Restarted Krylov subspace model-reduction methods for RCL circuit simulation

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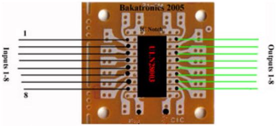
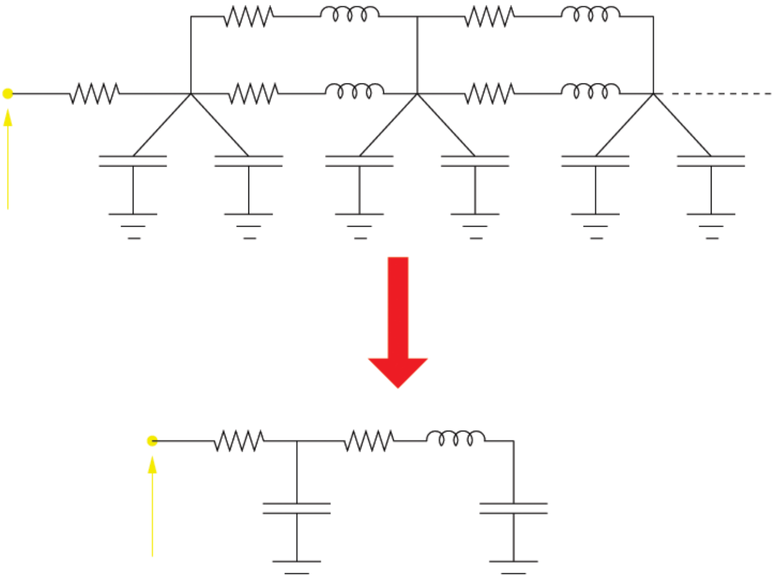
June 3, 2009 / Qualifying Exam



Primary application

Reduced size, physically viable RLC circuit models



Model Represented as DAE

(Differential Algebraic Equation)

Input-Output system

$$
\begin{array}{ccc}
u_1(t) \;\longrightarrow & & \longrightarrow\; y_1(t) \\
u_2(t) \;\longrightarrow & \boxed{\begin{aligned} Ex' &= Ax + Bu \\ y &= B^T x, \end{aligned}} & \longrightarrow\; y_2(t) \\
\vdots & & \vdots \\
u_p(t) \;\longrightarrow & & \longrightarrow\; y_p(t)
\end{array}
$$

where $A, E \in \mathbb{R}^{N \times N}$ are sparse, $B \in \mathbb{R}^{N \times p}$.

- $N \gg p$ typically large, e.g. $N = \mathcal{O}\left(10^9\right)$
- $x(t) \in \mathbb{R}^N$ (*state-space* variable) represents internal state.
- *Behavior* of model: $y = F(u)$

Transfer Function

Relates Output directly to Input

In the frequency domain, $Y(s) = H(s)U(s)$ with *transfer function*

$$H(s) = B^T(sE - A)^{-1}B \quad \in \quad (\mathbb{C} \cup \infty)^{p \times p}$$

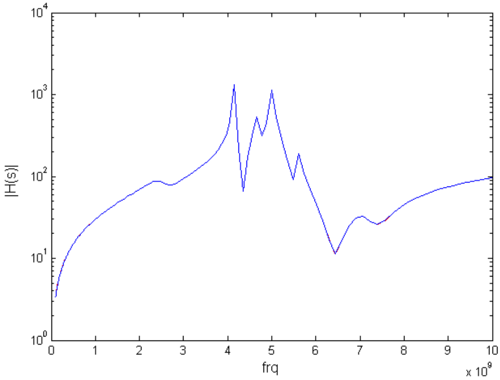
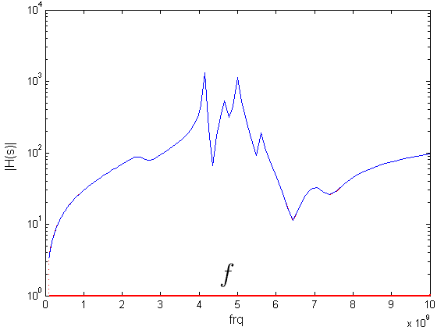
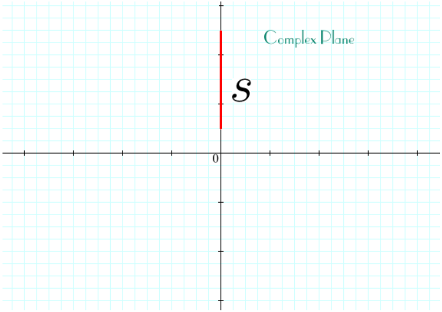


