SYSTEM-THEORETIC AND INTERPOLATORY METHODS FOR PARAMETRIC MODEL REDUCTION

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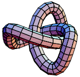

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Overview

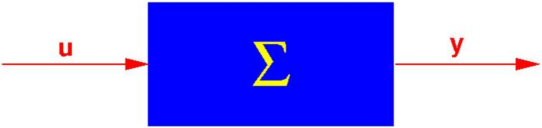
Dynamical Systems

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

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

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

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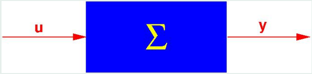

Reduced-Order System

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

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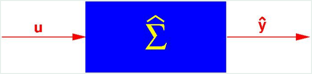

Goal:

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

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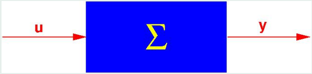

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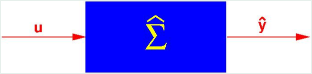


Goal:

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

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.

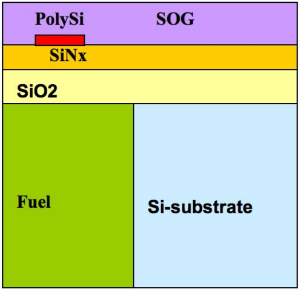
Source: The Oberwolfach Benchmark Collection http://www.imtek.de/simulation/benchmark

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_i, $i = 1, 2, 3$, diagonal.



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Motivation

Applications in Microsystems/MEMS Design

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.

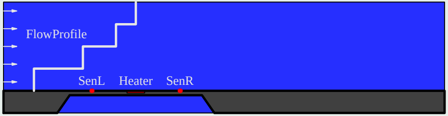


Figure: Anemometer model generated using ANSYS

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.

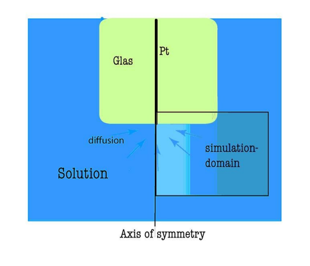
  Film coefficient depending on the applied potential is to be preserved.

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.



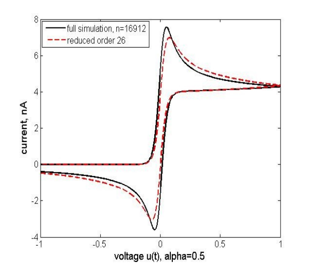


Figure: Schematic diagram of experimental set-up and corresponding voltammogram

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...

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...

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

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

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

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

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

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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

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

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

Problem

Approximate the dynamical system

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

by reduced-order system

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

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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:

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

allows easy parameter preservation for projection based model reduction.

Parametric System

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

Applications:

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

Model Reduction for Linear Parametric Systems

Parametric System

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Applications:

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

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 with 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: $W \neq V$,

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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

$$\begin{aligned} \operatorname{span}\left\{(s_1 E - A)^{-1}B, \ldots, (s_k E - A)^{-1}B\right\} &\subset \operatorname{Ran}(V), \\ \operatorname{span}\left\{(s_1 E - A)^{-T}C^T, \ldots, (s_k E - A)^{-T}C^T\right\} &\subset \operatorname{Ran}(W), \end{aligned}$$

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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Remarks:

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

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

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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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Remarks:

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

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

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Assume

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

Reduced-order model

Petrov-Galerkin-type projection

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$$
\begin{aligned}
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\hat{A}(p) &= W^T A_0 V + a_1(p) W^T A_1 V + \ldots + a_{q_A}(p) W^T A_{q_A} V, \\
\hat{B}(p) &= W^T B_0 \quad + b_1(p) W^T B_1 \quad + \ldots + b_{q_B}(p) W^T B_{q_B}, \\
\hat{C}(p) &= \quad C_0 V + \quad c_1(p) C_1 V + \ldots + \quad c_{q_C}(p) C_{q_C} V.
\end{aligned}
$$

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 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/'09]: Arnoldi-MGS method, employ recursive dependance of multi-moments, numerically robust, r often larger as with [Farle et al.].

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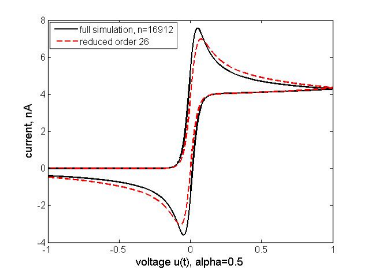
Electro-chemical SEM:

compute cyclic voltammogram based on FEM model

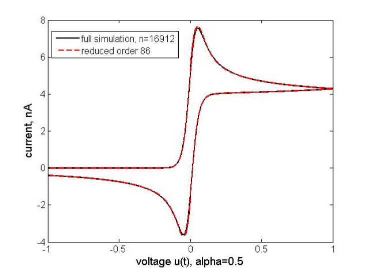
$$E\dot{x}(t) = (A_0 + p_1 A_1 + p_2 A_2)x(t) + Bu(t), \quad y(t) = c^T x(t),$$

where $n = 16.912$, $m = 3$, A_i diagonal.

