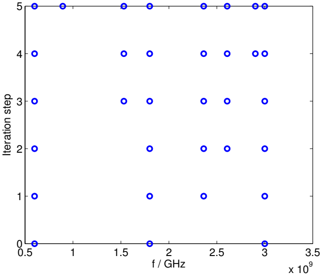

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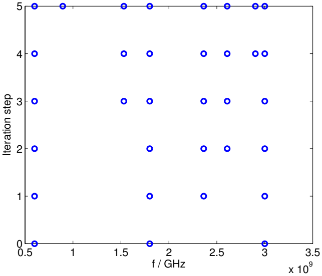


- global stopping criterion [Grimme,Gallivan'98] $\sum_{i=1}^{l} 2^{i-l} \frac{|\mathcal{H}_r^{(i)}(s) - \mathcal{H}_r^{(i-1)}(s)|}{|\mathcal{H}_r^{(i)}(s)|} \leqslant \varepsilon$

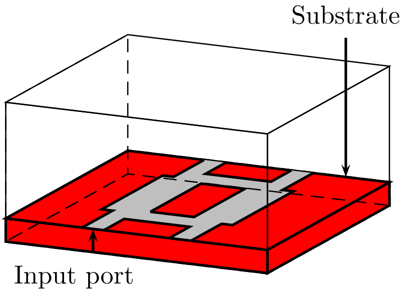
Outline

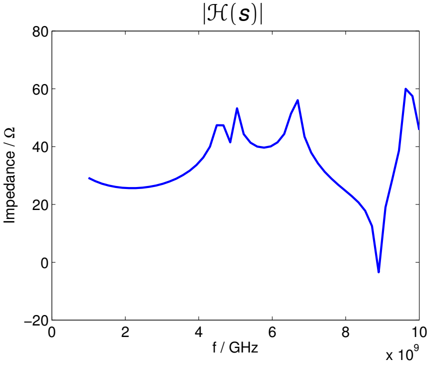
Model Order Reduction — Numerical Results

- model problems have a frequency range in $[f_{\text{min}}, f_{\text{max}}]$
- computed reduced order models have fixed size $n = 25(50)$
- SPRIM uses expansion point $s_0 = \frac{f_{\text{min}} + f_{\text{max}}}{2}$
- expansion point selection based on relative error 10^{-9}
- strategy finally leads to $l = 8$ expansion points $s_1, \ldots, s_8$
- Rational Arnoldi (RA) and Adaptive Order Rational Arnoldi (AORA) repeated 5 times
- RA uses fixed sizes $j = n/l$ for each Krylov subspace $\mathcal{K}_j$
- AORA adaptively increases each $\mathcal{K}_{j_i}$

Model Order Reduction — Numerical Results

Branchline Coupler





- size $N = 73385$, discretized using FIT
- frequency range $[f_{\text{min}}, f_{\text{max}}] = [10^9, 10^{10}]$

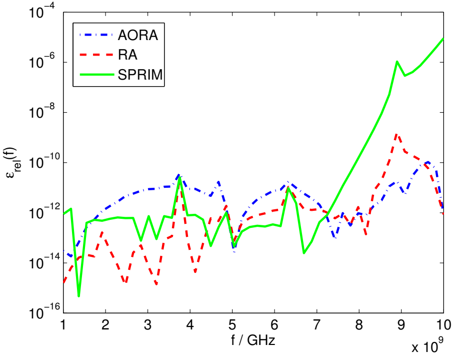
Model Order Reduction — Numerical Results