Figure: $\|H(s)\|$ vs. frequency for $N = 1841$ test model

We consider $H(s)$ over $s \in S$.

$$S = 2\pi i f, \quad f \in [f_{\min}, f_{\max}]$$





Transfer Function

Transfer function

$$H(s) = B^T(sE - A)^{-1}B$$

- $H(s) \in (\mathbb{C} \cup \infty)^{p \times p}$ is relatively small
- Explicitly computing $H(s)$ is not feasible!
- But computing

$$H_n(s) = B_n^T(sE_n - A_n)^{-1}B_n \quad \in \quad (\mathbb{C} \cup \infty)^{p \times p}$$

is *easy* for small $A_n, E_n \in \mathbb{R}^{n \times n}$, $B_n \in \mathbb{R}^{n \times p}$, where $n \ll N$.

Reduced model via projection

- Project A,E,B onto a subspace of $\mathbb{R}^N$.

$$A_n := V_n^T A V_n, \quad E_n := V_n^T E V_n, \quad B_n := V_n^T B,$$

  where $V_n \in \mathbb{R}^{N \times n}$ has full rank

- Reduced model transfer function:

$$H_n(s) = B_n^T (sE_n - A_n)^{-1} B_n$$

Outline

Transfer function

Single-matrix formulation

Let $s_0 \in \mathbb{C}$ be a point for which $s_0 E - A$ is invertible.
$H(s)$ can be re-expressed as

$$
\begin{aligned}
H(s) &= B^T (sE - A)^{-1} \\
&= B^T \left[(s - s_0)E + s_0 E - A\right]^{-1} B \\
&= B^T \left(I - (s - s_0)\widehat{H}\right)^{-1} R
\end{aligned}
$$

where

$$
\widehat{H} := -(s_0 E - A)^{-1} E \quad \text{and} \quad R := (s_0 E - A)^{-1} B.
$$

(*Single matrix formulation*)

Moments of the transfer function about s_0

Single-matrix formulation: $H(s) = B^T \left(I - (s - s_0)\widehat{H} \right)^{-1} R$

Via Neumann (geometric series) expansion,

$$
\begin{aligned}
H(s) &= B^T \left(\sum_{j=0}^{\infty} (s - s_0)^j \widehat{H}^j \right) R \\
&= \sum_{j=0}^{\infty} (s - s_0)^j M_j
\end{aligned}
$$

where $M_j = B^T \widehat{H}^j R$.

- This is exactly the Taylor series expansion about s_0 !
- M_j are *moments* (i.e. derivatives) of $H(s)$ at s_0

Moment matching

Taylor series of $H(s)$ about s_0:

$$H(s) = \sum_{j=0}^{\infty} (s - s_0)^j M_j$$

with moments $M_j = B^T \widehat{H}^j R$.

- Reduced model $H_n(s)$ will *match n moments* about s_0.

$$H_n(s) = H(s) + \mathcal{O}\left((s - s_0)^n\right)$$

Moment matching

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- Reduced model $H_n(s)$ will *match n moments* about s_0.

- Natural home for $H_n(s)$ is the n-th *block-Krylov* subspace

$$\mathcal{K}_n\left(\widehat{H}, R\right) := \operatorname{span}\left\{R, \widehat{H}R, \widehat{H}^2 R, \ldots, \widehat{H}^{n-1} R\right\}$$

Krylov subspace projection:
Overview

- Pick $s_0 \in \mathbb{C}$, compute matrices $\widehat{H}(s_0)$, $R(s_0)$
- Generate a full rank matrix $V_n \in \mathbb{R}^{N \times n}$ such that

$$\mathcal{K}_n\left(\widehat{H}, R\right) \subseteq \operatorname{colspan} V_n$$

- Compute projections

$$A_n := V_n^T A V_n, \text{ etc.}$$

- Reduced order model is

$$H_n(s) = B_n^T (sE_n - A_n)^{-1} B_n$$

Outline

Pole decomposition of model

Poles of $H(s)$ are $\mu \in \mathbb{C} \cup \infty$ such that $\|H(\mu)\| = \infty$.

