Model Order Reduction for Maxwell Equations based on Moment Matching

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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
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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, $N = 32'924$. 

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

\[
\begin{align*}
\frac{\partial (\varepsilon E)}{\partial t} &= -\sigma E + \nabla \times H \\
\frac{\partial (\mu H)}{\partial t} &= -\nabla \times E \\
0 &= \nabla \cdot (\varepsilon E), \quad 0 = \nabla \cdot (\mu H)
\end{align*}
\]

\(\varepsilon\) electric permittivity, \(\mu\) magnetic permeability, \(\sigma\) electric conductivity.
Maxwell’s Equations

\[
\frac{\partial (\varepsilon E)}{\partial t} = -\sigma E + \nabla \times H \\
\frac{\partial (\mu H)}{\partial t} = -\nabla \times E \\
(0 = \nabla \cdot (\varepsilon E), \ 0 = \nabla \cdot (\mu H))
\]

\(\varepsilon\) electric permittivity, \(\mu\) magnetic permeability, \(\sigma\) electric conductivity.

Discrete equations:

\[
M_\varepsilon \dot{E} = -M_\sigma E + GH + B_E u \\
M_\mu \dot{H} = -G^T E + B_H u + \text{b.c.}
\]

\(0 = D_E M_\varepsilon E, \ 0 = D_H M_\mu H\)

\[y = C_E E + C_H H\]

- \(u\) input, \(y\) output
- \(M_\varepsilon, M_\mu\) are sym. pos. def., \(M_\sigma\) sym. pos. semidef. (mass matrices)
- \(G\) highly singular! (curl operator)
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Model Order Reduction

\[
\begin{align*}
\mathcal{M}\dot{x} &= Ax + Bu \\
(0 &= Dx) \\
y &= Cx
\end{align*}
\]

\[
\mathcal{M} = \begin{pmatrix} M_\varepsilon & 0 \\ 0 & M_\mu \end{pmatrix}, \quad \mathcal{A} = \begin{pmatrix} -M_\sigma & G \\ -G^T & 0 \end{pmatrix}, \quad x = \begin{pmatrix} E \\ H \end{pmatrix}.
\]
Model Order Reduction

\[
\begin{align*}
M\dot{x} &= Ax + Bu \\
(0 &= Dx) \\
y &= Cx
\end{align*}
\]

\[
\begin{align*}
M = \begin{pmatrix} M_\varepsilon & 0 \\
0 & M_\mu \end{pmatrix}, \quad A = \begin{pmatrix} -M_\sigma & G \\
-G^T & 0 \end{pmatrix}, \quad x = \begin{pmatrix} E \\
H \end{pmatrix}.
\end{align*}
\]

Model Order Reduction: find full rank \( S, T \in \mathbb{R}^{2n,r} \) such that \( r \ll 2n \) and use instead

\[
\begin{align*}
(S^*MT)\dot{\tilde{x}} &= (S^*AT)\tilde{x} + (S^*B)u \\
(0 &= (DT)\tilde{x}) \\
\tilde{y} &= (CT)\tilde{x}
\end{align*}
\]

\[\|y - \tilde{y}\| \text{ small}\]
Model Order Reduction

\[ \dot{\mathcal{M}} \dot{x} = \mathcal{A} x + \mathcal{B} u \]
\[ (0 = \mathcal{D} x) \]
\[ y = \mathcal{C} x \]

\[ \mathcal{M} = \begin{pmatrix} M_\varepsilon & 0 \\ 0 & M_\mu \end{pmatrix}, \quad \mathcal{A} = \begin{pmatrix} -M_\sigma & G \\ -G^T & 0 \end{pmatrix}, \quad x = \begin{pmatrix} E \\ H \end{pmatrix}. \]

