Workshop on
Numerical Methods for Uncertainty Quantification
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Perspectives of Parametric Model Order Reduction for UQ

Peter Benner

Max Planck Institute for Dynamics of Complex Technical Systems
Computational Methods in Systems and Control Theory
Magdeburg, Germany

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MoreSim_4_Nano

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Overview

Motivation

Statistical Quantities

Goal

For a random variable (field, process) $\mathbf{x}$ on a probability space $(\Omega, \mathcal{F}, \mathcal{P})$, compute statistical information like

expected value $\mathbb{E}(\mathbf{x}) := \int_\Omega \mathbf{x}(\omega)\, \mathbf{d}\mathcal{P}(\omega)$;

standard deviation $\mathrm{std}_\mathbf{x} := \sqrt{\mathrm{var}\,(\mathbf{x})}$,

where $\mathrm{var}\,(\mathbf{x}) := \mathbb{E}\left((\mathbf{x} - \mathbb{E}(\mathbf{x}))^2\right)$ is the **variance** of $\mathbf{x}$;

$k\sigma$ **values** (*e.g.*, $k = 3, 6$) or **higher order moment**, where $\mathbf{x}$ solves a problem described by a system of (partial or ordinary) differential equations subject to uncertain data and/or differential operator:

$$\mathcal{L}(\xi, \omega)\mathbf{x}(\xi, \omega) = f(\xi, \omega) \quad \text{a.e. in } \Omega,\ \xi \in G.$$

Motivation

Computing Statistical Quantities

Intrusive vs. non-intrusive methods

- non-intrusive methods use a standard solver for the deterministic problem resulting from using a particular realization of the random variable,
- intrusive methods use special codes based on simultaneous discretization w.r.t. to random and spatial variables, require new solvers, often better convergence properties.

Basic methods for computing statistical quantities:

- non-intrusive: Monte Carlo (MC) and variants, stochastic collocation,
- intrusive: stochastic Galerkin.

Here: non-intrusive methods.

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Here: non-intrusive methods.

Motivating Example

from BMBF research network MoreSim4Nano

VLSI design in the presence of inaccurate lithography

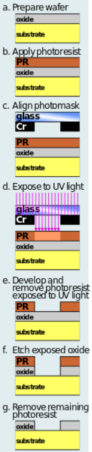
- Analyze the influence of variations during the lithography or variations of the materials on the electric field.
- Consider time-harmonic Maxwell's equations

$$\nabla \times (\mu^{-1} \nabla \times \mathbf{E}) + i\,\omega\,\sigma\,\mathbf{E} - \omega^2\,\epsilon\,\mathbf{E} = i\,\omega\,\mathbf{J}$$

with uncertain material parameters μ, σ, and ϵ.

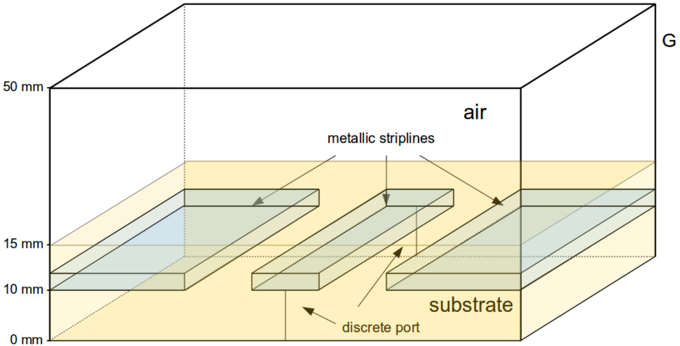
- The (approximate) distribution of the parameters is provided by industrial partners. We assume the parameters to be log-normally distributed, i.e., the probability density function is

$$f_p(x) = \frac{1}{\sqrt{2\pi}\sigma_p x} \exp\left(-\frac{(\ln(x) - \mu_p)^2}{2\sigma_p^2}\right) \quad \text{if } x \in \mathbb{R},\ x \geq 0.$$



Numerical Example

Consider a coplanar waveguide with dielectric overlay consisting of three perfectly conducting striplines situated at a height of 10mm in a shielded box with perfect electric conductor (PEC) boundary.



