INTERPOLATORY AND SYSTEM-THEORETIC METHODS FOR PARAMETRIC MODEL REDUCTION

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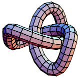

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Overview

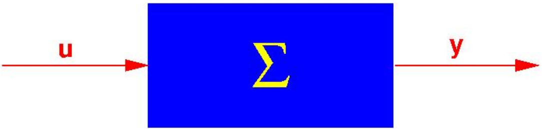
Dynamical Systems

$$\Sigma(p) : \begin{cases} E(p)\dot{x}(t;p) = f(t, x(t;p), u(t), p), \quad x(t_0) = x_0, & \text{(a)} \\ y(t;p) = g(t, x(t;p), u(t), p) & \text{(b)} \end{cases}$$

with

- (generalized) states $x(t;p) \in \mathbb{R}^n$ ($E \in \mathbb{R}^{n\times n}$),
- inputs $u(t) \in \mathbb{R}^m$,
- outputs $y(t;p) \in \mathbb{R}^q$, (b) is called output equation,
- $p \in \mathbb{R}^d$ is a parameter vector.

E singular $\Rightarrow$ (a) is system of differential-algebraic equations (DAEs)
otherwise $\Rightarrow$ (a) is system of ordinary differential equations (ODEs)



Model Reduction for Dynamical Systems

Original System

$$\Sigma(p): \begin{cases} E(p)\dot{x} = f(t, x, u, p), \\ y = g(t, x, u, p). \end{cases}$$

- states $x(t; p) \in \mathbb{R}^n$,
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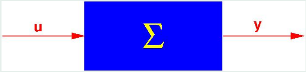
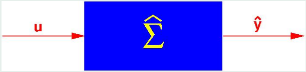


Reduced-Order System

$$\widehat{\Sigma}(p): \begin{cases} \hat{E}(p)\dot{\hat{x}} = \widehat{f}(t, \hat{x}, u, p), \\ \hat{y} = \widehat{g}(t, \hat{x}, u, p). \end{cases}$$

- states $\hat{x}(t; p) \in \mathbb{R}^r$, $r \ll n$
- inputs $u(t) \in \mathbb{R}^m$,
- outputs $\hat{y}(t; p) \in \mathbb{R}^q$,
- parameters $p \in \mathbb{R}^d$.



Goal:

$\|y - \hat{y}\| <$ tolerance $\cdot \|u\|$ for all admissible input signals and relevant parameter settings.

Model Reduction for Dynamical Systems

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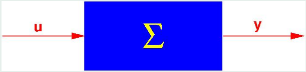

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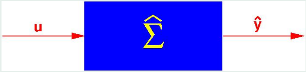

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Motivation

Applications in Microsystems/MEMS Design

Compact models for electro-thermic simulation

- Goal: controlling the thermic behavior in ICs and MEMS.
- Joule effect: electric current flowing through a conductor induces heat.
- For ICs: dissipate heat.

  For MEMS: employ Joule effect for designing MEMS with switching behavior ("hotplate").
- Spatial discretization of heat equation using FEM leads to large-scale system; generate compact models for MST model library, essential parameters for heat exchange need to be preserved symbolically:
  - film coefficients (convection boundary conditions),
  - heat conductivity/exchange coefficients.

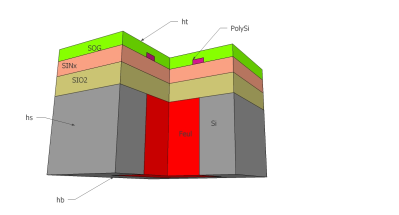
Source: The Oberwolfach Benchmark Collection http://www.imtek.de/simulation/benchmark

Compact models for electro-thermic simulation

Example: 3 film coefficients (top, bottom, side) $\Longrightarrow$

$$
\begin{aligned}
E\dot{x}(t) &= (A_0 + \sum_{i=1}^{3} p_i A_i)x(t) + bu(t) \\
y(t) &= c^T x(t)
\end{aligned}
$$

- $n = 4,257$,
- $A_0 =$ discrete Laplacian,
- A_i, $i = 1, 2, 3$, diagonal.



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Motivation

Applications in Microsystems/MEMS Design

Electro-chemical scanning electron microscope (SEM)

- Used for high resolution measurements of chemical reactivity and topography of surfaces, in particular for biological systems and nano-structures.
- Based on measuring current through a micro-electrode which is moved through electrolyte along surface.
- Measurements lead to cyclic voltammogram, plotting the current vs. applied potential.
- Mathematical model: Multi-species diffusion equations with mixed boundary conditions, defined by Butler-Volmer equation.

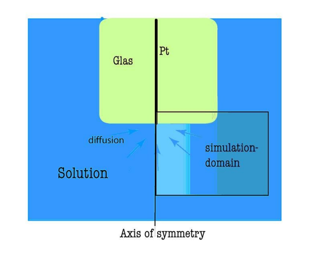
  Film coefficient depending on the applied potential is to be preserved.

Electro-chemical scanning electron microscope (SEM)

Example: 2 film coefficients $\Longrightarrow$

$$E\dot{x}(t) = (A_0 + p_1 A_1 + p_2 A_2)x(t) + Bu(t), \quad y(t) = c^T x(t).$$

FEM model: $n = 16,912$, $m = 3$ inputs, A_1, A_2 diagonal.



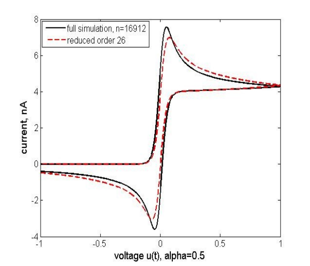


Figure: Schematic diagram of experimental set-up and corresponding voltammogram

Flow sensor (anemometer)

- Sensor measuring flow rates of fluids or gas.
- Based on one heater with thermo-sensors on both sides.
- Design process requires compact model, in which flow velocity and, possibly, material parameters (viscosity, density) appear as symbolic quantities.
- Mathematical model: Linear convection-diffusion equation.

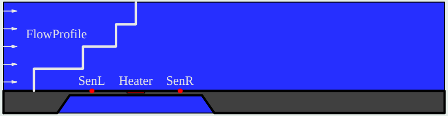


Figure: Anemometer model generated using ANSYS

Flow sensor (anemometer)

Parameter study based on reduced-order model:

- Full model: $n = 29,008$.
- Reduced-order Model: $r = 75$
  12 parameter interpolation points,
  BT ($tol = 10^{-4}$) $\Rightarrow$ $2 \le r_j \le 9$,
  $\max_{\omega,p} |R(\jmath\omega, p)| \le 6.5 \cdot 10^{-4}$
  ($R := G - \hat{G}$).
- Visualize frequency-response for $p \in [0, 1]$ (100 frequencies, 1000 parameter values).
- Generation of movie:

  $>$ 11 days with full model;
  93 sec. with reduced-order model!

[Baur/Benner, AT 2009]

Model Reduction Basics

Simulation-Free Methods

1. Modal Truncation
2. Guyan-Reduction/Substructuring
3. Padé-Approximation, Moment-Matching, and Krylov Subspace Methods ($\rightsquigarrow$ interpolatory methods)
4. Balanced Truncation ($\rightsquigarrow$ system-theoretic methods)
5. many more...

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Simulation-Free Methods

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5. many more...

Joint feature of many methods: Galerkin or Petrov-Galerkin-type projection of state-space onto low-dimensional subspace $\mathcal{V}$ along $\mathcal{W}$: assume $x \approx VW^T x =: \tilde{x}$, where

$$\mathrm{range}\,(V) = \mathcal{V}, \quad \mathrm{range}\,(W) = \mathcal{W}, \quad W^T V = I_r.$$

Then, with $\hat{x} = W^T x$, we obtain $x \approx V\hat{x}$ and

$$\|x - \tilde{x}\| = \|x - V\hat{x}\|.$$

Linear Parametric Systems

Linear, time-invariant systems depending on parameters

$$\begin{aligned} E(p)\dot{x}(t;p) &= A(p)x(t;p) + B(p)u(t), \quad & A(p), E(p) \in \mathbb{R}^{n\times n}, \\ y(t;p) &= C(p)x(t;p), & B(p) \in \mathbb{R}^{n\times m}, C(p) \in \mathbb{R}^{q\times n}. \end{aligned}$$

Laplace Transformation / Frequency Domain

Application of Laplace transformation ($x(t;p) \mapsto x(s;p)$, $\dot{x}(t;p) \mapsto sx(s;p)$) to linear system with $x(0) = 0$:

$$sE(p)x(s;p) = A(p)x(s;p) + B(p)u(s), \quad y(s;p) = C(p)x(s;p),$$

yields I/O-relation in frequency domain:

$$y(s;p) = \Big(\underbrace{C(p)(sE(p) - A(p))^{-1}B(p)}_{=:G(s;p)} \Big) u(s)$$

$G(s;p)$ is the parameter-dependent transfer function of $\Sigma(p)$.

