Numerical Methods for Model Reduction of Large-Scale Dynamical Systems

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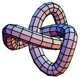
TECHNISCHE UNIVERSITÄT CHEMNITZ



NUMERISCHE SIMULATION PARALLELE SFB 393

Sonderforschungsbereich 393
“Parallele Numerische Simulation für Physik und Kontinuumsmechanik”

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Overview

Thanks to

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- Thilo Penzl for LyaPack.
- Members of the working group MIIT: Ulrike Baur, Matthias Pester, Jens Saak, Viatcheslav Sokolov.

Problem

Given a physical problem with dynamics described by the states $x \in \mathbb{R}^n$, where n is the dimension of the state space.

Because of redundancies, complexity, etc., we want to describe the dynamics of the system using a reduced number of states.

This is the task of model reduction (also: dimension reduction, order reduction).

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Example: Image Compression by Truncated SVD

- A digital image with $n_x \times n_y$ pixels can be represented as matrix $X \in \mathbb{R}^{n_x \times n_y}$, where x_{ij} contains color information of pixel (i, j).
- Memory: $4 \cdot n_x \cdot n_y$ bytes.

Theorem: (Schmidt-Mirsky/Eckart-Young)

Best rank-r approximation to $X \in \mathbb{R}^{n_x \times n_y}$ w.r.t. spectral norm:

$$\widehat{X} = \sum\nolimits_{k=1}^{r} \sigma_j u_j v_j^T,$$

where $X = U\Sigma V^T$ is the singular value decomposition (SVD) of X.
The approximation error is $\|X - \widehat{X}\|_2 = \sigma_{k+1}$.

Idea for dimension reduction

Instead of X save $u_1, \ldots, u_r$, $\sigma_1 v_1, \ldots, \sigma_r v_r$.
$\rightsquigarrow$ memory $= r \times (n_x + n_y)$ bytes.

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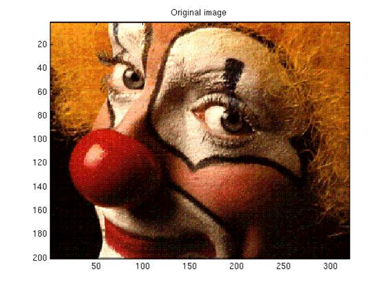

320×200 pixel
$\rightsquigarrow \approx 256$ kb

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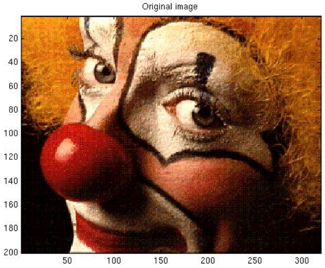

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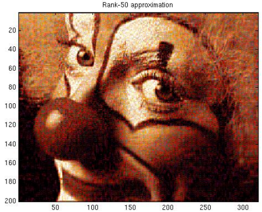
- rank $r = 50$, ≈ 104 kb



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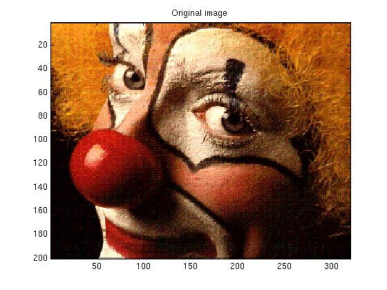

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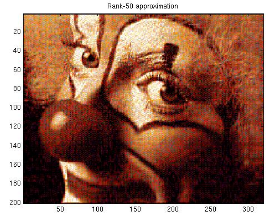
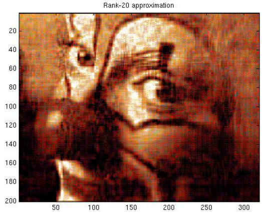