Model provided by CST AG Darmstadt/TEMF, TU Darmstadt.

Details

- Below a height of $15mm$ the box is filled with substrate which has another physical behavior than the air in the rest of the box.
- Denote the lower part of the box as sub-domain 1 and the upper part as sub-domain 2.
- Therefore the parameters ϵ_r and σ have to be split in ϵ_r^1, ϵ_r^2, σ^1 and σ^2.
- The relative permeability μ_r takes the same value for substrate and air.
- The system is excited with $u = 1$ Ampere at the front side of the box and the voltage along the port is integrated as the output y.
- The used frequency is $\omega = 0.6 \cdot 10^9$ Hz.
- Distributions for parameters provided by industrial partner.

Model provided by CST AG Darmstadt/TEMF, TU Darmstadt.

Discretized System

As we want to work with an affine form of the PDE, we rewrite the system in the following way

$$\nabla \times ((\mu_r \mu_0)^{-1} \nabla \times \mathbf{E}) + i\omega(\sigma^1 \chi_{G_1} + \sigma^2 \chi_{G_2})\mathbf{E} \\ -\omega^2 \epsilon_0 (\epsilon_r^1 \chi_{G_1} + \epsilon_r^2 \chi_{G_2})\mathbf{E} = i\omega \mathbf{J},$$

which leads to the affine discretized system

$$\mu_r A_{\mu_0} \mathbf{e} + i\omega(\sigma^1 A^1 + \sigma^2 A^2)\mathbf{e} - \omega^2(\epsilon_r^1 A_{\epsilon_0}^1 + \epsilon_r^2 A_{\epsilon_0}^2)\mathbf{e} = B_J u, \\ y = L\mathbf{e},$$

where u (current) is the single input of the system, y (voltage) the single output and B, C are the associated matrices.
Besides that, the matrices A^i and $A_{\epsilon_0}^i$ are zero on domain $j \neq i$, for $i, j = 1, 2$.

Numerical Results

- FEM discretization in FEniCS with Nédélec elements ($18,755$ dofs).
- Use stochastic collocation (Stroud and sparse grids) and basic Monte Carlo implemented in MATLAB®.
- We need 10 points for the Stroud integration and use a comparable sparse grid with 11 points which is the Hermite-Genz-Keister level 1 for a 5-dimensional parameter space. (The sparse grid is generated by use of the SGMGA code [Burkardt '10]).
- As reference solution, we use a Monte Carlo simulation which operates on $1,000,000$ realizations of the parameter vector.

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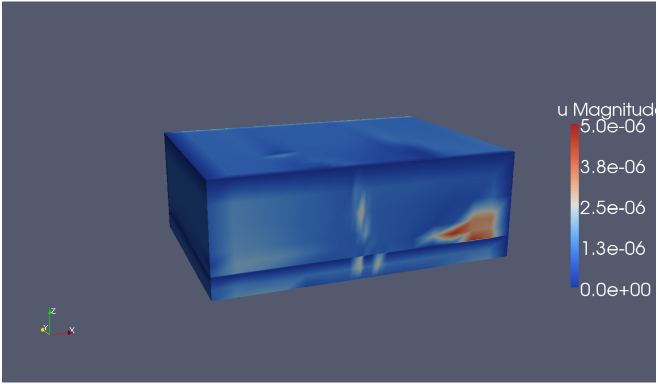
Numerical Results

We compute the maximum relative error for Stroud

$$err^{\text{Stroud}}_{rel,\mathbb{E}(\mathbf{e})} = max_{x\in G}(|(\text{Stroud} - \text{MC})/\text{MC}|) = 6.6901 \cdot 10^{-5}.$$

The relative error is shown in the following picture.