Model Order Reduction: find full rank \( S, T \in \mathbb{R}^{2n,r} \) such that \( r \ll 2n \) and use instead

\[ \hat{\mathcal{M}} \hat{\dot{x}} = \hat{\mathcal{A}} \hat{x} + \hat{\mathcal{B}} u \]
\[ (0 = \hat{\mathcal{D}} \hat{x}) \]
\[ \hat{y} = \hat{\mathcal{C}} \hat{x} \]
\[ \| y - \hat{y} \| \text{ small} \]
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

\[
\begin{align*}
(V^* M_\varepsilon V) \, \dot{e} &= -(V^* M_\sigma V) \, e + (V^* GW) \, h + (V^* B_E) \, u \\
(W^* M_\mu W) \, \dot{h} &= -(W^* G^T V) \, e + (W^* B_H) \, u \\
(0 &= (D_E M_\varepsilon V) \, e , \quad 0 = (D_H M_\mu W) \, h) \\
\tilde{y} &= (C_E V) \, e + (C_H W) \, h \\
\| y - \tilde{y} \| & \text{ small}
\end{align*}
\]
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{align*}
\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 + \tilde{B}_H u \\
(0 &= \tilde{D}_E e, \quad 0 = \tilde{D}_H h) \\
\tilde{y} &= \tilde{C}_E e + \tilde{C}_H h
\end{align*}

$\|y - \tilde{y}\|$ small
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Moment-Matching — Basic Idea

\[
\mathbf{M} = \begin{pmatrix} M_\varepsilon & 0 \\ 0 & M_\mu \end{pmatrix}, \quad \mathbf{A} = \begin{pmatrix} -M_\sigma & G \\ -G^T & 0 \end{pmatrix}, \quad \mathbf{B} = \begin{pmatrix} B_E \\ B_H \end{pmatrix}, \quad \mathbf{C} = \begin{pmatrix} C_E & C_H \end{pmatrix}.
\]
Moment-Matching — Basic Idea

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Transfer function

\[ \mathcal{H}(s) = \mathcal{C}\mathcal{P} \left( s\mathbf{M} - \mathbf{A} \right)^{-1} \mathbf{B} \quad (\mathcal{P} \text{ projector to divergence-free part}) \]
Moment-Matching — Basic Idea

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

\[
\mathcal{H}(s) = \mathcal{C} \mathcal{P} (s\mathcal{M} - \mathcal{A})^{-1} \mathcal{B} \quad (\mathcal{P} \text{ projector to divergence-free part })
\]

Taylor/Laurent expansion at some expansion point \( s_j \):

\[
\mathcal{A}_j := (s_j\mathcal{M} - \mathcal{A})^{-1} \mathcal{M}, \quad \mathcal{B}_j := (s_j\mathcal{M} - \mathcal{A})^{-1} \mathcal{B}, \quad \mathcal{C}_j := \mathcal{C} \mathcal{P} (s_j\mathcal{M} - \mathcal{A})^{-1}.
\]
Moment-Matching — Basic Idea

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

Transfer function

\[ \mathcal{H}(s) = CP \left( sM - A \right)^{-1} B \quad \text{(} P \text{ projector to divergence-free part)} \]

Taylor/Laurent expansion at some expansion point \( s_j \):

\[ A_j := (s_jM - A)^{-1} M, \quad B_j := (s_jM - A)^{-1} B, \quad C_j := CP \left( s_jM - A \right)^{-1}. \]

\[ \Rightarrow \mathcal{H}(s) = \sum_{p=0}^{\infty} \chi_j^{(p)} CP \left[ -A_j \right]^p B_j (s - s_j)^p = \sum_{p=0}^{\infty} \gamma_j^{(p)} CP \left[ -A_j \right]^p B (s - s_j)^p \]
Moment-Matching — Basic Idea

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

Transfer function

\[
\mathcal{H}(s) = \mathcal{CP} (s\mathcal{M} - \mathcal{A})^{-1} \mathcal{B} \quad (\mathcal{P} \text{ projector to divergence-free part })
\]

Taylor/Laurent expansion at some expansion point \(s_j\):