Linear Parametric Systems

Linear, time-invariant systems depending on parameters

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Problem

Approximate the dynamical system

$$\begin{aligned} E(p)\dot{x} &= A(p)x + B(p)u, & A(p), E(p) &\in \mathbb{R}^{n\times n}, \\ y &= C(p)x, & B(p) \in \mathbb{R}^{n\times m}&, C(p) \in \mathbb{R}^{q\times n}, \end{aligned}$$

by reduced-order system

$$\begin{aligned} \hat{E}(p)\dot{\hat{x}} &= \hat{A}(p)\hat{x} + \hat{B}(p)u, & \hat{A}(p), \hat{E}(p) &\in \mathbb{R}^{r\times r}, \\ \hat{y} &= \hat{C}(p)\hat{x}, & \hat{B}(p) \in \mathbb{R}^{r\times m}&, \hat{C}(p) \in \mathbb{R}^{q\times r}, \end{aligned}$$

of order $r \ll n$, such that

$$\|y - \hat{y}\| = \|Gu - \hat{G}u\| \leq \|G - \hat{G}\|\|u\| < \text{tolerance} \cdot \|u\|.$$

$\Longrightarrow$ Approximation problem: $\min_{\text{order}\,(\hat{G})\leq r} \|G - \hat{G}\|$.

Model Reduction for Linear Parametric Systems

Problem

Approximate the dynamical system

$$\begin{array}{rcll} E(p)\dot{x} & = & A(p)x + B(p)u, & A(p), E(p) \in \mathbb{R}^{n\times n}, \\ y & = & C(p)x, & B(p) \in \mathbb{R}^{n\times m}, C(p) \in \mathbb{R}^{q\times n}, \end{array}$$

by reduced-order system

$$\begin{array}{rcll} \hat{E}(p)\dot{\hat{x}} & = & \hat{A}(p)\hat{x} + \hat{B}(p)u, & \hat{A}(p), \hat{E}(p) \in \mathbb{R}^{r\times r}, \\ \hat{y} & = & \hat{C}(p)\hat{x}, & \hat{B}(p) \in \mathbb{R}^{r\times m}, \hat{C}(p) \in \mathbb{R}^{q\times r}, \end{array}$$

of order $r \ll n$, such that

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Parametric System

$$\Sigma(p) : \begin{cases} E(p)\dot{x}(t;p) &= A(p)x(t;p) + B(p)u(t), \\ y(t;p) &= C(p)x(t;p). \end{cases}$$

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Appropriate representation:

$$\begin{array}{rcl} E(p) & = & E_0 + e_1(p)E_1 + \ldots + e_{q_E}(p)E_{q_E}, \\ A(p) & = & A_0 + a_1(p)A_1 + \ldots + a_{q_A}(p)A_{q_A}, \\ B(p) & = & B_0 + b_1(p)B_1 + \ldots + b_{q_B}(p)B_{q_B}, \\ C(p) & = & C_0 + c_1(p)C_1 + \ldots + c_{q_C}(p)C_{q_C}, \end{array}$$

allows easy parameter preservation for projection based model reduction.

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Applications:

- Repeated simulation for varying material or geometry parameters, boundary conditions,
- Optimization and design.

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Applications:

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Additional model reduction goal:

preserve parameters as symbolic quantities in reduced-order model:

$$\widehat{\Sigma}(p): \left\{ \begin{array}{rcl} \hat{E}(p)\dot{\hat{x}}(t;p) & = & \hat{A}(p)\hat{x}(t;p) + \hat{B}(p)u(t), \\ \hat{y}(t;p) & = & \hat{C}(p)\hat{x}(t;p) \end{array} \right.$$

with states $\hat{x}(t;p) \in \mathbb{R}^r$.

Computation of reduced-order model by projection

Given a linear (descriptor) system $E\dot{x} = Ax + Bu,\ y = Cx$ with transfer function $G(s) = C(sE - A)^{-1}B,$ a reduced-order model is obtained using projection matrices $V, W \in \mathbb{R}^{n\times r}$ with $W^TV = I_r$ ($\rightsquigarrow (VW^T)^2 = VW^T$ is projector) by computing

$$\hat{E} = W^TEV,\ \hat{A} = W^TAV,\ \hat{B} = W^TB,\ \hat{C} = CV.$$

Petrov-Galerkin-type (two-sided) projection: $W \neq V$,

Galerkin-type (one-sided) projection: $W = V$.

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Petrov-Galerkin-type (two-sided) projection: $W \neq V$,

Galerkin-type (one-sided) projection: $W = V$.

Rational Interpolation/Moment-Matching

Choose V, W such that

$$G(s_j) = \hat{G}(s_j), \quad j = 1, \ldots, k,$$

and

$$\frac{d^i}{ds^i} G(s_j) = \frac{d^i}{ds^i} \hat{G}(s_j), \quad i = 1, \ldots, K_j, \quad j = 1, \ldots, k.$$

Theorem (simplified) [Grimme '97, Villemagne/Skelton '87]

If

$$\begin{aligned} \operatorname{span}\left\{(s_1E-A)^{-1}B,\ldots,(s_kE-A)^{-1}B\right\} &\subset \operatorname{Ran}(V),\\ \operatorname{span}\left\{(s_1E-A)^{-T}C^T,\ldots,(s_kE-A)^{-T}C^T\right\} &\subset \operatorname{Ran}(W), \end{aligned}$$

then

$$G(s_j)=\hat{G}(s_j),\quad \frac{d}{ds}G(s_j)=\frac{d}{ds}\hat{G}(s_j),\quad \text{for } j=1,\ldots,k.$$

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$$G(s_j)=\hat{G}(s_j), \quad \frac{d}{ds}G(s_j)=\frac{d}{ds}\hat{G}(s_j), \quad \text{for } j=1,\ldots,k.$$

Remarks:

computation of V, W from rational Krylov subspaces, e.g.,

- dual rational Arnoldi/Lanczos [Grimme '97],
- Iterative Rational Krylov-Algo. [Antoulas/Beattie/Gugercin '07].

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\end{aligned}$$

then

$$G(s_j)=\hat{G}(s_j),\quad \frac{d}{ds}G(s_j)=\frac{d}{ds}\hat{G}(s_j),\quad \text{for } j=1,\ldots,k.$$

Remarks:

using Galerkin/one-sided projection yields $G(s_j)=\hat{G}(s_j)$, but in general

$$\frac{d}{ds}G(s_j)\neq\frac{d}{ds}\hat{G}(s_j).$$

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$$G(s_j)=\hat{G}(s_j), \quad \frac{d}{ds}G(s_j)=\frac{d}{ds}\hat{G}(s_j), \quad \text{for } j=1,\ldots,k.$$

Remarks:

$k=1$, standard Krylov subspace(s) of dimension $K \rightsquigarrow$ moment-matching methods/Padé approximation,

$$\frac{d^i}{ds^i}G(s_1)=\frac{d^i}{ds^i}\hat{G}(s_1), \quad i=0,\ldots,K-1(+K).$$

Parametric Systems

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Assume

$$\begin{aligned} E(p) &= E_0 + e_1(p)E_1 + \ldots + e_{q_E}(p)E_{q_E}, \\ A(p) &= A_0 + a_1(p)A_1 + \ldots + a_{q_A}(p)A_{q_A}, \\ B(p) &= B_0 + b_1(p)B_1 + \ldots + b_{q_B}(p)B_{q_B}, \\ C(p) &= C_0 + c_1(p)C_1 + \ldots + c_{q_C}(p)C_{q_C}. \end{aligned}$$