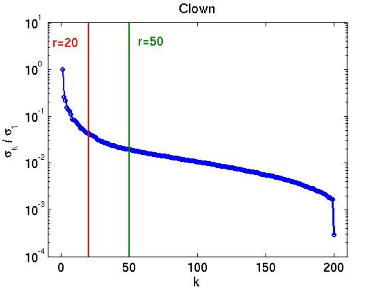
- rank $r = 20$, ≈ 42 kb

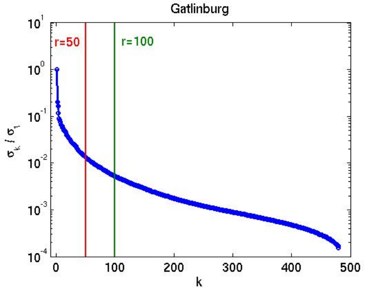


Background

Image data compression via SVD works, if the singular values decay (exponentially).

Singular Values of the Image Data Matrices





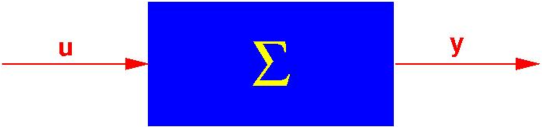
Systems Theory

Dynamical Systems

$$\Sigma : \left\{ \begin{array}{rcl} \dot{x}(t) & = & f(t, x(t), u(t)), \quad x(t_0) = x_0, \\ y(t) & = & g(t, x(t), u(t)) \end{array} \right.$$

with

- states $x(t) \in \mathbb{R}^n$,
- inputs $u(t) \in \mathbb{R}^m$,
- outputs $y(t) \in \mathbb{R}^p$.



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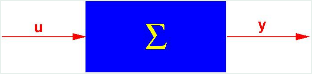

Goal:

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

Model Reduction for Dynamical Systems

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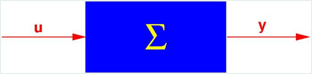

Reduced-Order System

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

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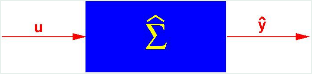

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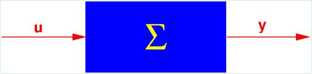

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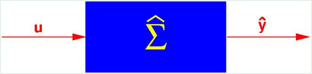

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Linear Systems in Frequency Domain

Linear, Time-Invariant (LTI) Systems

$$\begin{aligned} f(t,x,u) &= Ax+Bu, \quad & A \in \mathbb{R}^{n\times n}, \quad B \in \mathbb{R}^{n\times m}, \\ g(t,x,u) &= Cx+Du, \quad & C \in \mathbb{R}^{p\times n}, \quad D \in \mathbb{R}^{p\times m}. \end{aligned}$$

Laplace Transformation / Frequency Domain

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

$$sx(s) = Ax(s) + Bu(s), \quad y(s) = Bx(s) + Du(s),$$

yields I/O-relation in frequency domain:

$$y(s) = \Big(\underbrace{B(sI_n - A)^{-1}C + D}_{=:G(s)} \Big) u(s)$$

G is the transfer function of Σ.

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Approximate the dynamical system

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by reduced-order system

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

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

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(Optimal) Control

Feedback Controllers

A feedback controller (dynamic compensator) is a linear system of order N, where

- input $=$ output of plant,
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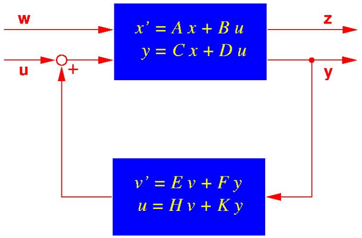
Modern (LQG-/$\mathcal{H}_2$-/$\mathcal{H}_\infty$-) control design: $N \geq n$

$\Rightarrow$ reduce order of original system.