Numerical Results

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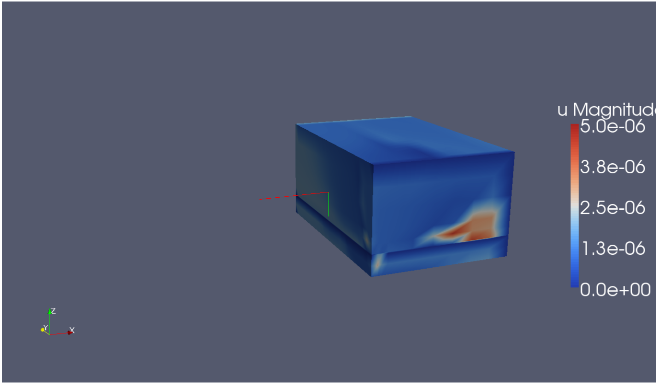
$$err^{\text{Stroud}}_{rel,\mathbb{E}(\mathbf{e})} = max_{x\in G}(|(\text{Stroud} - \text{MC})/\text{MC}|) = 6.6901 \cdot 10^{-5}.$$

The relative error on the right half of the box is shown in the following picture.



Motivation

Model Reduction for UQ?

Both, MC or SC require repeated solution of

$$\mu_r A_{\mu_0}\mathbf{e} + i\omega(\sigma^1 A^1 + \sigma^2 A^2)\mathbf{e} - \omega^2(\epsilon_r^1 A_{\epsilon_0}^1 + \epsilon_r^2 A_{\epsilon_0}^2)\mathbf{e} = B_J u, \quad y = L\mathbf{e},$$

given a realization of the parameter vector $p = [\,\mu_r, \sigma^1, \sigma^2, \epsilon_0^1, \epsilon_0^2\,]^T$.

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given a realization of the parameter vector $p = [\,\mu_r, \sigma^1, \sigma^2, \epsilon_0^1, \epsilon_0^2\,]^T$. Computing the quantity of interest y for a given (scaled) frequency ω and input u can be interpreted as evaluating

$$y(\omega, p) = G(i\omega, p)u(\omega, p)$$

with the rational transfer function

$$G(s,p) = L\left(s^2(\epsilon_r^1 A^1_{\epsilon_0} + \epsilon_r^2 A^2_{\epsilon_0}) + s(\sigma^1 A^1 + \sigma^2 A^2) + \mu_r A_{\mu_0}\right)^{-1} B_J.$$

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$$G(s,p) = L\left(s^2(\epsilon_r^1 A_{\epsilon_0}^1 + \epsilon_r^2 A_{\epsilon_0}^2) + s(\sigma^1 A^1 + \sigma^2 A^2) + \mu_r A_{\mu_0}\right)^{-1} B_J.$$

Using inverse Laplace transformation (assuming $\mathbf{e}(0) = 0$), this yields a 2nd order ODE system:

$$\begin{aligned}
\underbrace{(\epsilon_r^1 A_{\epsilon_0}^1 + \epsilon_r^2 A_{\epsilon_0}^2)}_{=:M(p)} \ddot{e}(t;p) + \underbrace{(\sigma^1 A^1 + \sigma^2 A^2)}_{=:D(p)} \dot{e}(t;p) + \underbrace{\mu_r A_{\mu_0}}_{=:K(p)} e(t;p) &= B_J u(t) \\
y(t;p) &= Le(t;p).
\end{aligned}$$

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given a realization of the parameter vector $p = [\,\mu_r, \sigma^1, \sigma^2, \epsilon_0^1, \epsilon_0^2\,]^T$. Corresponding rational transfer function

$$G(s,p) = L\left(s^2 M(p) + sD(p) + K(p)\right)^{-1} B_J.$$

and 2nd order ODE system:

$$M(p)\ddot{e}(t;p) + D(p)\dot{e}(t;p) + K(p) = B_J u(t), \qquad y(t;p) = Le(t;p).$$

Or, in 1st order formulation, setting $x := [\,e,\, \dot{e}\,]^T$,

$$\underbrace{\begin{bmatrix} I_n & \\ & M(p) \end{bmatrix}}_{=:E(p)} \dot{x} = \underbrace{\begin{bmatrix} 0 & I_n \\ -K(p) & -D(p) \end{bmatrix}}_{=:A(p)} x + \underbrace{\begin{bmatrix} 0 \\ B_J \end{bmatrix}}_{=:B} u,$$

$$y = [\,L,\, 0\,]\, x =: Cx.$$

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Model Reduction for UQ?