Petrov-Galerkin-type projection

For given projection matrices $V, W \in \mathbb{R}^{n \times r}$ with $W^T V = I_r$ ($\rightsquigarrow (VW^T)^2 = VW^T$ is projector), compute

$$
\begin{aligned}
\hat{E}(p) &= W^T E_0 V + e_1(p) W^T E_1 V + \ldots + e_{q_E}(p) W^T E_{q_E} V, \\
&= \hat{E}_0 + e_1(p)\hat{E}_1 + \ldots + e_{q_E}(p)\hat{E}_{q_E}, \\
\hat{A}(p) &= W^T A_0 V + a_1(p) W^T A_1 V + \ldots + a_{q_A}(p) W^T A_{q_A} V, \\
&= \hat{A}_0 + a_1(p)\hat{A}_1 + \ldots + a_{q_A}(p)\hat{A}_{q_A}, \\
\hat{B}(p) &= W^T B_0 + b_1(p) W^T B_1 + \ldots + b_{q_B}(p) W^T B_{q_B}, \\
&= \hat{B}_0 + b_1(p)\hat{B}_1 + \ldots + b_{q_B}(p)\hat{B}_{q_B}, \\
\hat{C}(p) &= C_0 V + c_1(p) C_1 V + \ldots + c_{q_C}(p) C_{q_C} V, \\
&= \hat{C}_0 + c_1(p)\hat{C}_1 + \ldots + c_{q_C}(p)\hat{C}_{q_C}.
\end{aligned}
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&= \hat{E}_0 + e_1(p)\hat{E}_1 + \ldots + e_{q_E}(p)\hat{E}_{q_E}, \\
\hat{A}(p) &= W^T A_0 V + a_1(p) W^T A_1 V + \ldots + a_{q_A}(p) W^T A_{q_A} V, \\
&= \hat{A}_0 + a_1(p)\hat{A}_1 + \ldots + a_{q_A}(p)\hat{A}_{q_A}, \\
\hat{B}(p) &= W^T B_0 + b_1(p) W^T B_1 + \ldots + b_{q_B}(p) W^T B_{q_B}, \\
&= \hat{B}_0 + b_1(p)\hat{B}_1 + \ldots + b_{q_B}(p)\hat{B}_{q_B}, \\
\hat{C}(p) &= C_0 V + c_1(p) C_1 V + \ldots + c_{q_C}(p) C_{q_C} V, \\
&= \hat{C}_0 + c_1(p)\hat{C}_1 + \ldots + c_{q_C}(p)\hat{C}_{q_C}.
\end{aligned}
$$

Parametric Model Reduction based on Multi-Moment Matching

Idea: choose appropriate frequency parameter $\hat{s}$ and parameter vector $\hat{p}$, expand into multivariate power series about $(\hat{s}, \hat{p})$ and compute reduced-order model, so that

$$G(s,p) = \hat{G}(s,p) + \mathcal{O}\left(|s-\hat{s}|^K + \|p-\hat{p}\|^L + |s-\hat{s}|^k \|p-\hat{p}\|^\ell\right),$$

i.e., first $K, L, k+\ell$ (mostly: $K = L = k+\ell$) coefficients (multi-moments) of Taylor/Laurent series coincide.

Algorithms:

- [Daniel et al. '04]: explicit computation of moments, numerically unstable.
- [Farle et al. '06/'07]: Krylov subspace approach, only polynomial parameter-dependance, numerical properties not clear, but appears to be robust.
- [Feng/B. '07–'10]: Arnoldi-MGS method, employ recursive dependance of multi-moments, numerically robust, r often larger as with [Farle et al.].

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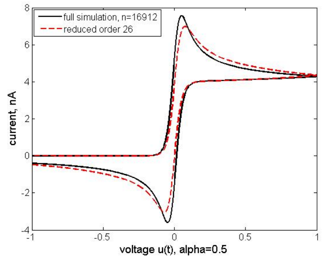
Electro-chemical SEM:

compute cyclic voltammogram based on FEM model

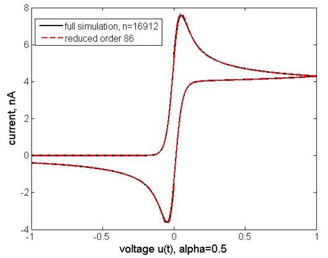
$$E\dot{x}(t) = (A_0 + p_1 A_1 + p_2 A_2)x(t) + Bu(t), \quad y(t) = c^T x(t),$$

where $n = 16,912$, $m = 3$, A_1, A_2 diagonal.

$K = L = k + \ell = 4 \;\Rightarrow\; r = 26$



$K = L = k + \ell = 9 \;\Rightarrow\; r = 86$



Parametric Model Reduction based on Multi-Moment Matching

Numerical Examples

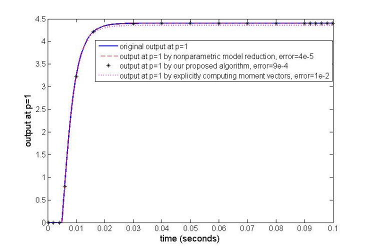
Anemometer:

FEM model

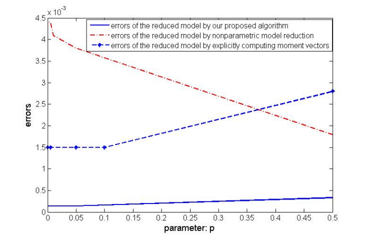
$$E\dot{x}(t) = (A_0 + p_1 A_1)x(t) + bu(t), \quad y(t) = c^T x(t),$$

where $n = 29,008$, $m = q = 1$.

Outputs for $p = 1$



Output errors for $p = 1$



Theorem 1 [BAUR/BEATTIE/B./GUGERCIN '07/'09]

Let
$$\begin{aligned}\hat{G}(s,p) &:= \hat{C}(p)(s\hat{E}(p)-\hat{A}(p))^{-1}\hat{B}(p)\\ &= C(p)V(sW^TE(p)V-W^TA(p)V)^{-1}W^TB(p)\end{aligned}$$

and suppose $\hat{p} = [\hat{p}_1, \ldots, \hat{p}_d]^T$ and $\hat{s} \in \mathbb{C}$ are chosen such that both $\hat{s}\,E(\hat{p}) - A(\hat{p})$ and $\hat{s}\,\hat{E}(\hat{p}) - \hat{A}(\hat{p})$ are invertible.

If
$$\left(\hat{s}\,E(\hat{p}) - A(\hat{p})\right)^{-1} B(\hat{p}) \in \mathrm{Ran}(V)$$

or
$$\left(C(\hat{p})\,(\hat{s}\,E(\hat{p}) - A(\hat{p}))^{-1}\right)^T \in \mathrm{Ran}(W),$$

then $G(\hat{s},\hat{p}) = \hat{G}(\hat{s},\hat{p})$.

Note: result extends to MIMO case using tangential interpolation:
Let $0 \neq b \in \mathbb{R}^m$, $0 \neq c \in \mathbb{R}^q$ be arbitrary.

a) If $(\hat{s}\,E(\hat{p}) - A(\hat{p}))^{-1} B(\hat{p})b \in \mathrm{Ran}(V)$, then $G(\hat{s},\hat{p})b = \hat{G}(\hat{s},\hat{p})b$;

b) If $\left(c^T C(\hat{p})\,(\hat{s}\,E(\hat{p}) - A(\hat{p}))^{-1}\right)^T \in \mathrm{Ran}(W)$, then $c^T G(\hat{s},\hat{p}) = c^T \hat{G}(\hat{s},\hat{p})$.

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Theorem 2 [Baur/Beattie/B./Gugercin '07/'09]

Suppose that $E(p)$, $A(p)$, $B(p)$, $C(p)$ are C^1 in a neighborhood of $\hat{p} = [\hat{p}_1, \ldots, \hat{p}_d]^T$ and that both $\hat{s}\,E(\hat{p}) - A(\hat{p})$ and $\hat{s}\,\hat{E}(\hat{p}) - \hat{A}(\hat{p})$ are invertible. If

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1. Assertion of theorem satisfies necessary conditions for surrogate models in trust region methods [Alexandrov/Dennis/Lewis/Torczon '98].
2. Approximation of gradient allows use of reduced-order model for sensitivity analysis.

Generic implementation of interpolatory PMOR

Define $\mathcal{A}(s,p) := sE(p) - A(p)$.