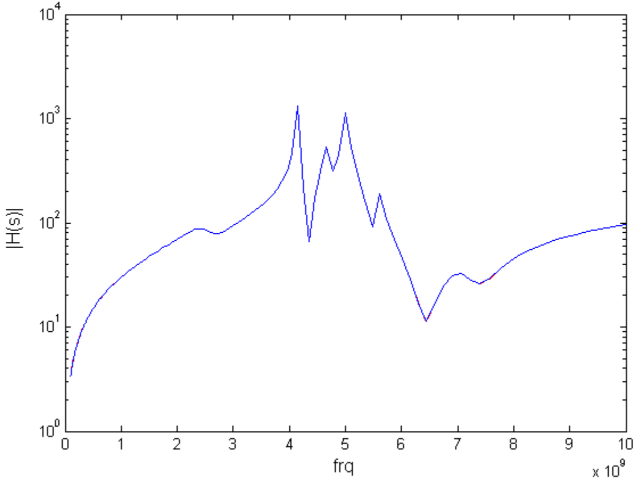
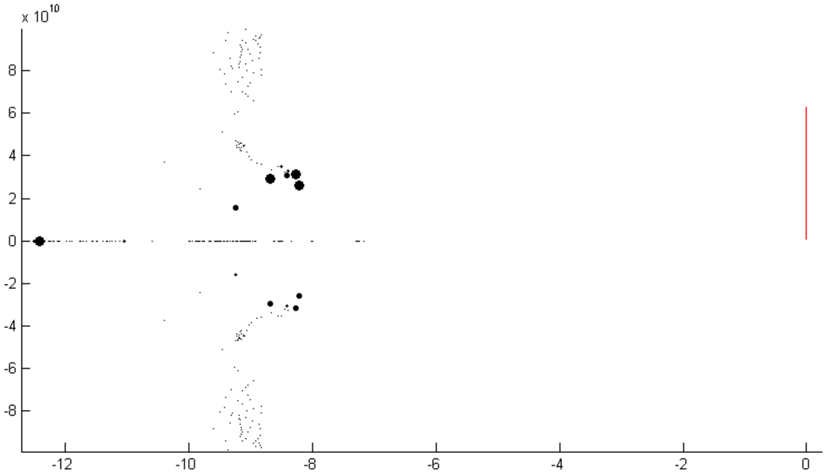


Figure: $\|H(s)\|$ vs. frequency ($s = 2\pi i f$)

Pole decomposition of model

Example: poles of a size $N = 1841$ test model



$\log_{10}$ scale on Re axis. Dot size indicates dominance.

Pole-residue decomposition of model

Poles as eigenvalues of $sE - A \in \mathbb{R}^{N\times N}$

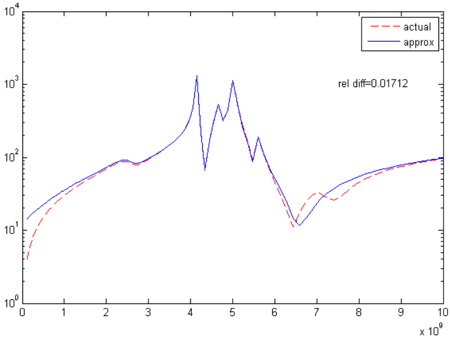
- Transfer function: $H(s) = B^T(sE - A)^{-1}B$
- If $sE - A$ has full set of N eigenvectors, eigenvalues μ_j then

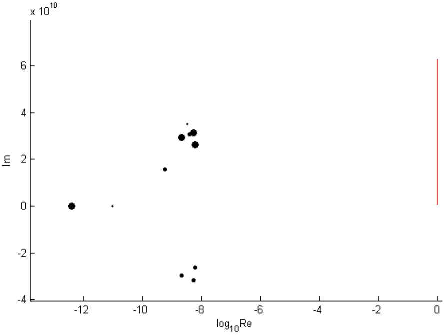
$$H(s) = X_\infty + \sum_{\substack{j=1 \\ \mu_j \neq \infty}}^{N} \frac{X_j}{s - \mu_j} \tag{$\star$}$$

- $\mu_j \in \mathbb{C} \cup \infty$ are the poles of $H(s)$. X_j are residues.
- *Dominant poles* associated with terms that dominate $(\star)$ on S.