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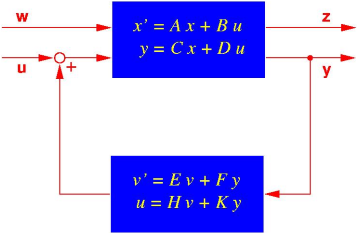

Micro Electronics

- Progressive miniaturization: **Moore's Law** states that the number of on-chip transistors doubles each 12 (now: 18) months.
- Verification of VLSI/ULSI chip design requires high number of simulations for different input signals.
- Increase in packing density requires modeling of interconnect to ensure that thermic/electro-magnetic effects do not disturb signal transmission.
- Linear systems in micro electronics occur through modified nodal analysis (MNA) for RLC networks, e.g., when
  - decoupling large linear subcircuits,
  - modeling transmission lines,
  - modeling pin packages in VLSI chips,
  - modeling circuit elements described by Maxwell's equation using partial element equivalent circuits (PEEC).

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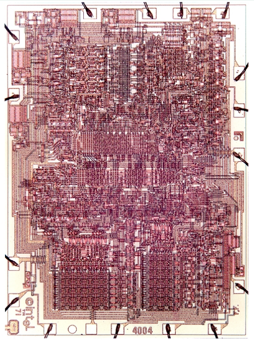
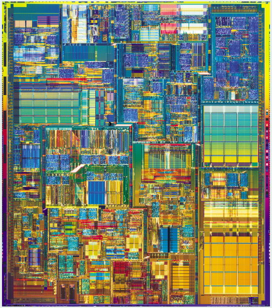
Example for Miniaturization

Intel 4004 (1971)



- 1 layer, 10μ technology,
- 2,300 transistors,
- 64 kHz clock speed.

Intel Pentium IV (2001)



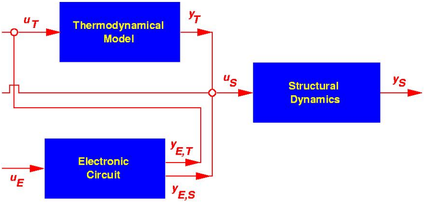
- 7 layers, 0.18μ technology,
- 42,000,000 transistors,
- 2 GHz clock speed,
- 2km of interconnect.

MEMS/Microsystems

Typical problem in MEMS simulation:
coupling of different models (thermic, structural, electric, electro-magnetic) during simulation.

Problems and Challenges:

- Reduce simulation times by replacing sub-systems with their reduced-order models.
- Stability properties of coupled system may deteriorate through model reduction even when stable sub-systems are replaced by stable reduced-order models.
- Multi-scale phenomena.



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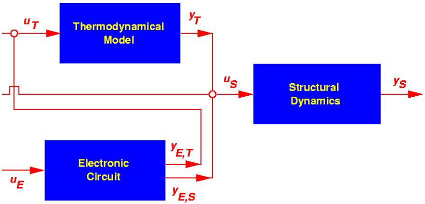

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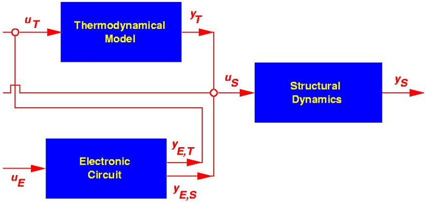

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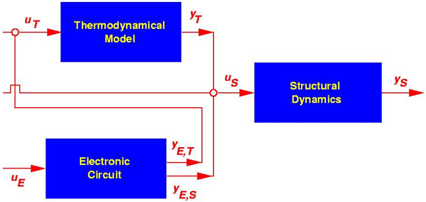

- Automatic generation of compact models.
- Satisfy desired error tolerance for all admissible input signals, i.e., want

$$\|y - \widehat{y}\| < \text{tolerance} \cdot \|u\| \qquad \forall u \in L_2(\mathbb{R}, \mathbb{R}^m).$$

$\Longrightarrow$ Need computable error bound/estimate!

- Preserve physical properties:
  - stability (poles of G in $\mathbb{C}^-$),
  - minimum phase (zeroes of G in $\mathbb{C}^-$),
  - passivity ("system does not generate energy").

Model Reduction

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- Satisfy desired error tolerance for all admissible input signals, i.e., want

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$\Longrightarrow$ Need computable error bound/estimate!