1. Select "frequencies" $s_1, \ldots, s_k \in \mathbb{C}$ and parameter vectors $p^{(1)}, \ldots, p^{(\ell)} \in \mathbb{R}^d$.
2. Compute (orthonormal) basis of
$$\mathcal{V} = \operatorname{span}\left\{\mathcal{A}(s_1,p^{(1)})^{-1}B(p^{(1)}), \ldots, \mathcal{A}(s_k,p^{(\ell)})^{-1}B(p^{(\ell)})\right\}.$$
3. Compute (orthonormal) basis of
$$\mathcal{W} = \operatorname{span}\left\{\mathcal{A}(s_1,p^{(1)})^{-H}C(p^{(1)})^T, \ldots, \mathcal{A}(s_k,p^{(\ell)})^{-T}C(p^{(\ell)})^T\right\}.$$
4. Set $V := [v_1, \ldots, v_{k\ell}]$, $\tilde{W} := [w_1, \ldots, w_{k\ell}]$, and $W := \tilde{W}(\tilde{W}^T V)^{-1}$. (Note: $r = k\ell$).
5. Compute $\begin{cases} \hat{A}(p) := W^T A(p) V, & \hat{B}(p) := W^T B(p) V, \\ \hat{C}(p) := W^T C(p) V, & \hat{E}(p) := W^T E(p) V. \end{cases}$

- If directional derivatives w.r.t. p are included in $\mathrm{Ran}(V)$, $\mathrm{Ran}(W)$, then also the Hessian of $G(\hat{s}, \hat{p})$ is interpolated by the Hessian of $\hat{G}(\hat{s}, \hat{p})$.
- Choice of optimal interpolation frequencies s_k and parameter vectors $p^{(k)}$ in general is an open problem.
- For prescribed parameter vectors $p^{(k)}$, we can use corresponding $\mathcal{H}_2$-optimal frequencies $s_{k,\ell}$, $\ell = 1, \ldots, r_k$ computed by IRKA, i.e., reduced-order systems $\hat{G}_*^{(k)}$ so that

$$\|G(., p^{(k)}) - \hat{G}_*^{(k)}(.)\|_{\mathcal{H}_2} = \min_{\substack{\mathrm{order}(\hat{G})=r_k \\ \hat{G} \text{ stable}}} \|G(., p^{(k)}) - \hat{G}^{(k)}(.)\|_{\mathcal{H}_2},$$

  where

$$\|G\|_{\mathcal{H}_2} := \left(\frac{1}{2\pi} \int_{-\infty}^{+\infty} \|G(\jmath\omega)\|_{\mathrm{F}}^2 d\omega \right)^{1/2}.$$

- Optimal choice of interpolation frequencies s_k and parameter vectors $p^{(k)}$ possible for special parameterized SISO systems.

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Theorem 3 [Baur/Beattie/B./Gugercin '09]

For special parameterized SISO systems,

$$A(p) \equiv A_0,\ E(p) \equiv E_0,\ B(p) = B_0 + p_1 B_1,\ C(p) = C_0 + p_2 C_1,$$

optimal choice possible, necessary conditions:
If $\hat{G}$ minimizes the approximation error w.r.t.

$$\|G - \hat{G}\|_{\mathcal{H}_2 \times \mathcal{L}_2(\Omega)}, \qquad p \in \Omega \subset \mathbb{R}^d,$$

and $\Lambda(\hat{A}, \hat{E}) = \{\hat{\lambda}_1, \ldots, \hat{\lambda}_r\}$ (all simple), then the interpolation frequencies satisfy

$$s_i = -\hat{\lambda}_i, \quad i = 1, \ldots, r,$$

and the parameter interpolation points $\{p^{(1)}, \ldots, p^{(r)}\}$ satisfy the interpolation conditions

$$\begin{aligned} G(-\hat{\lambda}_k, p^{(k)}) &= \hat{G}(-\hat{\lambda}, p^{(k)}), \\ \frac{\partial}{\partial s} G(-\hat{\lambda}, p^{(k)}) &= \frac{\partial}{\partial s}\hat{G}(-\hat{\lambda}, p^{(k)}), \quad \nabla_p G(-\hat{\lambda}, p^{(k)}) = \nabla_p \hat{G}(-\hat{\lambda}, p^{(k)}). \end{aligned}$$

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Proof:

$$\|G\|_{\mathcal{H}_2 \times \mathcal{L}_2(\Omega)} = \|L^T \tilde{G} L\|_{\mathcal{H}_2}, \quad \text{where } \tilde{G}(s) = \begin{bmatrix} C_0 \\ C_1 \end{bmatrix} (sE - A)^{-1} [\, B_0, B_1 \,],\ L = \begin{bmatrix} 1 & 0 \\ \frac{1}{2} & \frac{1}{2\sqrt{3}} \end{bmatrix}$$

$\Longrightarrow$ Computation via IRKA applied to $\tilde{G}$.

- FD discretization ($n = 400$, $m = q = 1$) yields

$$\dot{x}(t) = (p_0 A_0 + p_1 A_1 + p_2 A_2)\, x(t) + B\, u(t),$$

  where $p_0 =$ diffusion coefficient; p_i, $i = 1, 2$, convection in x_i direction, $p \in [0, 1]^3$.

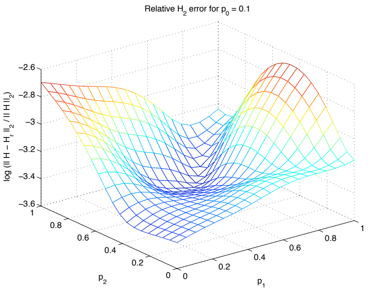
- Parameter vectors for interpolation:

$$\begin{array}{lll} p^{(1)} = (0.8, 0.5, 0.5), & p^{(2)} = (0.8, 0, 0.5), & p^{(3)} = (0.8, 1, 0.5), \\ p^{(4)} = (0.1, 0.5, 0.5), & p^{(5)} = (0.1, 0, 1), & p^{(6)} = (0.1, 1, 1). \end{array}$$

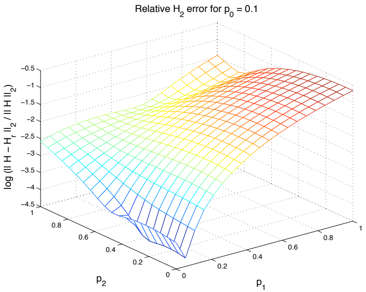
- Compare implementations:
  - generic rational PMOR ($\equiv$ fix interpolation frequencies),
  - IRKA-based rational PMOR ($\equiv$ optimize interpolation frequencies).

- Reduced-order model: $r_1 = r_2 = r_3 = 3$, $r_4 = r_5 = r_6 = 4 \Rightarrow$ $r = 21$.

Relative $\mathcal{H}_2$ Error for $p_0 = 0.1$

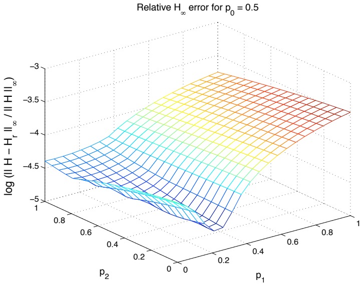


IRKA, 5 steps



generic

Relative $\mathcal{H}_\infty$ Error for $p_0 = 0.1$



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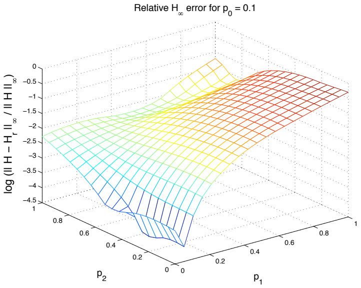


generic

- Important requirement for a compact model of thermal conduction is boundary condition independence.
- The thermal problem is modeled by the heat equation, where heat exchange through device interfaces is modeled by convection boundary conditions containing film coefficients $\{p_i\}_{i=1}^3$, to describe the heat exchange at the ith interface.
- Spatial semi-discretization leads to

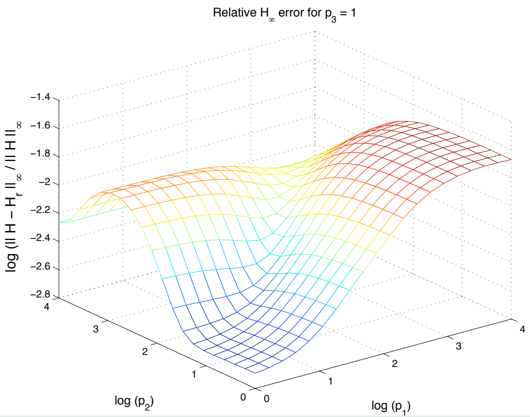
$$E\dot{x}(t) = (A_0 + \sum_{i=1}^{3} p_i A_i)x(t) + bu(t), \quad y(t) = c^T x(t),$$

where $n = 4,257$, A_i, $i = 1, 2, 3$, are diagonal.

Source: C.J.M Lasance, *Two benchmarks to facilitate the study of compact thermal modeling phenomena*, IEEE. Trans. Components and Packaging Technologies, Vol. 24, No. 4, pp. 559–565, 2001.