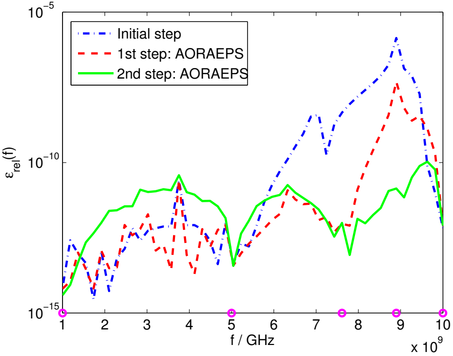
Branchline Coupler

relative error

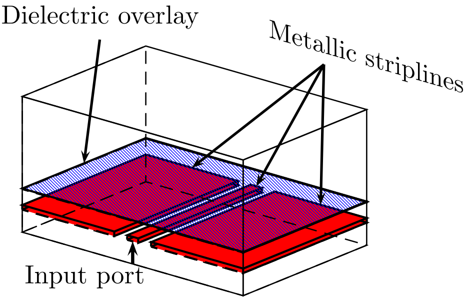
$$\epsilon_{rel}(f) = \frac{|\mathcal{H}(s) - \tilde{\mathcal{H}}(s)|}{|\mathcal{H}(s)|},$$

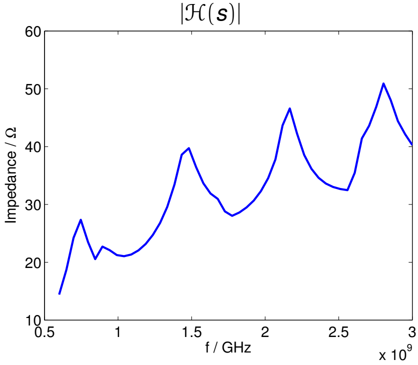
$s = 2\pi i f$ with $f \in [10^9, 10^{10}]$ displayed as reference





Coplanar Waveguide





- size $N = 32924$, discretized using FIT
- frequency range $[f_{\min}, f_{\max}] = [0.6 \cdot 10^9, 3.0 \cdot 10^9]$

relative error

$$\epsilon_{rel}(f) = \frac{|\mathcal{H}(s) - \tilde{\mathcal{H}}(s)|}{|\mathcal{H}(s)|},$$

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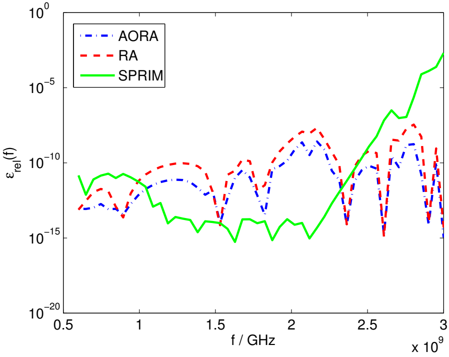

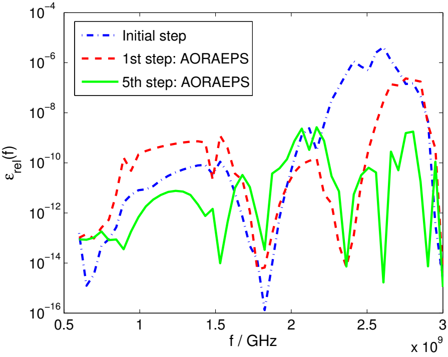

Outline

- Maxwell's Equations
- Model Order Reduction
  - MOR for Maxwell Equations
  - Model Order Reduction Based on Moment Matching
  - Numerical Results
- **Modified Adaptive-Order Rational Arnoldi Method**
  - Savings for the AORA method
  - QMR Method
  - Simplified QMR
  - QMR with Subspace Recycling
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Lemma

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- Lemma requires that shifts $s_1, \ldots, s_l$ are selected in the same order
- new shift s_{l+1} can be injected at any time
- only new shift s_{l+1} requires to solve systems with $s_{l+1}\mathcal{M} - \mathcal{A}$
- $\longrightarrow$ mAORA (modified AORA)

Solving Systems in the Modified AORA Method

Recall

- $\mathcal{J}\,(s\mathcal{M} - \mathcal{A})$ is **complex-symmetric**, where $\mathcal{J} = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}$
- Schur complement $\mathcal{S}(s) = s^2 M_\varepsilon + sM_\sigma + GM_\mu^{-1}G^T$ is **complex-symmetric**

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- Save memory and time: Only compute factorization of $A(s_*)$ for some characteristic shift $s_*=2\pi i\sqrt{f_{\min}f_{\max}}$.
- For all $s_j\neq s_*$ use (recycling) Krylov subspace method as wrapper.