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Or, in 1st order formulation, setting $x := [\,e,\, \dot{e}\,]^T$,

$$E(p)\dot{x} = A(p)x + Bu, \quad y = Cx.$$

Goal: Faster simulation/evaluation of parametric ODE system/transfer function
$\rightsquigarrow$ parametric model order reduction (PMOR).

Introduction to Model Order Reduction

Model Reduction

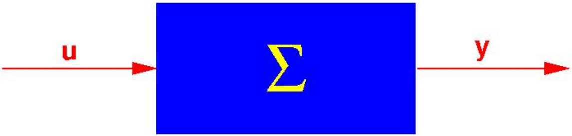
Dynamical Systems

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

with

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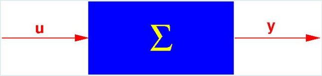
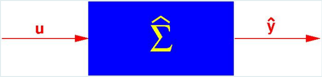


Reduced-Order System

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

- 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.

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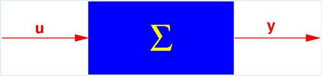

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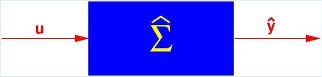

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Model Reduction Basics

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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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

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

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 $\Sigma(p)$.

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Model Reduction for Linear Parametric Systems

Problem

Approximate the dynamical system

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

by reduced-order system

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

of order $r \ll n$, such that for any feasible p,

$$||y - \hat{y}|| = \left|\left|Gu - \hat{G}u\right|\right| \le \left|\left|G - \hat{G}\right|\right| \, ||u|| < \text{tolerance} \cdot ||u|| \, .$$

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

Model Reduction for Linear Parametric Systems

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

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Model Reduction for Linear Parametric Systems

Parametric System

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

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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.

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.

Model Reduction for Linear Parametric Systems

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.

Additional model reduction goal:

preserve parameters as symbolic quantities in reduced-order model:

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

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

Interpolatory Model Reduction

Short Introduction

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 truncation matrices $V, W \in \mathbb{R}^{n\times r}$ with $W^T V = I_r$ ($\rightsquigarrow (VW^T)^2 = VW^T$ is projector) by computing

$$\hat{E} = W^T EV,\ \hat{A} = W^T AV,\ \hat{B} = W^T B,\ \hat{C} = CV.$$

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

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

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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

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

Interpolatory Model Reduction

Short Introduction

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

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,

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

Interpolatory Model Reduction

Notation

Parametric Systems

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

Assume

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

Interpolatory Model Reduction

Structure-Preservation

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

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

PMOR 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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PMOR based on Multi-Moment Matching

Numerical Examples

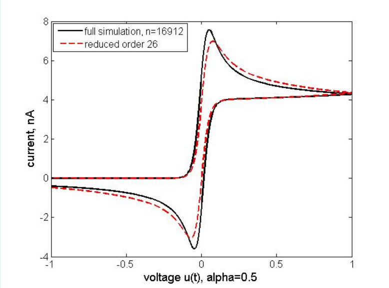
Electro-chemical SEM:

compute cyclic voltammogram based on FEM model

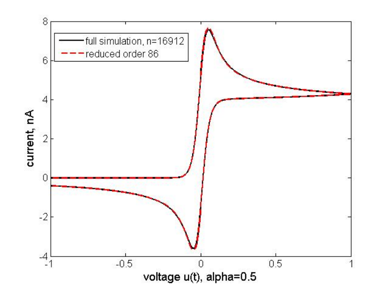
$$E\dot{x}(t) = (A_0 + p_1 A_1 + p_2 A_2)x(t) + Bu(t), \quad y(t) = c^T x(t),$$

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

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



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



PMOR based on Multi-Moment Matching

Numerical Examples

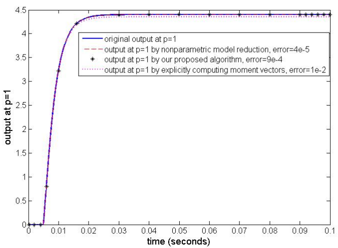
Anemometer:

FE model

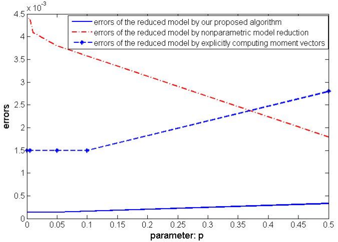
$$E\dot{x}(t) = (A_0 + p_1 A_1)x(t) + bu(t), \quad y(t) = c^T x(t),$$

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

Outputs for $p = 1$



Output errors for $p = 1$



PMOR based on Rational Interpolation

Theory: Interpolation of the Transfer Function

Theorem 1 [Baur/Beattie/B./Gugercin '07/'09]

Let
$$\hat{G}(s,p) := \hat{C}(p)(s\hat{E}(p) - \hat{A}(p))^{-1}\hat{B}(p) = C(p)V(sW^T E(p)V - W^T A(p)V)^{-1}W^T B(p)$$

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

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 $c^T G(\hat{s},\hat{p}) = c^T \hat{G}(\hat{s},\hat{p})$.

PMOR based on Rational Interpolation

Theory: Interpolation of the Transfer Function

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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.

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

PMOR based on Rational Interpolation

Theory: Interpolation of the Parameter Gradient

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

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

and

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

then

$$\nabla_p G(\hat{s}, \hat{p}) = \nabla_p G_r(\hat{s}, \hat{p}), \qquad \frac{\partial}{\partial s} G(\hat{s}, \hat{p}) = \frac{\partial}{\partial s} \hat{G}(\hat{s}, \hat{p}).$$

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Let $0 \neq b \in \mathbb{R}^m$, $0 \neq c \in \mathbb{R}^q$ be arbitrary. If $(\hat{s}\,E(\hat{p}) - A(\hat{p}))^{-1} B(\hat{p}) b \in \mathrm{Ran}(V)$ and $\left(c^T C(\hat{p})\,(\hat{s}\,E(\hat{p}) - A(\hat{p}))^{-1}\right)^T \in \mathrm{Ran}(W)$, then $\nabla_p c^T G(\hat{s}, \hat{p}) b = \nabla_p c^T \hat{G}(\hat{s}, \hat{p}) b$.

PMOR based on Rational Interpolation

Theory: Interpolation of the Parameter Gradient

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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.

PMOR based on Rational Interpolation

Algorithm

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 $\begin{cases} \hat{A}(p) := W^T A(p) V, & \hat{B}(p) := W^T B(p) V, \\ \hat{C}(p) := W^T C(p) V, & \hat{E}(p) := W^T E(p) V. \end{cases}$

PMOR based on Rational Interpolation

Remarks

- 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

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

  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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- 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

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

  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.

PMOR based on Rational Interpolation

Numerical Example: 2D Convection-Diffusion Equation

- 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:

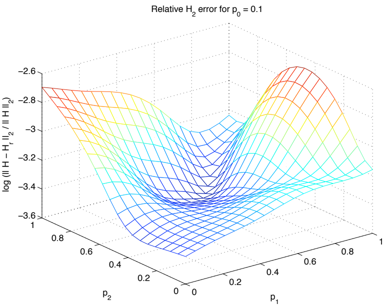
$$\begin{aligned} p^{(1)} &= (0.8, 0.5, 0.5), & p^{(2)} &= (0.8, 0, 0.5), & p^{(3)} &= (0.8, 1, 0.5), \\ p^{(4)} &= (0.1, 0.5, 0.5), & p^{(5)} &= (0.1, 0, 1), & p^{(6)} &= (0.1, 1, 1). \end{aligned}$$

- Compare implementations:
  - generic rational PMOR ($\equiv$ fix interpolation frequencies),
  - IRKA-based rational PMOR ($\equiv$ optimize interpolation frequencies).
- Reduced-order model: $r_1 = r_2 = r_3 = 3$, $r_4 = r_5 = r_6 = 4 \Rightarrow r = 21.$