Choose 2 interpolation points for parameters ("important" configurations), 8/7 interpolation frequencies are picked H_2 optimal by IRKA.
$\Longrightarrow$ $k = 2, \ell = 8, 7$, hence $r = 15$.

$p_3 = 1,\ p_1, p_2 \in [1, 10^4]$.



Idea (for simplicity, $E = I_n$)

- A system Σ, realized by (A, B, C, D), is called balanced, if solutions P, Q of the Lyapunov equations

$$AP + PA^T + BB^T = 0, \qquad A^T Q + QA + C^T C = 0,$$

satisfy: $P = Q = \mathrm{diag}(\sigma_1, \ldots, \sigma_n)$ with $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_n > 0$.

- $\{\sigma_1, \ldots, \sigma_n\}$ are the Hankel singular values (HSVs) of Σ.
- Compute balanced realization of the system via state-space transformation

$$\begin{aligned} \mathcal{T} : (A, B, C, D) &\mapsto (TAT^{-1}, TB, CT^{-1}, D) \\ &= \left(\begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}, \begin{bmatrix} B_1 \\ B_2 \end{bmatrix}, \begin{bmatrix} C_1 & C_2 \end{bmatrix}, D \right) \end{aligned}$$

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Idea (for simplicity, $E = I_n$)

- A system Σ, realized by (A, B, C, D), is called balanced, if solutions P, Q of the Lyapunov equations

$$AP + PA^T + BB^T = 0, \qquad A^T Q + QA + C^T C = 0,$$

  satisfy: $P = Q = \mathrm{diag}(\sigma_1, \dots, \sigma_n)$ with $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_n > 0$.
- $\{\sigma_1, \dots, \sigma_n\}$ are the Hankel singular values (HSVs) of Σ.
- Compute balanced realization of the system via state-space transformation

$$\begin{aligned} \mathcal{T} : (A, B, C, D) &\mapsto (TAT^{-1}, TB, CT^{-1}, D) \\ &= \left(\begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}, \begin{bmatrix} B_1 \\ B_2 \end{bmatrix}, \begin{bmatrix} C_1 & C_2 \end{bmatrix}, D \right) \end{aligned}$$

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Motivation:

HSV are system invariants: they are preserved under $\mathcal{T}$ and determine the energy transfer given by the Hankel map

$$\mathcal{H} : L_2(-\infty, 0) \mapsto L_2(0, \infty) : u_- \mapsto y_+.$$

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In balanced coordinates ... energy transfer from u_- to y_+:

$$E := \sup_{\substack{u \in L_2(-\infty,0] \\ x(0)=x_0}} \frac{\int_0^\infty y(t)^T y(t)\, dt}{\int_{-\infty}^0 u(t)^T u(t)\, dt} = \frac{1}{\|x_0\|_2} \sum_{j=1}^n \sigma_j^2 x_{0,j}^2$$

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$\Longrightarrow$ Truncate states corresponding to "small" HSVs

$\Longrightarrow$ analogy to best approximation via SVD, therefore balancing-related methods are sometimes called SVD methods.

Implementation: SR Method

1. Compute (Cholesky) factors of the solutions of the Lyapunov equations,
$$P = S^T S, \quad Q = R^T R.$$
2. Compute SVD
$$SR^T = [\, U_1, \; U_2 \,] \begin{bmatrix} \Sigma_1 & \\ & \Sigma_2 \end{bmatrix} \begin{bmatrix} V_1^T \\ V_2^T \end{bmatrix}.$$
3. Set
$$W = R^T V_1 \Sigma_1^{-1/2}, \qquad V = S^T U_1 \Sigma_1^{-1/2}.$$
4. Reduced model is $(W^T AV, W^T B, CV, D)$.

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Properties:

- Reduced-order model is stable with HSVs $\sigma_1, \ldots, \sigma_r$.
- Adaptive choice of r via computable error bound:

$$\|y - \hat{y}\|_2 \leq \left(2 \sum\nolimits_{k=r+1}^{n} \sigma_k\right) \|u\|_2.$$

- General misconception:
  complexity $\mathcal{O}(n^3)$ – true for several implementations (e.g., MATLAB, SLICOT, MorLAB).

But: recent developments in Numerical Linear Algebra yield matrix equation solvers with sparse linear systems complexity!

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Solving Large-Scale Lyapunov Equations

General form for $A, W = W^T \in \mathbb{R}^{n \times n}$ given and $P \in \mathbb{R}^{n \times n}$ unknown:

$$0 \quad = \quad \mathcal{L}(Q) := A^T Q + QA + W.$$

In large scale applications from semi-discretized control problems for PDEs,

- $n = 10^3 - 10^6$ ($\Longrightarrow$ $10^6 - 10^{12}$ unknowns!),
- A has sparse representation ($A = -M^{-1}K$ for FEM),
- W low-rank with $W \in \{BB^T, C^TC\}$, where $B \in \mathbb{R}^{n \times m}$, $m \ll n$, $\quad C \in \mathbb{R}^{q \times n}$, $p \ll n$.
- Standard (Schur decomposition-based) $\mathcal{O}(n^3)$ methods are not applicable!

- For $A \in \mathbb{R}^{n\times n}$ stable, $B \in \mathbb{R}^{n\times m}$ $(w \ll n)$, consider Lyapunov equation
$$AX + XA^T = -BB^T.$$
- ADI Iteration: [Wachspress 1988]
$$\begin{aligned}(A + p_k I)X_{(k-1)/2} &= -BB^T - X_{k-1}(A^T - p_k I)\\ (A + \overline{p_k} I){X_k}^T &= -BB^T - X_{(k-1)/2}(A^T - \overline{p_k} I)\end{aligned}$$
with parameters $p_k \in \mathbb{C}^-$ and $p_{k+1} = \overline{p_k}$ if $p_k \notin \mathbb{R}$.
- For $X_0 = 0$ and proper choice of p_k: $\lim_{k\to\infty} X_k = X$ (super)linearly.
- Re-formulation using $X_k = Y_k Y_k^T$ yields iteration for Y_k...

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Factored ADI Iteration

Lyapunov equation $0 = AX + XA^T + BB^T$.

Setting $X_k = Y_k Y_k^T$, some algebraic manipulations $\Longrightarrow$

Algorithm [Penzl '97/'00, Li/White '99/'02, B. 04, B./Li/Penzl '99/'08]

$$V_1 \leftarrow \sqrt{-2\mathrm{Re}\,(p_1)}(A + p_1 I)^{-1} B, \qquad Y_1 \leftarrow V_1$$

FOR $j = 2, 3, \ldots$

$$V_k \leftarrow \sqrt{\frac{\mathrm{Re}\,(p_k)}{\mathrm{Re}\,(p_{k-1})}} \left(V_{k-1} - (p_k + \overline{p_{k-1}})(A + p_k I)^{-1} V_{k-1}\right)$$

$$Y_k \leftarrow \begin{bmatrix} Y_{k-1} & V_k \end{bmatrix}$$

$$Y_k \leftarrow \mathrm{rrlq}(Y_k, \tau) \qquad \text{\% column compression}$$

At convergence, $Y_{k_{\max}} Y_{k_{\max}}^T \approx X$, where

$$Y_{k_{\max}} = \begin{bmatrix} V_1 & \ldots & V_{k_{\max}} \end{bmatrix}, \qquad V_k = \boxed{} \in \mathbb{C}^{n \times m}.$$

Note: Implementation in real arithmetic possible by combining two steps.

Factored Galerkin-ADI Iteration

Lyapunov equation $0 = AX + XA^T + BB^T$

Projection-based methods for Lyapunov equations with $A + A^T < 0$:

1. Compute orthonormal basis $\mathrm{range}(Z)$, $Z \in \mathbb{R}^{n\times r}$, for subspace $\mathcal{Z} \subset \mathbb{R}^n$, $\dim \mathcal{Z} = r$.
2. Set $\hat{A} := Z^T AZ$, $\hat{B} := Z^T B$.
3. Solve small-size Lyapunov equation $\hat{A}\hat{X} + \hat{X}\hat{A}^T + \hat{B}\hat{B}^T = 0$.
4. Use $X \approx Z\hat{X}Z^T$.

Examples:

- Krylov subspace methods, i.e., for $m = 1$:

$$\mathcal{Z} = \mathcal{K}(A, B, r) = \mathrm{span}\{B, AB, A^2B, \ldots, A^{r-1}B\}$$

[Jaimoukha/Kasenally '94, Jbilou '02–'08].

- K-PIK [Simoncini '07],

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Examples:

- ADI subspace [B./R.-C. Li/Truhar '08]:

$$\mathcal{Z} = \mathrm{colspan}\left[\; V_1, \quad \ldots, \quad V_r \;\right].$$

Note: ADI subspace is rational Krylov subspace [J.-R. Li/White '02].