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



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



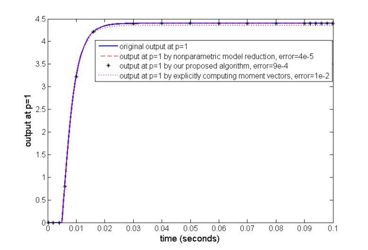
Anemometer:

FEM model

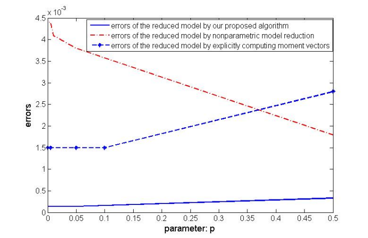
$$E\dot{x}(t) = (A_0 + p_1 A_1)x(t) + bu(t), \quad y(t) = c^T x(t),$$

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

Outputs for $p = 1$



Output errors for $p = 1$



Theorem [Beattie/B./Gugercin '07]

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

1. if $(\hat{s}\, E(\hat{p}) - A(\hat{p}))^{-1} B(\hat{p}) \in \mathrm{Ran}(V)$, then $G(\hat{s}, \hat{p}) = \hat{G}(\hat{s}, \hat{p})$;
2. if $\left(C(\hat{p})\, (\hat{s}\, E(\hat{p}) - A(\hat{p}))^{-1} \right)^T \in \mathrm{Ran}(W)$, then $G(\hat{s}, \hat{p}) = \hat{G}(\hat{s}, \hat{p})$;
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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
$$\mathcal{W} = \operatorname{span}\left\{\mathcal{A}(s_1,p^{(1)})^{-H}C(p^{(1)})^H, \ldots, \mathcal{A}(s_k,p^{(\ell)})^{-H}C(p^{(\ell)})^H\right\}.$$
4. Set $V := [v_1, \ldots, v_{k\ell}]$, $\tilde{W} := [w_1, \ldots, w_{k\ell}]$, and $W := \tilde{W}(\tilde{W}^H V)^{-1}$. (Note: $r = k\ell$).
5. Compute $\begin{cases} \hat{A}(p) := W^H A(p) V, & \hat{B}(p) := W^H B(p) V, \\ \hat{C}(p) := W^H C(p) V, & \hat{E}(p) := W^H E(p) V. \end{cases}$

- 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

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

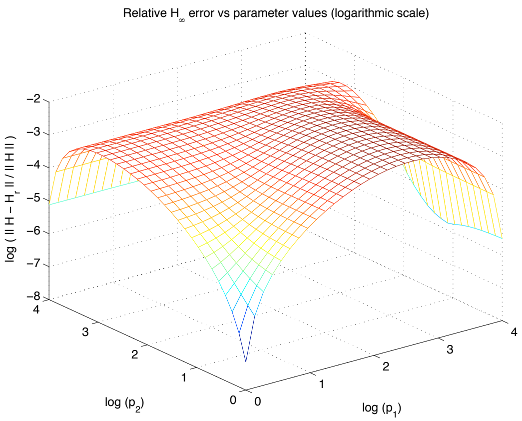
where $n = 4257$, A_i, $i = 1, 2, 3$, are diagonal.

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 4 interpolation points for parameters ("important" configurations), 6 interpolation frequencies are picked H_2 optimal by IRKA.

$\Longrightarrow \quad k = 6, \ell = 4,$ hence $r = 24.$

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



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

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

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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$\Longrightarrow$ 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
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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:

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

- General misconception (not at RICE, though — contributions by Antoulas, Gugercin, Heinkenschloss, Sorensen, Zhou): complexity $\mathcal{O}(n^3)$ – true for several implementations (e.g., MATLAB, SLICOT, MorLAB).

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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 $W \in \{BB^T, C^T C\}$, where $B \in \mathbb{R}^{n \times m}$, $m \ll n$, $C \in \mathbb{R}^{q \times n}$, $p \ll n$.
- 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

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

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

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],

$$\mathcal{Z} = \mathcal{K}(A, B, r) \cup \mathcal{K}(A^{-1}, B, r).$$

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 $\hat{A} := Z^T A Z$, $\hat{B} := Z^T B$.
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].

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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].