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\mathcal{A}_j := (s_j\mathcal{M} - \mathcal{A})^{-1} \mathcal{M}, \quad \mathcal{B}_j := (s_j\mathcal{M} - \mathcal{A})^{-1} \mathcal{B}, \quad \mathcal{C}_j := \mathcal{CP} (s_j\mathcal{M} - \mathcal{A})^{-1}.
\]

\[
\Rightarrow \mathcal{H}(s) = \sum_{p=0}^{\infty} \mathcal{CP} \left[ -\mathcal{A}_j \right]^p \mathcal{B}_j (s - s_j)^p = \sum_{p=0}^{\infty} \mathcal{C}_j \left[ -\mathcal{A}_j \right]^p \mathcal{B} (s - s_j)^p
\]

\(X_j^{(p)}\) input moments, Taylor coefficients \(Z_j^{(p)} = \mathcal{CP} X_j^{(p)} = Y_j^{(p)} \mathcal{B}\) output moments.
Krylov Subspace Methods

Krylov subspace

\[ \mathcal{K}_p(A, b) = \text{span}\{b, Ab, \ldots, A^{p-1}b\} \]
Krylov Subspace Methods

Krylov subspace

\[ \mathcal{K}_p(A, b) = \text{span}\{b, Ab, \ldots, A^{p-1}b\} \]

- input Krylov subspace

\[ X_j^{(p)} \in \mathcal{K}_p(A_j, B_j). \]

- output Krylov subspace

\[ (Y_j^{(p)})^* \in \mathcal{K}_p(A_j^*, C_j^*). \]
Krylov Subspace Methods

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\[ \mathcal{K}_p(A, b) = \text{span}\{b, Ab, \ldots, A^{p-1}b\} \]

- input Krylov subspace
  \[ X_j^{(p)} \in \mathcal{K}_p(A_j, B_j). \]
- output Krylov subspace
  \[ (Y_j^{(p)})^* \in \mathcal{K}_p(A_j^*, C_j^*). \]
- Lanczos-type methods [PVL, Gragg’74, Gutknecht’92, Feldmann, Freund’94, …] generate dual basis \( T \equiv T_r \in \mathbb{R}^{2n,r} \) and \( S \equiv S_r \in \mathbb{R}^{2n,r} \) of \( \mathcal{K}_r(A_j, B_j) \) and \( \mathcal{K}_r(A_j^*, C_j^*) \) such that \( S^* T = I \rightarrow \) matches 2r moments \( Z_j^{(0)}, \ldots, Z_j^{(2r-1)} \)
Krylov Subspace Methods

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\[ \mathcal{K}_p(A, b) = \text{span}\{b, Ab, \ldots, A^{p-1}b\} \]

- input Krylov subspace

\[ \chi_j^{(p)} \in \mathcal{K}_p(A_j, B_j). \]

- output Krylov subspace

\[ (Y_j^{(p)})^* \in \mathcal{K}_p(A_j^*, C_j^*). \]

- Lanczos-type methods \([PVL, Gragg'74, Gutknecht'92, Feldmann, Freund'94, \ldots]\) generate dual basis \(T \equiv T_r \in \mathbb{R}^{2n,r}\) and \(S \equiv S_r \in \mathbb{R}^{2n,r}\) of \(\mathcal{K}_r(A_j, B_j)\) and \(\mathcal{K}_r(A_j^*, C_j^*)\) such that \(S^* T = I \rightarrow\) matches \(2r\) moments \(Z_j^{(0)}, \ldots, Z_j^{(2r-1)}\)

- 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 \(\mathcal{K}_r(A_j, B_j)\) 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

\[ \mathcal{M} = \begin{pmatrix} M_\varepsilon & 0 \\ 0 & M_\mu \end{pmatrix}, \quad \mathcal{A} = \begin{pmatrix} -M_\sigma & G \\ -G^T & 0 \end{pmatrix}. \]

\[ \mathcal{M} \dot{x} = \mathcal{A} x + B u \]

\[ y = C x \]
Structure-Preserving Moment Matching Methods

Structure Preservation for Maxwell Equations

\[ \mathcal{M} = \begin{pmatrix} M_\varepsilon & 0 \\ 0 & M_\mu \end{pmatrix}, \quad \mathcal{A} = \begin{pmatrix} -M_\sigma & G \\ -G^T & 0 \end{pmatrix}. \]

\[
\begin{align*}
(S^* \mathcal{M} T) \dot{x} & = (S^* \mathcal{A} T) \ddot{x} + (S^* \mathcal{B}) u \\
\ddot{y} & = (\mathcal{C} T) \ddot{x}
\end{align*}
\]
Structure-Preserving Moment Matching Methods