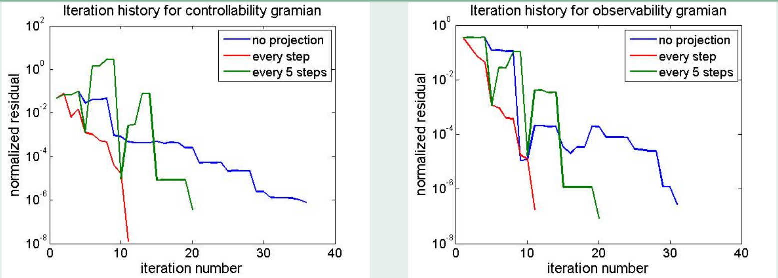
Factored Galerkin-ADI Iteration

Numerical example

FEM semi-discretized control problem for parabolic PDE:

- optimal cooling of rail profiles,
- $n = 20,209,\ m = 7,\ p = 6.$

Good ADI shifts



CPU times: 80s (projection every 5th ADI step) vs. 94s (no projection).

Computations by Jens Saak.

Factored Galerkin-ADI Iteration

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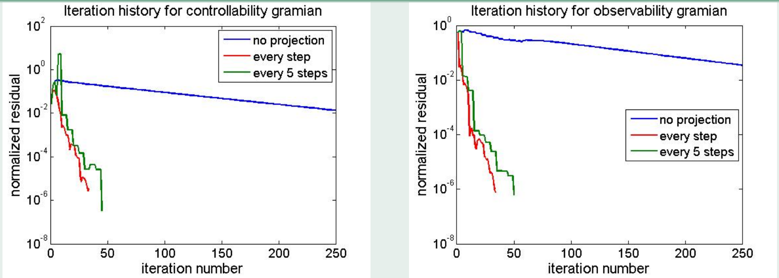


CPU times: 368s (projection every 5th ADI step) vs. 1207s (no projection).

Computations by Jens Saak.

Idea: for selected parameter values $p^{(j)}$, $j = 1, \ldots, k$, compute reduced-order models $\hat{G}_j(s)$ of $G(s; p^{(j)})$ by BT.

Parametric reduced-order system by Lagrange interpolation:

$$\begin{aligned} \hat{G}(s;p) &= \sum_{j=1}^{k} L_j(p)\hat{G}_j(s) = \sum_{j=1}^{k} \left(\prod_{i=1, i\neq j}^{k} \frac{p - p^{(i)}}{p^{(i)} - p^{(j)}} \right) \hat{C}_j^T (sI_{r_j} - \hat{A}_j)^{-1} \hat{B}_j \\ &= \begin{bmatrix} \hat{C}_1(p) \\ \vdots \\ \hat{C}_k(p) \end{bmatrix}^T \begin{bmatrix} (sI_{r_1} - \hat{A}_1)^{-1} & & \\ & \ddots & \\ & & (sI_{r_k} - \hat{A}_k)^{-1} \end{bmatrix} \begin{bmatrix} \hat{B}_1 \\ \vdots \\ \hat{B}_k \end{bmatrix} \end{aligned}$$

Note: no discretization/grid for frequency parameter s necessary!

Related ideas:

- use barycentric interpolation for improved stability and easy incorporation of new interpolation data;
- employ (rational) Hermite interpolation w.r.t. p;
- use sinc interpolation.

Combination of interpolation error and balanced truncation bound $\Longrightarrow$

$$\sup_{\substack{s\in\mathbb{C}^+\\ p\in[a,b]}} \|G(s;p)-\hat{G}(s;p)\| = \sup_{\substack{s\in\mathbb{C}^+\\ p\in[a,b]}} \|G(s;p)-\sum_{j=0}^{k} L_j(p)\hat{G}_j(s)\|$$

$$\leq \sup_{\substack{s\in\mathbb{C}^+\\ p\in[a,b]}} \|G(s;p)-\sum_{j=0}^{k} L_j(p)G_j(s)\| + \sup_{\substack{s\in\mathbb{C}^+\\ p\in[a,b]}} \|\sum_{j=0}^{k} L_j(p)(G_j(s)-\hat{G}_j(s))\|$$

$$\leq \sup_{\substack{s\in\mathbb{C}^+\\ p\in[a,b]}} \|R_k(G,s,p)\| + \mathrm{tol}\cdot \sup_{p\in[a,b]} |\sum_{j=0}^{k} L_j(p)|$$

with remainder $R_k(G,s,p) = G(s;p)-\hat{G}(s;p)$

$$R_k(G,s,p) = \frac{1}{(k+1)!}\left(\frac{\partial^{k+1}}{\partial p^{k+1}} G(s;\xi(p))\right)\prod_{i=0}^{k}(p-p_i)$$

at $\xi(p)\in[\min_j p_j, \max_j p_j]$.

Convection-diffusion equation

$$
\begin{aligned}
\frac{\partial T}{\partial t}(t,\xi) &= \Delta T(t,\xi) + p \cdot \nabla T(t,\xi) + b(\xi)u(t) \quad \xi \in (0,1)^2 \\
&\Downarrow \quad \mathit{FDM\ with\ } n = 400 \\
\frac{d}{dt}x(t) &= (A + p\,A_1)\,x(t) + b\,u(t), \quad b = e_1 \\
y(t) &= c^T x(t), \quad c^T = [1, 1, \cdots, 1]
\end{aligned}
$$

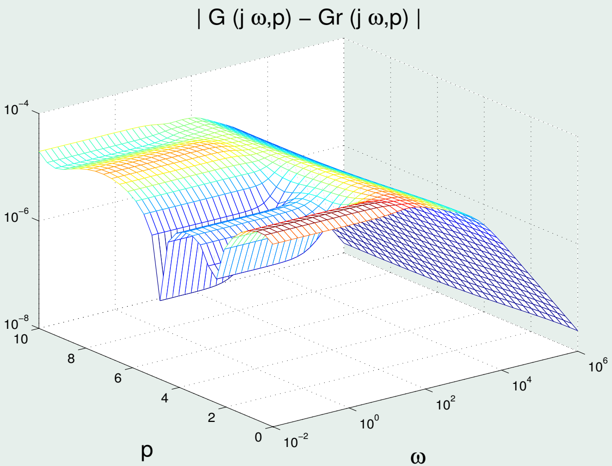
1. Choose $p_0, \cdots, p_5 \in [0,\ 10]$ as Chebyshev points;
2. prescribe BT error bound for $\hat{G}(s; p_j)$ by tol$=10^{-4}$
   $\Rightarrow$ systems of reduced order $r_j \in \{3, 4\}$;
3. error estimate for $\hat{G}(s; p)$ obtained by Lagrange interpolation:

$$\sup_{\substack{\omega \in [10^{-2}, 10^6] \\ p \in [0,10]}} |G(\jmath\omega, p) - \hat{G}(\jmath\omega, p)| \leq 3.3 \times 10^{-5}.$$

PMOR Using BT $(d = 1)$

Numerical Examples – Convection-Diffusion Equation

$|G(\jmath\omega; p) - \hat{G}(\jmath\omega; p)|$

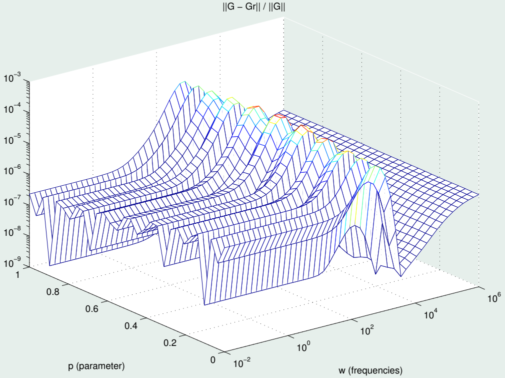


Anemometer: FEM model

$$E\dot{x}(t) = (A_0 + p_1 A_1)x(t) + bu(t), \quad y(t) = c^T x(t),$$

where $n = 29,008$, $m = q = 1$.

Relative Error $|G(\jmath\omega, p) - \hat{G}(\jmath\omega, p)| \,/\, |G(\jmath\omega, p)|$



Parametric Model Reduction Using Balanced Truncation on Sparse Grids [*Baur/B. '09*]

Disadvantage of interpolating BT reduced-order models:
for d-dimensional parameter spaces $p \in [0,1]^d$ with $d \geq 2$
we need many interpolation points $\Rightarrow$ many times BT,

i.e. very high complexity!