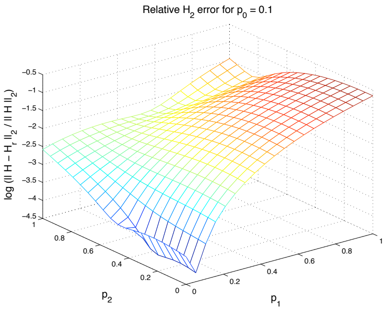
PMOR based on Rational Interpolation

Numerical Example: 2D Convection-Diffusion Equation

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



IRKA, 5 steps



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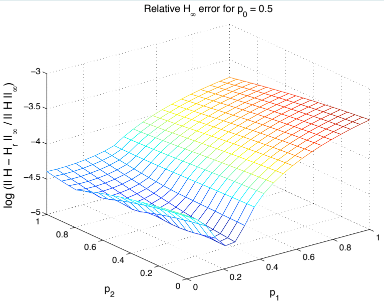
PMOR based on Rational Interpolation

Numerical Example: 2D Convection-Diffusion Equation

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



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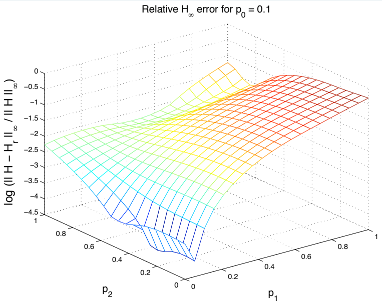


generic

PMOR based on Rational Interpolation

Numerical Example: Thermal Conduction in a Semiconductor Chip

- 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.

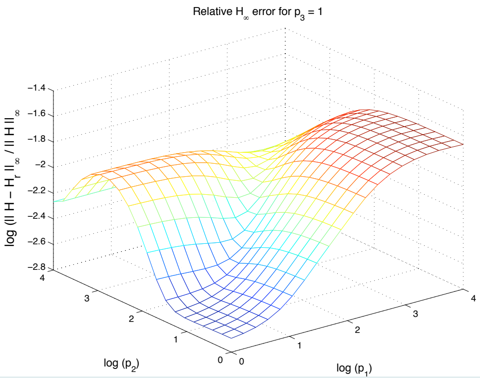
Source: C.J.M Lasance, *Two benchmarks to facilitate the study of compact thermal modeling phenomena*, IEEE. Trans. Components and Packaging Technologies, Vol. 24, No. 4, pp. 559–565, 2001.

PMOR based on Rational Interpolation

Numerical Example: Thermal Conduction in a Semiconductor Chip

Choose 2 interpolation points for parameters ("important" configurations), 8/7 interpolation frequencies are picked $\mathcal{H}_2$ optimal by IRKA. $\Longrightarrow$ $k = 2, \ell = 8, 7$, hence $r = 15$.

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



Model Reduction for Linear Parameter-Varying Systems

LPV Systems

Linear parameter-varying (LPV) systems = linear parametric systems with time-dependent parameters:

$$\Sigma : \quad \begin{cases} \dot{x}(t) = A_0 x(t) + \sum_{i=1}^{q} p_i(t) A_i x(t) + B_0 u(t), \\ y(t) = Cx(t), \quad x(0) = x_0, \end{cases}$$

Model Reduction for Linear Parameter-Varying Systems

LPV Systems: A Special Class of Bilinear Systems

Note that LPV systems

$$\dot{x}(t) = A_0 x(t) + \sum_{i=1}^{q} p_i(t) A_i x(t) + B_0 u_0(t), \quad y = Cx,$$

can be incorporated into the class of bilinear systems

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where $A_i \in \mathbb{R}^{n \times n}, \ B \in \mathbb{R}^{n \times m}, \ C \in \mathbb{R}^{p \times n}$. For this, the parameter dependent terms $p_i(t)$ are interpreted as additional inputs, resulting in a MIMO bilinear system with $q + k$ input variables:

$$u(t) := \begin{bmatrix} p_1(t) & \dots & p_q(t) & u_0(t) \end{bmatrix},$$
$$B := \begin{bmatrix} \mathbf{0} & \dots & \mathbf{0} & B_0 \end{bmatrix}.$$

Remark: Applying bilinear MOR, this automatically yields structure-preserving MOR techniques for LPV systems!