Structure Preservation for Maxwell Equations

\[ \mathcal{M} = \begin{pmatrix} M_\varepsilon & 0 \\ 0 & M_\mu \end{pmatrix}, \quad \mathcal{A} = \begin{pmatrix} -M_\sigma & G \\ -G^T & 0 \end{pmatrix}. \]

\[ \hat{\mathcal{M}} \hat{x}' = \hat{\mathcal{A}} \hat{x} + \hat{\mathcal{B}} u \]

\[ \tilde{y} = \hat{\mathcal{C}} \tilde{x} \]
Structure-Preserving Moment Matching Methods

Structure Preservation for Maxwell Equations

\[
\mathcal{M} = \begin{pmatrix} M_\varepsilon & 0 \\ 0 & M_\mu \end{pmatrix}, \quad \mathcal{A} = \begin{pmatrix} -M_\sigma & G \\ -G^T & 0 \end{pmatrix}.
\]

\[
\hat{\mathcal{M}} \dot{\hat{x}} = \hat{\mathcal{A}} \hat{x} + \hat{\mathcal{B}} u \\
\hat{y} = \hat{\mathcal{C}} \hat{x}
\]

- Lanczos-type methods: NO! $S \neq T$!
Structure-Preserving Moment Matching Methods

Structure Preservation for Maxwell Equations

\[
\mathbf{M} = \begin{pmatrix} M_\varepsilon & 0 \\ 0 & M_\mu \end{pmatrix}, \quad \mathbf{A} = \begin{pmatrix} -M_\sigma & G \\ -G^T & 0 \end{pmatrix}.
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\[
\hat{\mathbf{M}} \dot{\hat{x}} = \hat{\mathbf{A}} \hat{x} + \hat{\mathbf{B}} u \\
\hat{y} = \hat{\mathbf{C}} \hat{x}
\]

- Lanczos-type methods: NO! \( S \neq T! \)
- Arnoldi-type methods: \( S = T = Q \), but block structure is lost
Structure-Preserving Moment Matching Methods

Structure Preservation for Maxwell Equations

\[
\mathcal{M} = \begin{pmatrix} M_\varepsilon & 0 \\ 0 & M_\mu \end{pmatrix}, \quad \mathcal{A} = \begin{pmatrix} -M_\sigma & G \\ -G^T & 0 \end{pmatrix}.
\]

\[
\hat{\mathcal{M}} \hat{x} = \hat{\mathcal{A}} \hat{x} + \hat{\mathcal{B}} u \\
\hat{\mathcal{Y}} = \hat{\mathcal{C}} \hat{x}
\]

- Lanczos-type methods: \textbf{NO!} $S \neq T$!
- Arnoldi-type methods: $S = T = Q$, but block structure is lost

\[
Q = \begin{bmatrix} V \\ W \end{bmatrix} \rightarrow \begin{bmatrix} V & 0 \\ 0 & W \end{bmatrix}
\]
Structure-Preserving Moment Matching Methods

Structure Preservation for Maxwell Equations

\[ \mathcal{M} = \begin{pmatrix} M_\varepsilon & 0 \\ 0 & M_\mu \end{pmatrix}, \quad \mathcal{A} = \begin{pmatrix} -M_\sigma & G \\ -G^T & 0 \end{pmatrix}. \]

\[ \hat{\mathcal{M}} \ddot{x} = \hat{\mathcal{A}} \ddot{x} + \hat{\mathcal{B}} u \]
\[ \hat{y} = \hat{\mathcal{C}} \hat{x} \]

- Lanczos-type methods: **NO!** \( S \neq T! \)
- Arnoldi-type methods: \( S = T = Q \), but block structure is lost