Thus:

employ sparse grid interpolation [*Zenger 91, Griebel 91, Bungartz 92*].

Main advantages:

- requires significantly fewer grid points,
- preserves asymptotic error decay with increasing grid resolution (up to logarithmic factor).

PMOR Using BT on Sparse Grids

Sparse Grids [*Zenger '91, Griebel '91, Bungartz '92*]

On $[0,\ 1]$, construct equidistant grid with mesh size $h_\ell = 2^{-\ell}$ and associated $(2^\ell - 1)$-dim. space of piecewise linear functions S_ℓ.

Hierarchical basis decomposition [*Yserentant '86*]

$$S_\ell = T_1 \oplus \cdots \oplus T_\ell$$

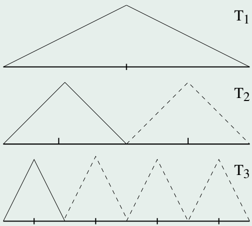
For $f \in C^2[0,\ 1]$ and interpolant $f_\mathrm{I} \in S_\ell$

$$f_\mathrm{I} = \sum_{i=1}^{\ell} f_i,\ \ f_i \in T_i,$$

the interpolation error is bounded by

$$\begin{aligned} \|f - f_\mathrm{I}\|_\infty &\leq c h_\ell^2. \\ \|f_i\|_\infty &\leq \frac{1}{2} 4^{-i} \|\frac{\partial^2 f}{\partial x^2}\|_\infty. \end{aligned}$$

Subspaces of S_ℓ



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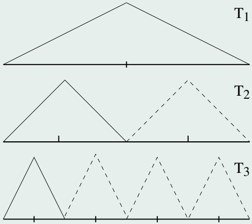


PMOR Using BT on Sparse Grids

Hierarchical basis decomposition in $d = 2$

On $[0,\ 1]^2$ construct rectangular grid with mesh size $h_{\ell_1} = 2^{-\ell_1}, h_{\ell_2} = 2^{-\ell_2}$ and $(2^\ell - 1)^2$-dim. space of piecewise bilinear functions $S_{\underline{\ell}}$ $\quad (\underline{\ell} := (\ell_1, \ell_2))$

Hierarchical basis decomposition:

$$S_{\underline{\ell}} = \bigoplus_{i_1=1}^{\ell} \bigoplus_{i_2=1}^{\ell} T_{\underline{i}}, \quad \underline{i} = (i_1, i_2)$$

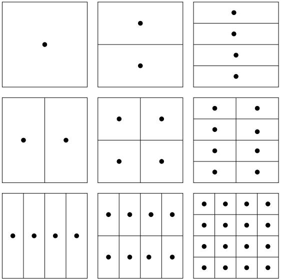
For $f : [0,\ 1]^2 \to \mathbb{R}$, $f^{(4)}_{x_1 x_1 x_2 x_2} \in C^0([0,\ 1]^2)$

$$f_{\mathrm{I}} = \sum_{i_1=1}^{\ell} \sum_{i_2=1}^{\ell} f_{\underline{i}}, \quad f_{\underline{i}} \in T_{\underline{i}}$$

the interpolation error is bounded

- $\|f - f_{\mathrm{I}}\|_\infty \leq \mathcal{O}(h_\ell^2)$
- $\|f_{\underline{i}}\|_\infty \leq \frac{1}{4} 4^{-i_1-i_2} \left\| \frac{\partial^4 f}{\partial x_1^2 \partial x_2^2} \right\|_\infty$

Subspaces of S_{33}:



supports of bases of $T_{11}, \ldots$

PMOR Using BT on Sparse Grids
Hierarchical basis decomposition in $d = 2$

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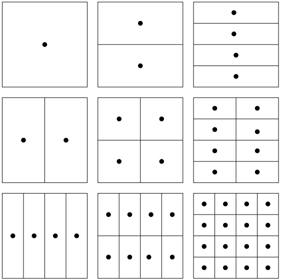


supports of bases of $T_{11}, \ldots$

PMOR Using BT on Sparse Grids

Sparse grids in $d = 2$ [*Zenger 91, Griebel 91, Bungartz 92*]

Sparse decomposition:

$$\tilde{S}_{\underline{\ell}} = \bigoplus_{i_1+i_2 \leq \ell+1} T_{\underline{i}}, \quad \underline{i} = (i_1, i_2)$$

with reduced dimension

$$\dim \tilde{S}_{\underline{\ell}} = 2^{\ell}(\ell - 1) + 1$$

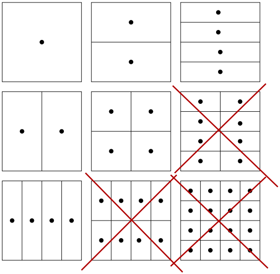
For $f : [0,\ 1]^2 \to \mathbb{R}$, $f^{(4)}_{x_1 x_1 x_2 x_2} \in C^0([0,\ 1]^2)$,

$$\tilde{f}_{\mathrm{I}} = \sum_{i_1+i_2 \leq \ell+1} f_{\underline{i}}, \qquad f_{\underline{i}} \in T_{\underline{i}},$$

the interpolation error is bounded:

$$\|f - \tilde{f}_{\mathrm{I}}\|_\infty \leq \mathcal{O}(h_\ell^2 \log(h_\ell^{-1})).$$

Subspaces of S_{33}:



supports of bases of $T_{11}, \ldots$

References

PMOR Using BT on Sparse Grids

Sparse grids in $d = 2$ [*Zenger 91, Griebel 91, Bungartz 92*]

Sparse decomposition:

$$\tilde{S}_{\underline{\ell}} = \bigoplus_{i_1+i_2 \leq \ell+1} T_{\underline{i}}, \quad \underline{i} = (i_1, i_2)$$

with reduced dimension

$$\dim \tilde{S}_{\underline{\ell}} = 2^{\ell}(\ell - 1) + 1$$

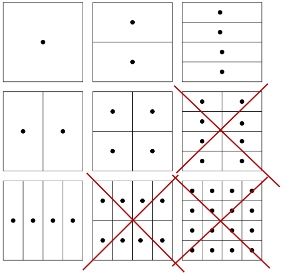
For $f : [0,\ 1]^2 \to \mathbb{R}$, $f^{(4)}_{x_1 x_1 x_2 x_2} \in C^0([0,\ 1]^2)$,

$$\tilde{f}_{\mathrm{I}} = \sum_{i_1+i_2 \leq \ell+1} f_{\underline{i}}, \qquad f_{\underline{i}} \in T_{\underline{i}},$$

the interpolation error is bounded:

$$\|f - \tilde{f}_{\mathrm{I}}\|_{\infty} \leq \mathcal{O}(h_{\ell}^2 log(h_{\ell}^{-1})).$$

Subspaces of S_{33}:



supports of bases of $T_{11}, \ldots$

PMOR Using BT on Sparse Grids

Sparse Grids [*Zenger '91, Griebel '91, Bungartz '92*]

On $[0,\ 1]^d$, construct grids with mesh size $h_{\underline{\ell}}$ ($\underline{i} := (i_1, \ldots, i_d) \in \mathbb{N}^d$).

For $f : [0,\ 1]^d \to \mathbb{R}$, $\frac{\partial^{2d} f}{\partial x_1^2 \ldots \partial x_d^2} \in C^0([0,\ 1]^d)$ search

interpolant f_{I} in space of piecewise d-linear functions:

	full grid space	sparse grid space
	$S_\ell = \bigoplus_{i_1=1}^{\ell} \cdots \bigoplus_{i_d=1}^{\ell} T_{\underline{i}}$	$\tilde{S}_\ell = \bigoplus_{\lvert\underline{i}\rvert_1 \leq \ell+d-1} T_{\underline{i}}$
dimension	$\mathcal{O}(h_\ell^{-d})$	$\mathcal{O}(h_\ell^{-1}\,(log(h_\ell^{-1}))^{d-1})$
$\lVert f - f_{\mathrm{I}} \rVert_\infty$	$\mathcal{O}(h_\ell^2)$	$\mathcal{O}(h_\ell^2\,(log(h_\ell^{-1}))^{d-1})$