Outline

QMR Method — Sketch

Two-sided Lanczos Method

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QMR for $Ax = b$ based on two-sided Lanczos method:

- $r_0 = b - Ax_0,\ v_1 = r_0/\|r_0\|$
- $x_k = x_0 + V_k y$
- quasi-minimize
$$\|b - Ax_k\| \leqslant \|V_{k+1}\| \cdot \left\| \|r_0\| e_1 - \underline{T_k} y \right\|$$
  $\longrightarrow y$ from least squares solution
  $\longrightarrow x$
- [Freund et al. '91,'93,'94]

Outline

Simplified QMR Method for J-Symmetric Matrices

- $A^T J = JA$, where $J = J^T$, J nonsingular
- use specific left initial guess $\tilde{v}_1 = Jv_1$

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- [Freund et al. '94,'95]
- Maxwell equations: complex-symmetric system A with complex-symmetric preconditioner P satisfy J-symmetry!

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QMR with Subspace Recycling

Krylov subspace methods with subspace recycling

- GCROT, GCRO-DR [De Sturler et al.'99,'06]
- recycling BiCG, recycling BiCGStab [Ahuja et al. '12,'13]

Main idea: $U, \tilde{U} \in \mathbb{C}^{n,r}$, $C = AU$, $\tilde{C} = A^T \tilde{U}$, $r \ll n$ given subspaces, $D_c = \tilde{C}^T C$.
Apply Lanczos (Arnoldi) to the systems

$$AV_k = V_{k+1} \underline{T_k},$$

$$A^T \tilde{V}_k = \tilde{V}_{k+1} \underline{\tilde{T}_k}$$

with updated initial guess and projected initial residual

$$x_0^{(new)} = x_0 + UD_c^{-1} \tilde{C}^T r_0, \; r_0^{(new)} = (I - CD_c^{-1} \tilde{C}^T) r_0.$$

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Apply Lanczos (Arnoldi) to the projected systems

$$(I - CD_c^{-1}\tilde{C}^T)AV_k = V_{k+1}\underline{T_k},$$

$$(I - \tilde{C}D_c^{-T}C^T)A^T\tilde{V}_k = \tilde{V}_{k+1}\underline{\tilde{T}_k}$$

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Recycling QMR/BiCG in a Nutshell

$$U, \tilde{U}, \; C = AU, \tilde{C} = A^T \tilde{U}, \; D_c = \tilde{C}^T C.$$

Changing the methods:

BiCG/QMR	Recycling BiCG/QMR
init x_0	$x_0^{(new)} = x_0 + UD_c^{-1}\tilde{C}^T r_0$
init $r_0 = b - Ax_0$	$r_0^{(new)} = (I - CD_c^{-1}\tilde{C}^T) r_0$
matvec Ax	$(I - CD_c^{-1}\tilde{C}^T)Ax$
matvec $A^T x$	$(I - \tilde{C}D_c^{-T} C^T)A^T x$
solution update $x = x + \alpha p$	$x = x + \alpha(I - UD_c^{-1}\tilde{C}^T)p$

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Preconditioning and simplified QMR: a little bit more tricky but similar