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

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

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

\[
H(s) = C (sM - A)^{-1} B, \quad H_r(s) = \hat{C} \left( s\hat{M} - \hat{A} \right)^{-1} \hat{B}
\]

\[
\| H(i\omega) - H_r(i\omega) \| \leq \ldots
\]

- multiple expansion points \( s_1, \ldots, s_l \in [f_{\text{min}}, f_{\text{max}}] \)
- 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

\[ \sum_{j=1}^{l} \mathcal{K}_{r_j}(A_j, B_j). \]
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

$$\sum_{j=1}^{l} \mathcal{K}_{r_j}(A_j, B_j).$$

**Lemma (Key-Lemma, Grimme,Gallivan’98)**

*If $s_j \neq s_k$ then*

$$A_k \cdot A_j^{p-1} B_j \in \mathcal{K}_p(A_j, B_j) + \mathcal{K}_1(A_k, B_k)$$
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

\[
\sum_{j=1}^{l} \mathcal{K}_r(A_j, B_j).
\]

Lemma (Key-Lemma, Grimme,Gallivan’98)

If \(s_j \neq s_k\) then

\[
A_k \cdot A_j^{p-1} B_j \in \mathcal{K}_p(A_j, B_j) + \mathcal{K}_1(A_k, B_k)
\]

\(\Rightarrow\) 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. $K_j(A_j, B_j)$, $j = 1, \ldots, l$ one after another using modified Gram-Schmidt.
Rational Arnoldi Methods

- Traditional Rational Arnoldi methods build $Q_r$ w.r.t. $K_{r_j}(A_j, B_j), j = 1, \ldots, l$ one after another using modified Gram-Schmidt.

\[ K_{r_1}(A_1, B_1) \]
Rational Arnoldi Methods

- Traditional Rational Arnoldi methods build $Q_r$ w.r.t. $K_{r_j}(A_j, B_j)$, $j = 1, \ldots, l$ one after another using modified Gram-Schmidt.

$$K_{r_1}(A_1, B_1) + K_{r_2}(A_2, B_2)$$
Rational Arnoldi Methods

- Traditional Rational Arnoldi methods build $Q_r$ w.r.t. $K_{r_j}(A_j, B_j), j = 1, \ldots, l$ one after another using modified Gram-Schmidt.

$$K_{r_1}(A_1, B_1) + K_{r_2}(A_2, B_2) + K_{r_3}(A_3, B_3)$$
Rational Arnoldi Methods

- Traditional Rational Arnoldi methods build \( Q_r \) w.r.t. \( K_{r_j}(A_j, B_j) \), \( j = 1, \ldots, l \) \textbf{one after another} using modified Gram-Schmidt.

\[
K_{r_1}(A_1, B_1) + K_{r_2}(A_2, B_2) + K_{r_3}(A_3, B_3) + K_{r_4}(A_4, B_4)
\]
Traditional Rational Arnoldi methods build $Q_r$ w.r.t. $K_{rj}(A_j, B_j)$, $j = 1, \ldots, l$ one after another using modified Gram-Schmidt.

$$\text{span } Q_r = K_{r1}(A_1, B_1) + K_{r2}(A_2, B_2) + \cdots + K_{rl}(A_l, B_l)$$
Rational Arnoldi Methods

- Traditional Rational Arnoldi methods build $Q_r$ w.r.t. $K_{r_j}(A_j, B_j), j = 1, \ldots, l$ one after another using modified Gram-Schmidt.

\[
\text{span } Q_r = K_{r_1}(A_1, B_1) + K_{r_2}(A_2, B_2) + \cdots + K_{r_l}(A_l, B_l)
\]

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

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

  \[
  \text{span } Q_r = \mathcal{K}_{r_1}(A_1, B_1) + \mathcal{K}_{r_2}(A_2, B_2) + \cdots + \mathcal{K}_{r_l}(A_l, B_l)
  \]

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

- Adaptive-Order Rational Arnoldi (AORA) [Lee, Chu, Feng’06] $Q_r$ is generated by interchangeably increasing the size $r_j$ of $\mathcal{K}_j(A_j, B_j)$. 
Rational Arnoldi Methods