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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

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

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

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

Modal Truncation

Idea:

Project state-space onto A-invariant subspace $\mathcal{V}$, where

$$\mathcal{V} = \operatorname{span}(v_1, \ldots, v_r),$$

v_k = eigenvectors corresp. to "dominant" modes $\equiv$ eigenvalues of A.

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Properties:

- Simple computation for large-scale systems, using, e.g., Krylov subspace methods (Lanczos, Arnoldi), Jacobi-Davidson method.
- Error bound:

$$\|G - \widehat{G}\|_\infty \leq \operatorname{cond}_2(T)\, \|C_2\|_2 \|B_2\|_2 \frac{1}{\min_{\lambda \in \Lambda(A_2)} |\operatorname{Re}(\lambda)|},$$

where $T^{-1}AT = \operatorname{diag}(A_1, A_2)$.

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Difficulties:

- Eigenvalues contain only limited system information.
- Dominance measures are difficult to compute.
  (Litz 1979: use Jordan canoncial form; otherwise merely heuristic criteria.)
- Error bound not computable for really large-scale probems.

Guyan Reduction (Static Condensation)

Partition states in inner and outer (master) nodes; eliminate inner nodes in stationary system.

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− Non-static behavior of the system is ignored.

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$$G(s) \quad = \quad m_0 + m_1(s - s_0) + m_2(s - s_0)^2 + \ldots$$
- As reduced-order model use rth Padé approximate $\widehat{G}$ to G:
$$G(s) = \widehat{G}(s) + \mathcal{O}((s - s_0)^{2r}),$$
i.e., $m_j = \widehat{m}_j$ for $j = 0, \ldots, 2r - 1$
$\rightsquigarrow$ moment matching if $s_0 < \infty$,
$\rightsquigarrow$ partial realization if $s_0 = \infty$.

Padé Approximation

Padé-via-Lanczos Method (PVL)

- Moments need not be computed explicitly; moment matching is equivalent to projecting state-space onto

$$\mathcal{V} = \mathrm{span}(\tilde{B}, \tilde{A}\tilde{B}, \ldots, \tilde{A}^{r-1}B) = \mathcal{K}(\tilde{A}, \tilde{B}, r)$$

(where $\tilde{A} = (s_0 E - A)^{-1}E$, $\tilde{B} = (s_0 E - A)^{-1}B$) along

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- PVL applies w/o changes for singular E if $s_0 \notin \Lambda(A, E)$:
  - for $s_0 \neq \infty$: Gallivan/Grimme/Van Dooren 1994, Freund/Feldmann 1996, Grimme 1997
  - for $s_0 = \infty$: B./Sokolov 2005

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- Good approximation quality only locally.
- Preservation of physical properties only in very special cases; usually requires post processing which (partially) destroys moment matching properties.

Balanced Truncation

Idea:

- 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 $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_n > 0$.

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- Compute balanced realization of the system via state-space transformation

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

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- Truncation $\rightsquigarrow (\widehat{A}, \widehat{B}, \widehat{C}, \widehat{D}) = (A_{11}, B_1, C_1, D)$.

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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

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$$E := \sup_{\substack{u \in L_2(-\infty,0] \\ x(0)=x_0}} \frac{\int\limits_0^\infty y(t)^T y(t)\, dt}{\int\limits_{-\infty}^0 u(t)^T u(t)\, dt} = \frac{1}{\|x_0\|_2} \sum_{j=1}^n \sigma_j^2 x_{0,j}^2$$

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

$\Longrightarrow$ complete analogy to best approximation via SVD!

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- Several related methods by variation of Gramians for
  - closed-loop model reduction (LQG balancing),
  - minimum-phase preservation (balanced stochastic truncation),
  - passivity preservation (positive-real balanced truncation).