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interpolant f_{I} in space of piecewise d-linear functions:

	full grid space $S_\ell = \bigoplus_{i_1=1}^{\ell} \cdots \bigoplus_{i_d=1}^{\ell} T_{\underline{i}}$	sparse grid space $\tilde{S}_\ell = \bigoplus_{\lvert\underline{i}\rvert_1 \le \ell+d-1} T_{\underline{i}}$
dimension	$\mathcal{O}(h_\ell^{-d})$	$\mathcal{O}(h_\ell^{-1}\ (log(h_\ell^{-1}))^{d-1})$
$\lVert f - f_{\mathrm{I}} \rVert_\infty$	$\mathcal{O}(h_\ell^2)$	$\mathcal{O}(h_\ell^2\ (log(h_\ell^{-1}))^{d-1})$

PMOR Using BT on Sparse Grids

Sparse Grids [*Zenger '91, Griebel '91, Bungartz '92*]

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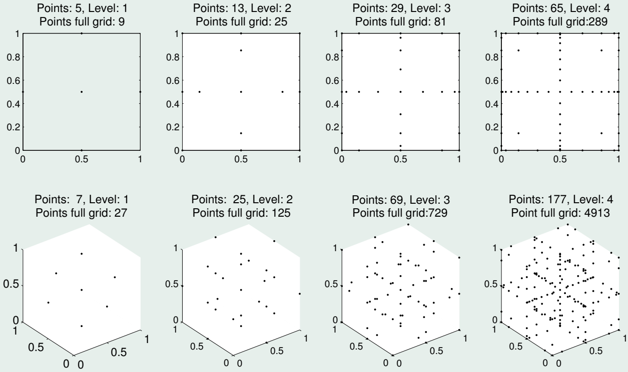
PMOR Using BT on Sparse Grids

MATLAB Sparse Grid Interpolation Toolbox [*Klimke/Wohlmuth '05, Klimke '07*]

Chebyshev-Gauß-Lobatto grid



PMOR Using BT on Sparse Grids

Algorithmic Framework

1. For level ℓ choose $\mathcal{O}(h_\ell^{-1}(log(h_\ell^{-1}))^{d-1})$ sparse grid points p_j.
2. Apply balanced truncation to $G_j(s) := G(s; p_j)$:

$$\hat{G}_j(s) = \hat{C}_j^T(sI_{r_j} - \hat{A}_j)^{-1}\hat{B}_j,$$

determine r_j by prescribed error tolerance:

$$\|G_j - \hat{G}_j\|_\infty \leq \mathrm{tol}.$$

3. Parametric reduced-order system:

$$\hat{G}(s; p) = \sum_{|\underline{i}|_1 \leq \ell+d-1} \phi_{\underline{i}}(p)\, c_{\underline{i}}(\hat{G}_1(s), \hat{G}_2(s), \cdots)$$

with interpolation error

$$\|G - \hat{G}\|_\infty \leq \mathrm{tol} \cdot C \cdot \sup_{p \in \mathcal{I}^d} \sum_{|\underline{i}|_1 \leq \ell+d-1} |\phi_{\underline{i}}(p)| + \mathcal{O}(h_\ell^2(log(h_\ell^{-1}))^{d-1}).$$

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PMOR Using BT on Sparse Grids
Algorithmic Framework

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$$\hat{G}_j(s) = \hat{C}_j^T(sI_{r_j} - \hat{A}_j)^{-1}\hat{B}_j,$$

   determine r_j by prescribed error tolerance:

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$$\hat{G}(s; p) = \sum_{|\underline{i}|_1 \leq \ell+d-1} \phi_{\underline{i}}(p)\, c_{\underline{i}}(\hat{G}_1(s), \hat{G}_2(s), \cdots)$$

   with interpolation error

$$\|G - \hat{G}\|_\infty \leq \mathrm{tol} \cdot C \cdot \sup_{p \in \mathcal{I}^d} \sum_{|\underline{i}|_1 \leq \ell+d-1} |\phi_{\underline{i}}(p)| + \mathcal{O}(h_\ell^2(log(h_\ell^{-1}))^{d-1}).$$

$$\begin{aligned}
\frac{\partial \mathbf{x}}{\partial t}(t,\xi) &= \Delta \mathbf{x}(t,\xi) + \mathbf{p}\cdot\nabla\mathbf{x}(t,\xi) + b(\xi)u(t), \quad \xi \in (0,1)^2 \\
&\Downarrow \quad \mathit{FDM\ with}\ n = 400 \\
\dot{x}(t) &= (A + p_1 A_1 + p_2 A_2)\, x(t) + b\, u(t)
\end{aligned}$$

- $b = e_1,\ c^T = [1, 1, \cdots, 1]$.
- Parameter space: $p_1, p_2 \in [0,\ 1]$.
- Chebyshev-Gauss-Lobatto grid with polynomial interpolation, level $\ell = 1 \Longrightarrow k = 5$ sparse grid points.
- Error tolerance for BT applied to $G(s; p^{(j)})$: 10^{-4} $\Longrightarrow$ system of reduced order $r_j = 3$ for $j = 1, \ldots, k$.
- Estimated interpolation error: 1.8×10^{-4}.

$$
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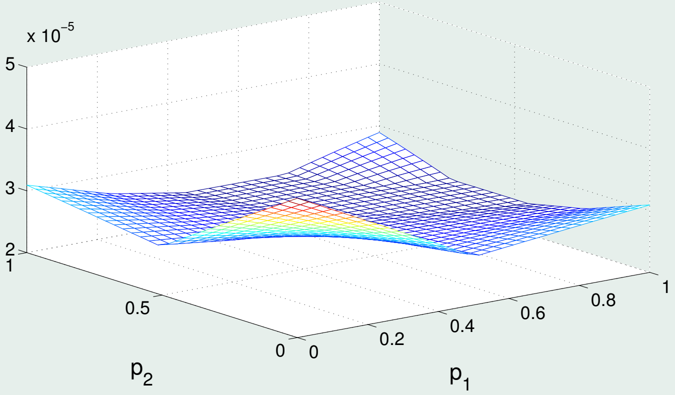
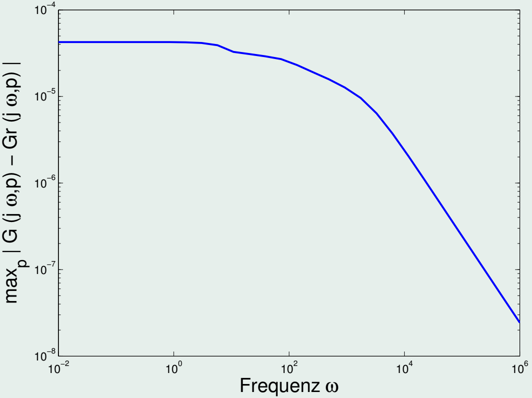
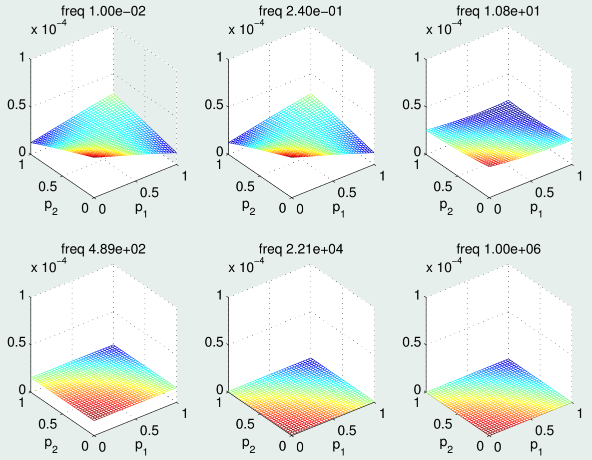
Absolute error of transfer function



L_∞ error of transfer function



Error of transfer function at certain frequencies



Conclusions and Outlook

- We have presented a general framework for interpolation-based model reduction of parametric systems.
- Applications: microsystems technology in particular, but also applicable to other areas where design and optimization are important.
- Approximation results for partial derivatives w.r.t. parameters $\rightsquigarrow$ sensitivities for process variations, optimization can be computed based on reduced-order model.
- Implementation of parametric model reduction based on multi-moment matching or rational Krylov methods (requires discretization w.r.t. frequency parameter) or balanced truncation (no discretization of frequency parameter).
- Efficiency of parametric model reduction methods can be enhanced when combined with sparse grid ideas.
- Wide variety of algorithmic possibilities, further need for optimization of interpolation point selection and error bounds, numerous possible applications.
- Explore connections to surrogate modeling in optimization: response surfaces, Kriging — hybrid methods?

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Workshop

Model Reduction for Complex Dynamical Systems

TU Berlin, 2-3 December 2010

http://www3.math.tu-berlin.de/modred2010/

organized by

Peter Benner	Michael Hinze
Matthias Bollhöfer	Patrick Lang
Heike Faßbender	Tatjana Stykel