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Model Reduction for Linear Parameter-Varying Systems

$\mathcal{H}_2$-Norm for Bilinear Systems

Similar to the linear case, there exist generalized transfer functions, i.e. for the SISO case:

$$H_k(s_1,\ldots,s_i) = C(s_kI - A_0)^{-1}A_1 \cdots (s_2I - A_0)^{-1}A_1(s_1I - A_0)^{-1}B.$$

Hence, we may define the $\mathcal{H}_2$-norm for bilinear systems:

$$||\Sigma||^2_{\mathcal{H}_2} := \mathrm{tr}\left(\sum_{k=1}^{\infty}\int_{-\infty}^{\infty}\ldots\int_{-\infty}^{\infty}\frac{1}{(2\pi)^k}\,\overline{H_k(i\omega_1,\ldots,i\omega_k)}H_k^T(i\omega_1,\ldots,i\omega_k)\right),$$

which can be computed via the solution of the generalized Lyapunov eq.:

$$\begin{aligned}||\Sigma||^2_{\mathcal{H}_2} &= CPC^T\\ &= (\mathrm{vec}(I_p))^T\,(C\otimes C)\left(-A_0\otimes I - I\otimes A_0 - \sum_{k=1}^{q}A_k\otimes A_k\right)^{-1}(B\otimes B)\,\mathrm{vec}(I_m).\end{aligned}$$

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Model Reduction for Linear Parameter-Varying Systems

Interpolation-Based MOR for Bilinear Systems

Studying $\mathcal{H}_2$-norm of the error system leads to an iterative procedure:

Algorithm 1 Bilinear IRKA

Input: A_0, A_k, B, C, $\hat{A}_0$, $\hat{A}_k$, $\hat{B}$, $\hat{C}$

Output: A_0^{opt}, A_k^{opt}, B^{opt}, C^{opt}

1: **while** (change in $\Lambda > \epsilon$) **do**

2: $R\Lambda R^{-1} = \hat{A}_0$, $\tilde{B} = R^{-1}\hat{B}$, $\tilde{C} = \hat{C}R$, $\tilde{A}_k = R^{-1}\hat{A}_k R$

3: $\text{vec}(V) = \left(-\Lambda \otimes I_n - I_{\hat{n}} \otimes A_0 - \sum_{k=1}^{m} \tilde{A}_k \otimes A_k\right)^{-1} \left(\tilde{B} \otimes B\right) \text{vec}(I_m)$

4: $\text{vec}(W) = \left(-\Lambda \otimes I_n - I_{\hat{n}} \otimes A_0^T - \sum_{k=1}^{m} \tilde{A}_k^T \otimes A_k^T\right)^{-1} \left(\tilde{C}^T \otimes C^T\right) \text{vec}(I_p)$

5: $V = \text{orth}(V)$, $W = \text{orth}(W)$

6: $\hat{A}_0 = \left(W^T V\right)^{-1} W^T A_0 V$, $\hat{A}_k = \left(W^T V\right)^{-1} W^T A_k V$,
$\hat{B} = \left(W^T V\right)^{-1} W^T B$, $\hat{C} = CV$

7: **end while**

8: $A_0^{opt} = \hat{A}_0$, $A_k^{opt} = \hat{A}_k$, $B^{opt} = \hat{B}$, $C^{opt} = \hat{C}$

Model Reduction for Linear Parameter-Varying Systems

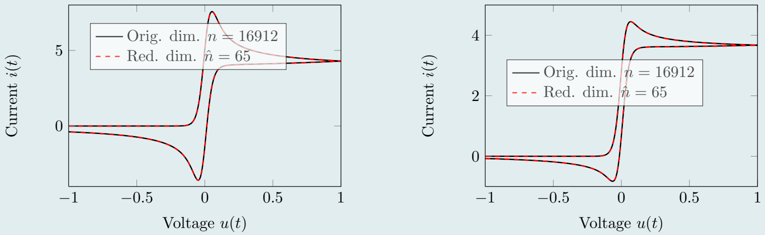
Numerical Example: Cyclic Voltammogramme