- Traditional Rational Arnoldi methods build $Q_r$ w.r.t. $K_{r_j}(A_j, B_j), j = 1, \ldots, l$ one after another using modified Gram-Schmidt.

$$\text{span } Q_r = K_{r_1}(A_1, B_1) + K_{r_2}(A_2, B_2) + \cdots + K_{r_l}(A_l, B_l)$$

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

- Adaptive-Order Rational Arnoldi (AORA) [Lee,Chu,Feng’06]
  $Q_r$ is generated by interchangeably increasing the size $r_j$ of $K_{r_j}(A_j, B_j)$.

  $$K_1(A_1, B_1)$$
Rational Arnoldi Methods

- Traditional Rational Arnoldi methods build $Q_r$ w.r.t. $K_r_j(A_j, B_j)$, $j = 1, \ldots, l$ one after another using modified Gram-Schmidt.

\[
\text{span } Q_r = K_{r_1}(A_1, B_1) + K_{r_2}(A_2, B_2) + \cdots + K_{r_l}(A_l, B_l)
\]

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  $Q_r$ is generated by interchangeably increasing the size $r_j$ of $K_{r_j}(A_j, B_j)$.

\[
K_1(A_1, B_1) + K_2(A_2, B_2)
\]
Rational Arnoldi Methods

- Traditional Rational Arnoldi methods build $Q_r$ w.r.t. $K_j(A_j, B_j)$, $j = 1, \ldots, l$ one after another using modified Gram-Schmidt.

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$$\text{span } Q_r = \mathcal{K}_{r_1}(A_1, B_1) + \cdots + \mathcal{K}_{r_l}(A_l, B_l)$$

- 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
Expansion Point Selection

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

\[
s_1 = 2 \pi i f_{\text{min}}, \quad s_2 = 2 \pi i \sqrt{f_{\text{min}} f_{\text{max}}}, \quad s_3 = 2 \pi i f_{\text{max}}
\]
Expansion Point Selection

- AORA called repeatedly $l = 1, 2, 3, \ldots$ with increasing number of expansion points $s_1, s_2, s_3, s_4$
Expansion Point Selection

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

$$s_1, s_2, s_3, s_4, s_5$$
Expansion Point Selection

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

\[ s_1, s_2, s_3, s_4, s_5, s_6 \]
Expansion Point Selection

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Expansion Point Selection

- AORA called repeatedly \( l = 1, 2, 3, \ldots \) with increasing number of expansion points \( s_1, \ldots, s_l \)

- relative error \( \frac{|\mathcal{H}_r^{(l)}(s) - \mathcal{H}_r^{(l-1)}(s)|}{|\mathcal{H}_r^{(l)}(s)|} \) between two computed reduced-order transfer functions used as measure [Köhler et al.’10’12]
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Expansion Point Selection

- AORA called repeatedly $l = 1, 2, 3, \ldots$ with increasing number of expansion points $s_1, \ldots, s_l$

- relative error $\frac{|H_r^{(l)}(s) - H_r^{(l-1)}(s)|}{|H_r^{(l)}(s)|}$ between two computed reduced-order transfer functions used as measure [Köhler et al.’10’12]

- global stopping criterion [Grimme,Gallivan’98] $\sum_{i=1}^{l} 2^{i-1} \frac{|H_r^{(i)}(s) - H_r^{(i-1)}(s)|}{|H_r^{(i)}(s)|} \leq \varepsilon$
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  - Numerical Results

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  - Savings for the AORA method
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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 $\mathcal{K}_{j_i}$
- size $N = 73385$, discretized using FIT
- frequency range $[f_{\text{min}}, f_{\text{max}}] = [10^9, 10^{10}]$
relative error

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

\( s = 2\pi i f \) with \( f \in [10^9, 10^{10}] \) displayed as reference
Model Order Reduction — Numerical Results

Coplanar Waveguide

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

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

\( s = 2\pi if \) with \( f \in [0.6 \cdot 10^9, 3.0 \cdot 10^9] \) displayed as reference
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Modified Adaptive-Order Rational Arnoldi Method

Repeatedly calling AORA method requires to recompute span\( Q_r \) from scratch.