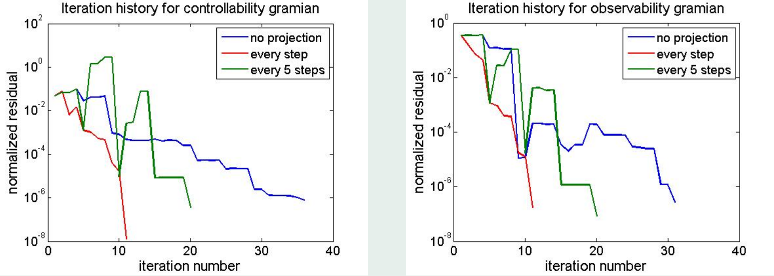
Factored Galerkin-ADI Iteration

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).

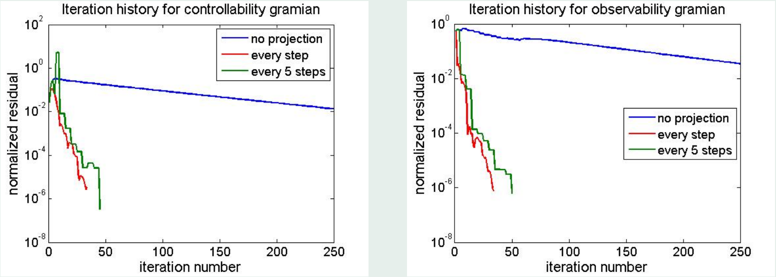
Computations by Jens Saak.

Factored Galerkin-ADI Iteration
Numerical example

FEM semi-discretized control problem for parabolic PDE:

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

Bad ADI shifts



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

Computations by Jens Saak.

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

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:

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

$$= \begin{bmatrix} \hat{C}_1(p) \\ \vdots \\ \hat{C}_k(p) \end{bmatrix}^T \begin{bmatrix} (sI_{r_1} - \hat{A}_1)^{-1} & & \\ & \ddots & \\ & & (sI_{r_k} - \hat{A}_k)^{-1} \end{bmatrix} \begin{bmatrix} \hat{B}_1 \\ \vdots \\ \hat{B}_k \end{bmatrix}$$

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

Current work: employ rational Hermite interpolation w.r.t. p.

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

PMOR Using BT $(d = 1)$

Numerical Example

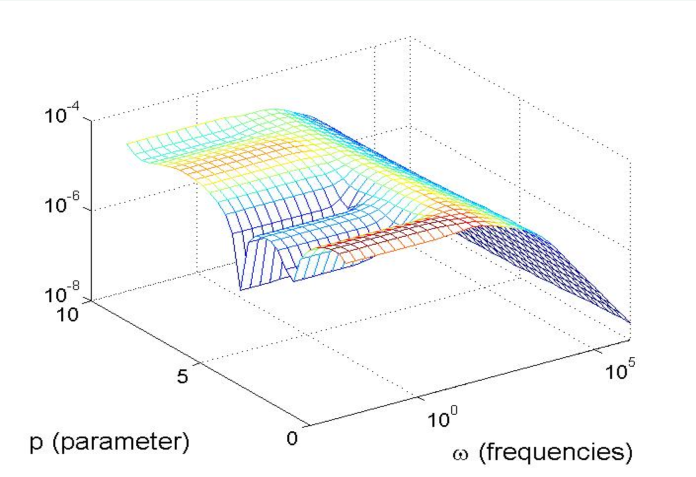
Convection-diffusion equation

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

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:

$$\sup_{\substack{s \in [\jmath 10^{-2}, \jmath 10^{6}] \\ p \in [0,10]}} \|G(s,p) - \hat{G}(s,p)\| \leq 2.6 \times 10^{-5}.$$

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



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 $f_\mathrm{I} \in S_\ell$

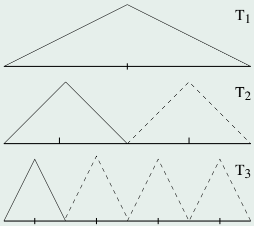
$$f_\mathrm{I} = \sum_{i=1}^{\ell} f_i,\ \ f_i \in T_i,$$

the interpolation error is bounded by

$$\|f - f_\mathrm{I}\|_\infty \leq ch_\ell^2.$$

$$\|f_i\|_\infty \leq \frac{1}{2} 4^{-i} \| \frac{\partial^2 f}{\partial x^2} \|_\infty.$$

Subspaces of S_ℓ



PMOR Using BT on Sparse Grids

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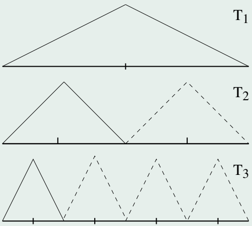


PMOR Using BT on Sparse Grids

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 $S_{\underline{\ell}}$ $\quad (\underline{\ell} := (\ell, \ell))$

Hierarchical basis decomposition:

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

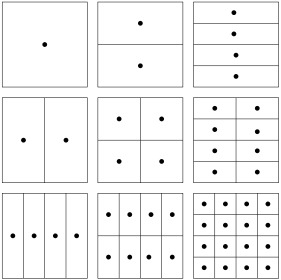
For $f : [0,\ 1]^2 \to \mathbb{R}$, $f^{(4)}_{x_1 x_1 x_2 x_2} \in C^0([0,\ 1]^2)$

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

the interpolation error is bounded

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

Subspaces of S_{33}:



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

PMOR Using BT on Sparse Grids

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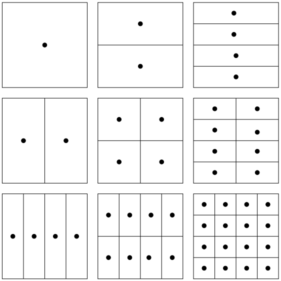

supports of bases of $T_{11}, \ldots$

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

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

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the interpolation error is bounded:

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

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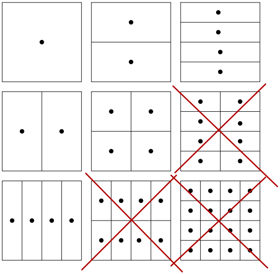

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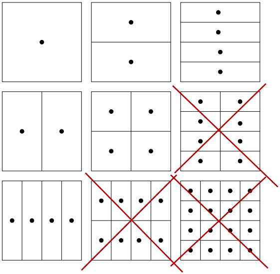

supports of bases of $T_{11}, \ldots$

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

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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 $\tilde{S}_\ell = \bigoplus_{\lvert\underline{i}\rvert_1 \le \ell+d-1} T_{\underline{i}}$
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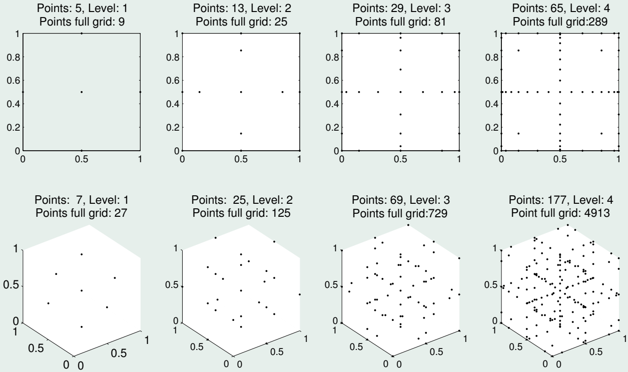
PMOR Using BT on Sparse Grids

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

Clenshaw-Curtis grid



1. For level ℓ choose $\mathcal{O}(h_\ell^{-1}(log(h_\ell^{-1}))^{d-1})$ sparse grid points.
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

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

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

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

- $b = e_1,\ c^T = [1, 1, \cdots, 1]$
- 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}.

PMOR Using BT on Sparse Grids

Numerical Examples — Convection-Diffusion Equation

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

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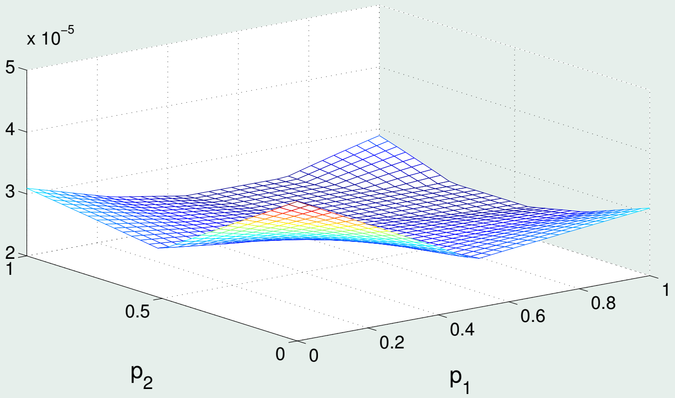
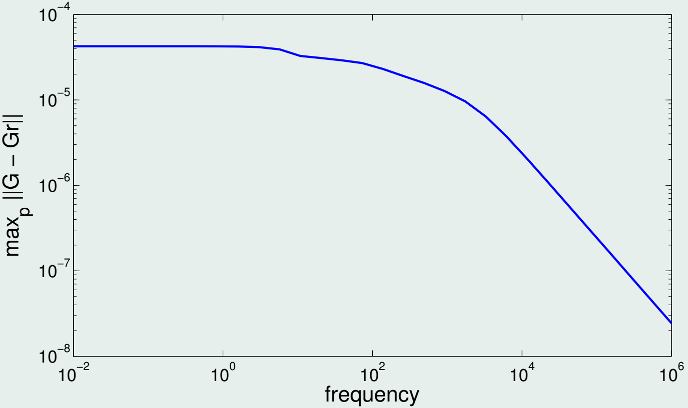
Absolute error of transfer function



H_∞ error of transfer function



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.

Announcement