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

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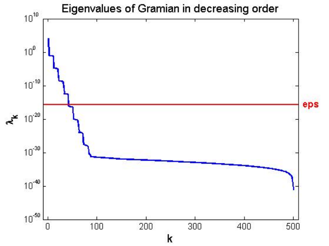
New algorithmic ideas from numerical linear algebra:

- Instead of Gramians P, Q compute $\widehat{S}, \widehat{R} \in \mathbb{R}^{n \times k}$, $k \ll n$, such that

$$P \approx \widehat{S}\widehat{S}^T, \quad Q \approx \widehat{R}\widehat{R}^T.$$

- Compute $\widehat{S}, \widehat{R}$ with problem-specific Lyapunov solvers of "low" complexity directly.



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New algorithmic ideas from numerical linear algebra:

Parallelization:

- Efficient parallel algorithms based on matrix sign function.
- Complexity $\mathcal{O}(n^3/q)$ on q-processor machine.
- Software library PLiCMR with WebComputing interface.

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Formatted Arithmetic:

For special problems from PDE control use implementation based on hierarchical matrices and matrix sign function method (Baur/B.), complexity $\mathcal{O}(n \log^2(n) r^2)$.

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New algorithmic ideas from numerical linear algebra:

Sparse Balanced Truncation:

- Sparse implementation using sparse Lyapunov solver (ADI+MUMPS/SuperLU).
- Complexity $\mathcal{O}(n(k^2 + r^2))$.
- Software:
  + MATLAB toolbox LYAPACK (PENZL 1999),
  + Software library SPARED with WebComputing interface.
    (BADÍA/B./QUINTANA-ORTÍ/QUINTANA-ORTÍ since 2003)

Comparison

Why is Balanced Truncation Superior?

Consider the approximation problem:

project x onto r-dim. subspace $\mathcal{V} \subset \mathbb{R}^n$ such that $\|x - V\hat{x}\| = \min!$

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Consequence: BT often needs the least states for a prescribed accuracy/yields the best accuracy for a prescribed number of states.

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Why is Balanced Truncation Not Always Superior?

Consider the approximation problem:

project x onto r-dim. subspace $\mathcal{V} \subset \mathbb{R}^n$ such that $\|x - V\hat{x}\| = \min!$

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- PVL pre-selects a "good" subspace by picking the expansion points close to assumed operating frequency.
- Balanced truncation aims at global minimization and thereby sometimes neglects local features.

Examples

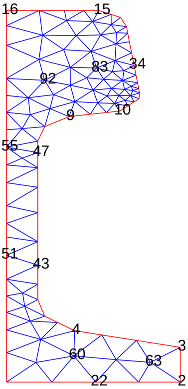
Optimal Control: Cooling of Steel Profiles

- Mathematical model: boundary control for linearized 2D heat equation.

$$
\begin{aligned}
c \cdot \rho \frac{\partial}{\partial t} x &= \lambda \Delta x, && \xi \in \Omega \\
\lambda \frac{\partial}{\partial n} x &= u_k - x, && \xi \in \Gamma_k, \ 1 \leq k \leq 7, \\
\frac{\partial}{\partial n} x &= 0, && \xi \in \Gamma_7.
\end{aligned}
$$

$\Longrightarrow m = 7, p = 6.$

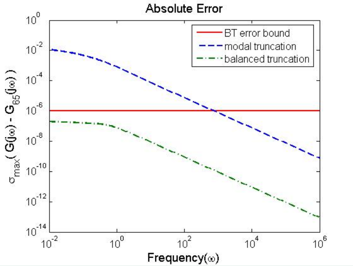
- FEM Discretization, different models for initial mesh ($n = 371$), 1, 2, 3, 4 steps of mesh refinement $\Rightarrow$ $n = 1357, 5177, 20209, 79841$.



Source: Physical model: courtesy of Mannesmann/Demag.

Math. model: Tröltzsch/Unger 1999/2001, Penzl 1999, Saak 2003.

$n = 1357$, Absolute Error



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- MT w/o static condensation, same order as BT model.