Pole decomposition example

Model size $N = 1841$. Truncated at 12 terms





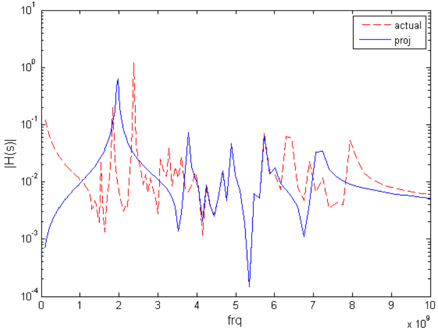
- Dominant poles determine features of the model on S.
- Ideally, reduced model consists of these dominant poles.

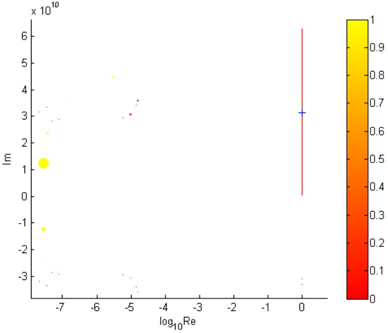
Background Summary

- Krylov subspace projection yields locally accurate approximate model around $s_0 \in \mathbb{C}$.
- We want to place s_0 for convergence near dominant poles.
- We do not know where dominant poles are.

Local convergence

Visual example: $N = 308$, Reduced model $n = 15$





Local convergence

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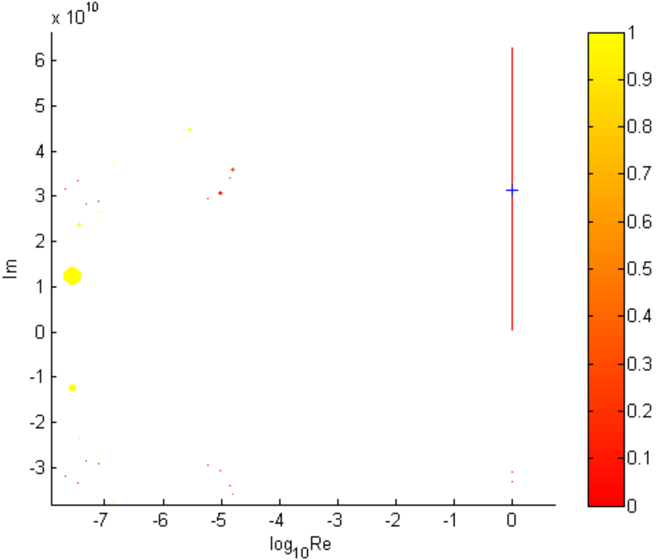

Local convergence

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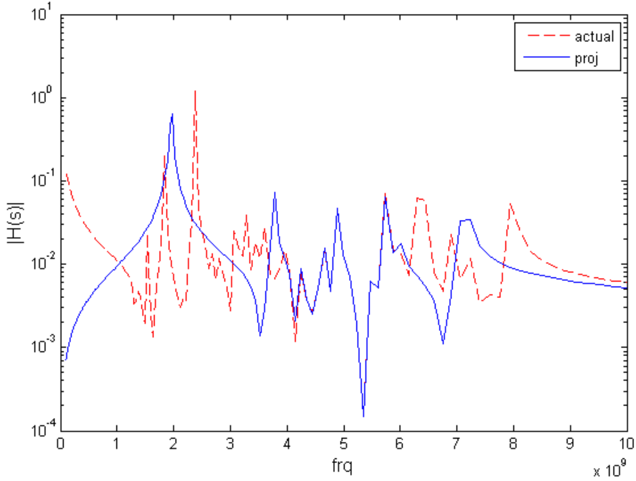

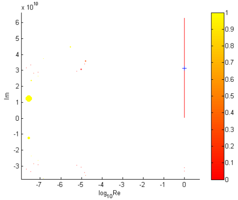

Outline

Krylov subspace

Recall that for matrices $\widehat{H}(s_0)$,$R(s_0)$, the reduced-order model transfer function $H_n(s)$:

- has Taylor series expansion

$$H_n(s) = \sum_{j=0}^{n-1} (s - s_0)^j M_j + \mathcal{O}\left((s - s_0)^n\right),$$

  where $M_j = B^T \widehat{H}^j R$

- lives in the n-th block-Krylov subspace

$$H_n(s) \in \mathcal{K}_n\left(\widehat{H}, R\right) := \text{span}\left\{R, \widehat{H}R, \widehat{H}^2 R, \ldots, \widehat{H}^{n-1} R\right\}$$

Arnoldi Process

Generates basis for Krylov subspace

Arnoldi process computes orthogonal basis matrix $V_n = [v_1\ v_2 \ldots v_n]$ for Krylov subspace $\mathcal{K}_n\left(\widehat{H}, r\right)$:

- $v_1 = r/\|r\|$
- $v_2 = \left(\widehat{H}v_1 \text{ orthogonalized against } v_1\right)$

  $\vdots$

- $v_n = \left(\widehat{H}v_{n-1} \text{ orthogonalized against } \{v_1, v_2, \ldots, v_{n-1}\}\right)$

Arnoldi Process

Computationally expensive

The n-th iteration of Arnoldi

$$v_n = \left(\widehat{H} v_{n-1} \text{ orthogonalized against } \{v_1, v_2, \ldots, v_{n-1}\}\right)$$

requires

- 1 Matrix-vector product
- $n-1$ inner products, $n-1$ SAXPYs $(\alpha x + y)$

Computing $v_n \in \mathbb{C}^N$ grinds to a halt with increasing n !

Thick-Restart

After m iterations of Arnoldi process,

- *Restart* the process.
- Keep (nearly) invariant subspace $Y \subset V_m$.
- Move s_0 to possibly better location. Adaptive, automated.

Current successful projection methods use *static* s_0 placement located for good global convergence, and no restarts.

Deflation

Extract invariant subspace from V_m

After a run (m iterations) of Arnoldi with $\widehat{H}(s_0)$,$R(s_0)$, matrix V_m is basis for $\mathcal{K}_m\left(\widehat{H}, R\right)$.

Deflation: Obtain $Y \subset \operatorname{span} V_m$ with property

$$\widehat{H}Y \approx YS$$

- $Y = [y_1\, y_2 \ldots y_\ell]$ is approximately $\widehat{H}$-invariant to some tolerance parameter τ.

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For *exactly* $\widehat{H}(s_0)$-invariant Y:

- Y is $\widehat{H}$-invariant for *any* s_0
- Y is eigenspace of $sE - A$ associated with 'captured' poles.

Selecting new s_0

- Dominant poles $\tilde{\mu}_j$ of reduced model $H_m(s)$ approximate dominant poles of the full model.
- We can use this info to select new expansion point s_0^1.

Thick-Restart Arnoldi with s_0^1

The next run of Arnoldi uses $\widehat{H}_1 := \widehat{H}(s_0^1)$, $R_1 := R(s_0^1)$, and Y to produce V^1.

- Each iteration, orthogonalize new $\widehat{H}v_j^1$ against $\{v_1^1, v_2^1, ..., v_j^1\}$ and $\{y_1, y_2, ..., y_\ell\}$.
- Eliminates from the search poles μ_j of the full model already 'discovered' on previous runs.

Thick-Restart Arnoldi with s_0^1

The next run of Arnoldi uses $\widehat{H}_1 := \widehat{H}(s_0^1)$, $R_1 := R(s_0^1)$, and Y to produce V^1.

Orthogonalization against known invariant subspace prevents redundancy (linear dependence) between V^1 and V^0, so

$$\widehat{V} = \begin{bmatrix} V^0 & V^1 \end{bmatrix}$$

has full rank.

Result of method

K runs of restarted Arnoldi yields

$$\widehat{V} := \begin{bmatrix} V^0 & V^1 & \cdots & V^{K-1} \end{bmatrix}$$

and

$$Y^j := \text{deflate}\left(V^{j-1}\right) \quad \text{for } j = 1, 2, ..., K-1.$$

- Each V^j is orthogonal to $\left\{Y^1, Y^2, ..., Y^j\right\}$.
- $\widehat{V}$ is possibly rank-deficient.
- $\text{colspan}\, V^j \neq \mathcal{K}_m\left(\widehat{H}_j, R_j\right)$ for $j > 0$.