Lemma

Suppose that

\[
\text{span} \ Q(l) = K_r(l) 1(s_1) + \cdots + K_r(l) l(s_l),
\]

\[
\text{span} \ Q(l+1) = K_r(l+1) 1(s_1) + \cdots + K_r(l+1) l(s_l) + K_r(l+1) l+1(s_{l+1}).
\]

such that

\[
r(l+1) 1 \leq r(l) 1 \cdots \leq r(l+1) l.
\]

Then

\[
K_r(l+1) 1(s_1) + \cdots + K_r(l+1) l(s_l)
\]

can be directly extracted from \( \text{span} \ Q(l) \).

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 \( s_{l+1} M - A \rightarrow mAORA \) (modified AORA).
Modified Adaptive-Order Rational Arnoldi Method

Repeatedly calling AORA method requires to recompute \( \text{span} Q_r \) from scratch.

Lemma

Suppose that

\[
\text{span} Q_r^{(l)} = \mathcal{K}_{r_1^{(l)}}(s_1) + \cdots + \mathcal{K}_{r_l^{(l)}}(s_l),
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\]

such that

\[
r_1^{(l+1)} \leq r_1^{(l)} \leq \cdots \leq r_l^{(l+1)} \leq r_l^{(l)}.
\]

Then \( \mathcal{K}_{r_1^{(l+1)}}(s_1) + \cdots + \mathcal{K}_{r_l^{(l+1)}}(s_l) \) can be directly extracted from \( \text{span} Q_r^{(l)} \).
Modified Adaptive-Order Rational Arnoldi Method

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- Lemma requires that shifts \( s_1, \ldots, s_{l} \) are selected in the same order
Repeatingly calling AORA method requires to recompute $\text{span}Q_r$ from scratch.

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such that

$$r_1^{(l+1)} \leq r_1^{(l)} \cdots r_{l+1}^{(l+1)} \leq r_l^{(l)}.$$

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- only new shift \( s_{l+1} \) requires to solve systems with \( s_{l+1}M - A \)
- \( \rightarrow \) mAORA (modified AORA)
Solving Systems in the Modified AORA Method

Recall

- $J(sM - A)$ is complex-symmetric, where $J = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}$
- Schur complement $S(s) = s^2 M_\varepsilon + sM_\sigma + GM_\mu^{-1}G^T$ is complex-symmetric
Solving Systems in the Modified AORA Method

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- $J(sM - A)$ is **complex-symmetric**, where $J = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}$

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- (modified) AORA requires solving a sequence complex-symmetric systems with varying shifts and varying right hand sides

$$A(s_j)x_{jp} = b_{jp}$$
Solving Systems in the Modified AORA Method

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- (modified) AORA requires solving a sequence complex-symmetric systems with varying shifts and varying right hand sides

$$A(s_j) x_{jp} = b_{jp}$$

- Save memory and time: Only compute factorization of $A(s_*)$ for some characteristic shift $s_* = 2\pi i \sqrt{f_{\text{min}} f_{\text{max}}}$. 

- For all $s_j \neq s_*$ use (recycling) Krylov subspace method as wrapper.
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QMR Method — Sketch

Two-sided Lanczos Method

\[ AV_k = V_{k+1} T_k, \quad A^T \tilde{V}_k = \tilde{V}_{k+1} \tilde{T}_k \]
QMR Method — Sketch

Two-sided Lanczos Method

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QMR for \( Ax = b \) based on two-sided Lanczos method:

- \( r_0 = b - Ax_0, \quad v_1 = r_0 / \| r_0 \| \)
- \( x_k = x_0 + V_k y \)
- quasi-minimize

\[ \| b - Ax_k \| \leq \| V_{k+1} \| \cdot \| r_0 \| e_1 - T_k y \| \]

\[ \rightarrow y \] from least squares solution

\[ \rightarrow x \]