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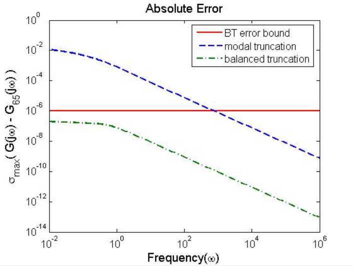

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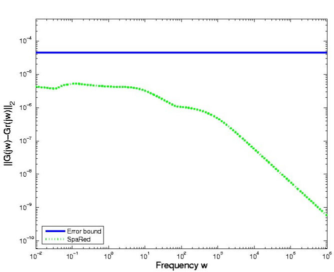
$n = 79841$, Absolute error

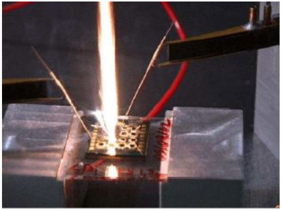


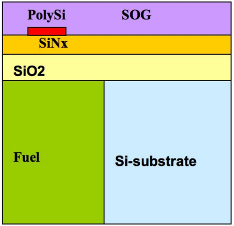
- BT model computed using SpaRed,
- computation time: 8 min.

Examples

MEMS: Microthruster

- Co-integration of solid fuel with silicon micromachined system.
- Goal: Ignition of solid fuel cells by electric impulse.
- Application: nano satellites.
- Thermo-dynamical model, ignition via heating an electric resistance by applying voltage source.
- Design problem: reach ignition temperature of fuel cell w/o firing neighbouring cells.
- Spatial FEM discretizatoin of thermo-dynamical model $\rightsquigarrow$ linear system, $m = 1$, $p = 7$.





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

Courtesy of C. Rossi, LAAS-CNRS/EU project "Micropyros".

Examples

MEMS: Microthruster

- axial-symmetric 2D model
- FEM discretisation using linear elements $\rightsquigarrow$ $n = 4,257$, $m = 1$, $p = 7$.
- Reduced model computed using SpaRed and Arnoldi(A, B).
- Order of reduced model: $r = 30$ ($r = 120$ for Arnoldi).

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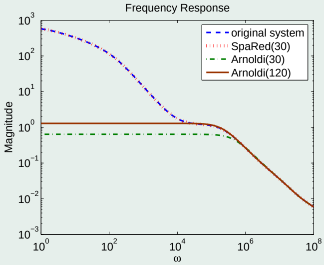
Frequency Response Analysis



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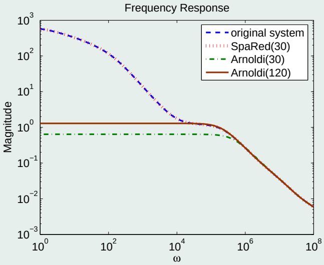
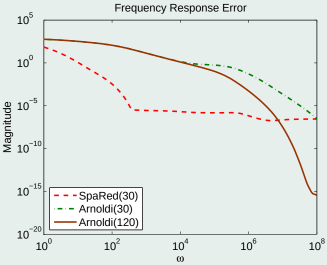
MEMS: Microthruster

- axial-symmetric 2D model
- FEM discretisation using linear elements $\rightsquigarrow$ $n = 4,257$, $m = 1$, $p = 7$.
- Reduced model computed using SpaRed and Arnoldi(A, B).
- Order of reduced model: $r = 30$ ($r = 120$ for Arnoldi).

Frequency Response Analysis



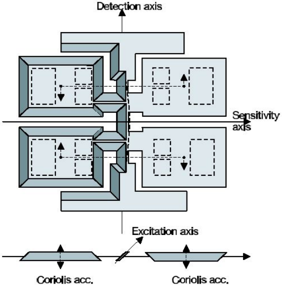
Absolute error



Examples
MEMS: Microgyroscope (Butterfly Gyro)

- By applying AC voltage to electrodes, wings are forced to vibrate in anti-phase in wafer plane.
- Coriolis forces induce motion of wings out of wafer plane yielding sensor data.