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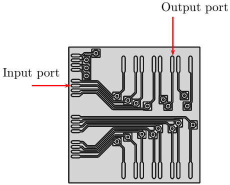
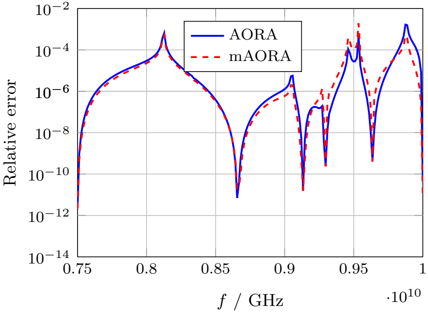
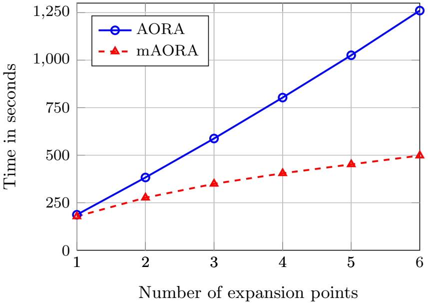
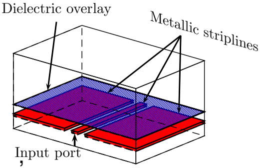
Modified AORA versus AORA









Sampling 20 frequencies $s_j = 2\pi\, i\, f_j$

$f_j \in [f_{\min}, f_{\max}] = [0.6 \cdot 10^9, 3 \cdot 10^9]$

Use complex-symmetric Schur complement system

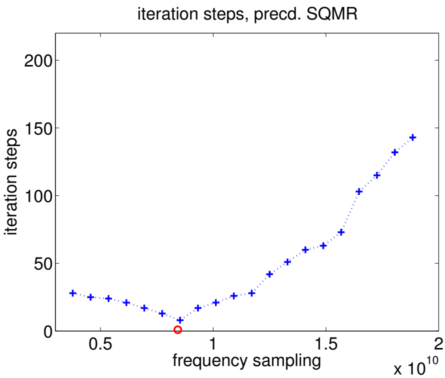
Preconditioner: *LU*-decomposition for $s_* = \sqrt{f_{\min} f_{\max}}$

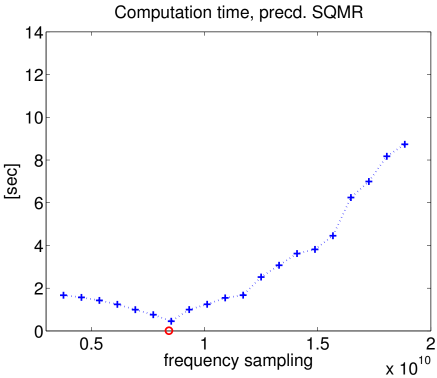
Comparison

- simplified QMR without subspace recycling
- simplified QMR using subspace recycling

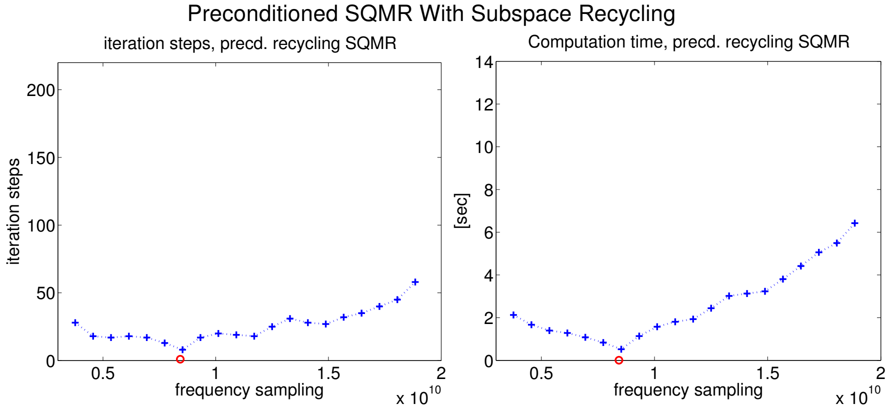
Preconditioner: LU decomposition for $\mathcal{S}(s_*)$

Preconditioned SQMR Without Subspace Recycling





Preconditioner: *LU* decomposition for $\mathcal{S}(s_*)$



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Conclusions

- (adaptive order) rational Arnoldi yields reduced order model for Maxwell equations
- main important structures can be preserved
- outer iteration: several calls of (modified) rational Arnoldi,
  inner iteration: preconditioned SQMR
- Recycling techniques $\rightarrow$ modified AORA, recycling SQMR

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