2 film coefficients $\Longrightarrow$

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

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

BIRKA Results, $r = 65$



Other Approaches

PMOR based on Rational Interpolation

- Transfer function interpolation (= output interpolation in frequency domain) [B./Baur '08]
- Matrix interpolation [Panzer/Mohring/Eid/Lohmann '10]
- Manifold interpolation [Amsallam/Farhat/... '08]
- Proper orthogonal/generalized decomposition (POD/PGD) [Kunisch/Volkwein, Hinze, Willcox, Nouy, ...]
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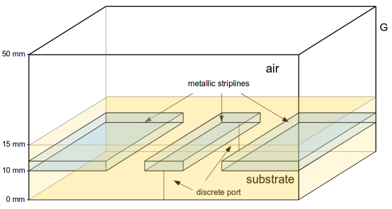
Reduced basis method

Numerical Example: Coplanar Waveguide

FEM (Nédélec) approximation of time-harmonic Maxwell equations, $n = 18,755$.

Coplanar waveguide



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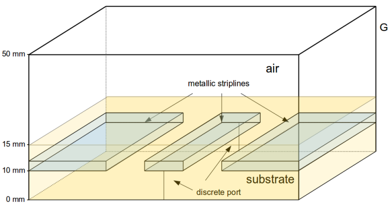
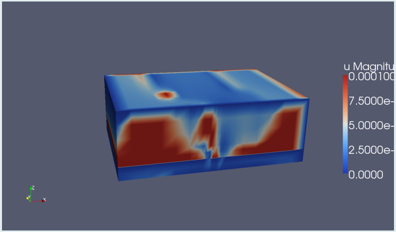


Relative errors for $r = 5$



Reference: basic MC(1,000,000)

Basic MC using RB model ≈ 2min (vs. 10 days for FEM model).

Reduced basis method

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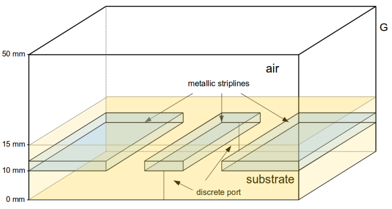
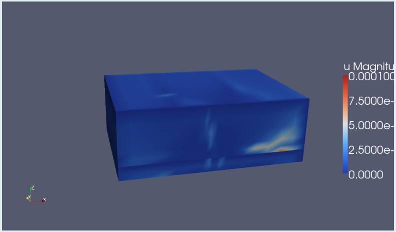


Relative errors for $r = 10$



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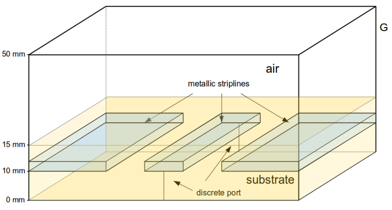
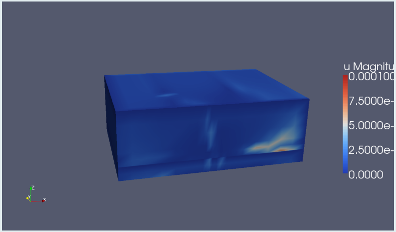


Relative errors for $r = 20$



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Conclusions and Outlook

- A variety of interpolatory and other PMOR methods can be used for standard forward uncertainty propagation problems if the model involves a number of uncertain parameters.
- Efficiency of parametric model reduction methods can be enhanced when combined with sparse grid ideas.
- Scaling with respect to number of parameters not well analyzed; so far, not all methods are applicable to problems with a large number of parameters, resulting, e.g., from Karhunen-Loéve and/or polynomial chaos expansion of random fields/processes.
- Wide variety of algorithmic possibilities, further need for optimization of interpolation point selection and error bounds, numerous possible applications.
- Combination with low-rank tensor techniques promising.
- Extension to nonlinear systems possible for most approaches.
- Currently working on stochastic RB method for Maxwell equations with uncertain geometry.

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