- Vibrating micro-mechanical gyroscope for inertial navigation.
- Rotational position sensor.



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

Courtesy of D. Billger (Imego Institute, Göteborg), Saab Bofors Dynamics AB.

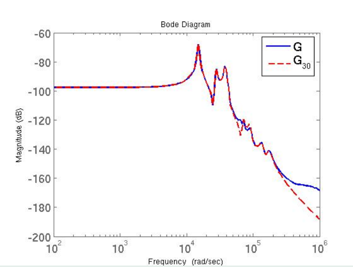
Examples

MEMS: Butterfly Gyro

- FEM discretization of structure dynamical model using quadratic tetrahedral elements (ANSYS-SOLID187)
  $\rightsquigarrow$ $n = 34,722$, $m = 1$, $p = 12$.
- Reduced model computed using SPARED, $r = 30$.

- FEM discretization of structure dynamical model using quadratic tetrahedral elements (ANSYS-SOLID187)
  $\rightsquigarrow$ $n = 34,722,\ m = 1,\ p = 12$.
- Reduced model computed using SpaRed, $r = 30$.

Frequency Repsonse Analysis



- FEM discretization of structure dynamical model using quadratic tetrahedral elements (ANSYS-SOLID187)
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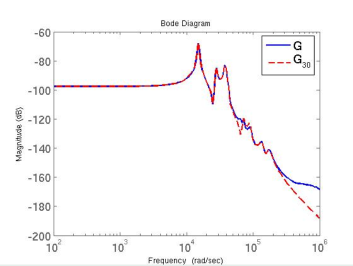
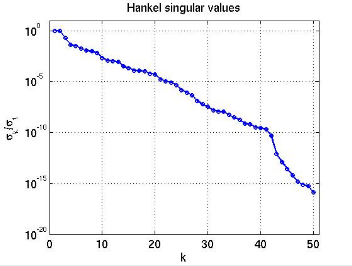
Frequency Repsonse Analysis



Hankel Singular Values



Parametric Models

$$\dot{x} = A(p)x + B(p)u, \quad y = C(p)x + D(p)u,$$

where $p \in \mathbb{R}^s$ are free parameters which should be preserved in the reduced-order model.

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- Frequently: B, C, D parameter independent,

$$A(p) = A_0 + p_1 A_1 + \ldots + p_s A_s.$$

  $\Rightarrow$ (Modified) linear model reduction methods applicable.

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- Multipoint expansion combined with Padé-type approx. possible.
- New idea: BT for reference parameters combined with interpolation yields parametric reduced-order models.

Current and Future Work

Parametric Models

Nonlinear Systems

- Linear projection

$$x \approx V\widehat{x}, \quad \dot{\widehat{x}} = W^T f(V\widehat{x}, u)$$

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Parametric Models

Nonlinear Systems

- Linear projection

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  is in general not model reduction!
- Need specific methods
  - POD + balanced truncation $\rightsquigarrow$ empirical Gramians (LALL/MARSDEN/GLAVASKI 1999/2002),
  - Approximate inertial manifold method ($\sim$ static condensation for nonlinear systems).

Parametric Models
Nonlinear Systems

- Linear projection

$$x \approx V\widehat{x}, \quad \dot{\widehat{x}} = W^T f(V\widehat{x}, u)$$

is in general not model reduction!

- Exploit structure of nonlinearities, e.g., in optimal control of linear PDEs with nonlinear BCs $\rightsquigarrow$
  - bilinear control systems $\dot{x} = Ax + \sum_j N_j x u_j + Bu$,
  - formal linear systems (cf. FÖLLINGER 1982)

$$\dot{x} = Ax + N\,g(Hx) + Bu = Ax + \begin{bmatrix} B & N \end{bmatrix} \begin{bmatrix} u \\ g(z) \end{bmatrix},$$

where $z := Hx \in \mathbb{R}^\ell$, $\ell \ll n$.

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Thanks for getting up early!