- [Freund et al. ’91,’93,’94]
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Simplified QMR Method for $J$-Symmetric Matrices

- $A^T J = JA$, where $J = J^T$, $J$ nonsingular
- use specific left initial guess $\tilde{v}_1 = Jv_1$
Simplified QMR Method for $J$-Symmetric Matrices

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  - half of the work can be skipped,
  - $A^T$ is not referenced,
  - computation time reduced,
  - structure exploited

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- simplified QMR can be generalized to preconditioned case, where preconditioner satisfies $P^T J = JP$
- [Freund et al. ’94,’95]
Simplified QMR Method for \( J \)-Symmetric Matrices

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- simplified QMR can be generalized to preconditioned case, where preconditioner satisfies \( P^T J = JP \)
- [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

\[
AV_k = V_{k+1} T_k,
\]

\[
A^T \tilde{V}_k = \tilde{V}_{k+1} \tilde{T}_k
\]

with updated initial guess and projected initial residual

\[
x_0^{(\text{new})} = x_0 + UD_c^{-1} \tilde{C}^T r_0, \ r_0^{(\text{new})} = (I - CD_c^{-1} \tilde{C}^T)r_0.
\]
QMR with Subspace Recycling

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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 projected systems

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

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

with updated initial guess and projected initial residual

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

<table>
<thead>
<tr>
<th>BiCG/QMR</th>
<th>Recycling BiCG/QMR</th>
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<tr>
<td>init (x_0)</td>
<td>(x_0^{(new)} = x_0 + UD_c^{-1}\tilde{C}^T r_0)</td>
</tr>
<tr>
<td>init (r_0 = b - Ax_0)</td>
<td>(r_0^{(new)} = (I - CD_c^{-1}\tilde{C}^T) r_0)</td>
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<tr>
<td>matvec (Ax)</td>
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<td>((I - \tilde{C}D_c^{-T} C^T)A^T x)</td>
</tr>
<tr>
<td>solution update (x = x + \alpha p)</td>
<td>(x = x + \alpha (I - UD_c^{-1}\tilde{C}^T)p)</td>
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</table>
Recycling QMR/BiCG in a Nutshell

\[ U, \bar{U}, C = AU, \bar{C} = A^T \bar{U}, D_c = \bar{C}^T C. \]

Changing the methods:

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

![Graph showing relative error and time in seconds for AORA and mAORA](image)

- **Relative error**
  - **f / GHz**
  - **AORA** vs **mAORA**

- **Time in seconds**
  - **Number of expansion points**
  - **AORA** vs **mAORA**

![Input port and output port](image)
Sampling 20 frequencies $s_j = 2\pi i f_j$

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

Use complex-symmetric Schur complement system

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

Comparison

- simplified QMR without subspace recycling
- simplified QMR using subspace recycling
Preconditioner: \( LU \) decomposition for \( S(s_*) \)

Preconditioned SQMR Without Subspace Recycling

- Iteration steps, precd. SQMR
- Computation time, precd. SQMR

```
<table>
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<tr>
<th>frequency sampling</th>
<th>iteration steps</th>
<th>computation time</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.5 x 10^{10}</td>
<td>0</td>
<td>0.5</td>
</tr>
<tr>
<td>1.0 x 10^{10}</td>
<td>50</td>
<td>1</td>
</tr>
<tr>
<td>1.5 x 10^{10}</td>
<td>100</td>
<td>2</td>
</tr>
<tr>
<td>2.0 x 10^{10}</td>
<td>200</td>
<td>8</td>
</tr>
</tbody>
</table>
```
Preconditioner: $LU$ decomposition for $S(s_*)$

**Preconditioned SQMR With Subspace Recycling**

- **Iteration steps, precd. recycling SQMR**
- **Computation time, precd. recycling SQMR**

![Graphs showing iteration steps and computation time for preconditioned recycling SQMR.](image)
Outline

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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 → modified AORA, recycling SQMR

This work was supported by the research network *MoreSim4Nano* funded by the German Federal Ministry of Education and Science (BMBF) with grant no. 05M10MBA.