Piecewise Krylov subspace

Compounded moment matching

Conjecture

1. $$\bigcup_{j=1}^{K-1} \mathcal{K}_m\left(\widehat{H}_j, R_j\right) \subset \operatorname{colspan}\widehat{V}.$$

2. If $\widehat{V}$ has full-rank, the reduced model of size $n = mK$ obtained by projection with $\widehat{V}$ matches *at least* m moments about each s_0^j.

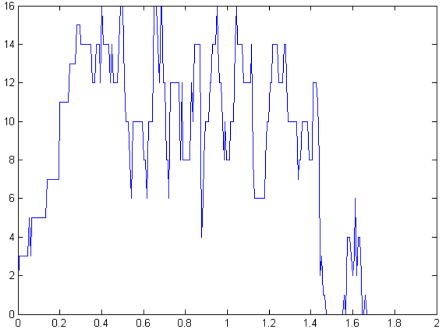
Outline

Preliminary results

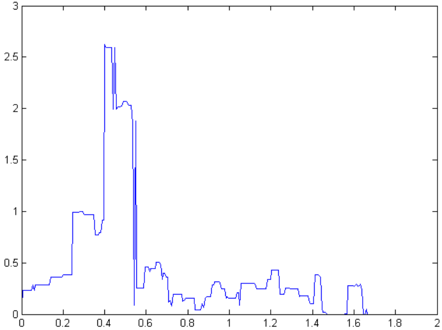
selecting good expansion points s_0

- Current working algorithm uses K pre-determined expansion points s_0^j placed along imaginary-axis.
- Covers entire segment S of interest.

Example: 1 run of $m = 15$, invariance tolerance $\tau = 10^{-4}$



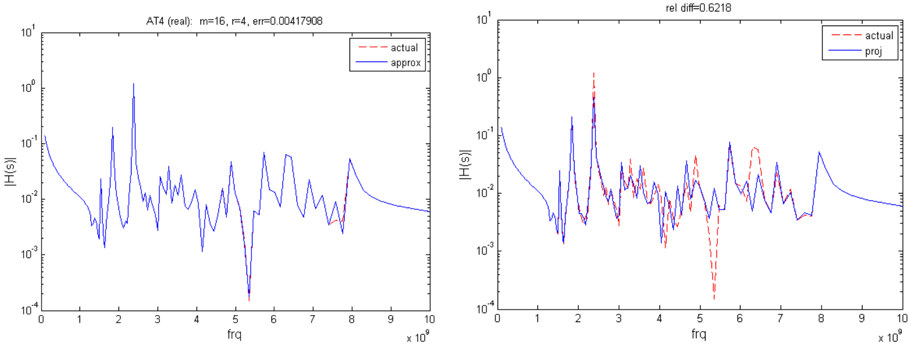
converged poles vs. s_0



wt vs. s_0

Preliminary results

Comparison of two reduced ($N = 308$, $n = 64$) models



New ($m = 16, K = 4, \tau = 10^{-6}$)   Standard ($s_0 = \pi 10^{10} \in \mathbb{R}$)

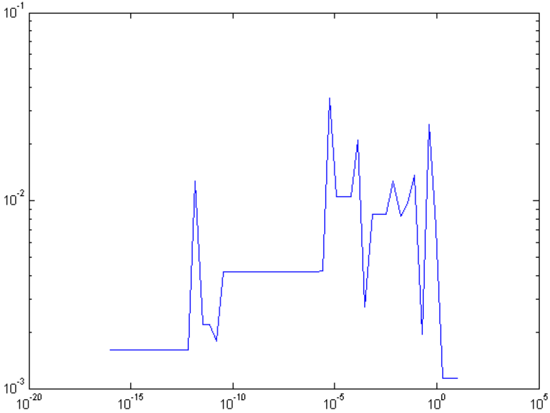
Figure: Standard reduced model requires size 125 to match accuracy of size 64 model using restarts.

Preliminary results

Weird effects of τ

Selecting invariance tolerance parameter τ is not trivial!

Same example model. $m = 16$, $K = 4$ reduced models



Relative (L^∞) error vs. τ

Take-home message

- Thick-restart Krylov methods are used in other applications, but have not been applied to model reduction.
- Existing multi expansion-point (s_0) methods are inefficient.
- Potential adaptivity of our method could result in robust algorithms.

Thank you