

SYSTEM-THEORETIC METHODS FOR MODEL REDUCTION OF LARGE-SCALE SYSTEMS: SIMULATION, CONTROL, AND INVERSE PROBLEMS

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Overview

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- Balancing Basics
- Balanced Truncation and Relatives
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3 Numerical Examples

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- Control

4 Conclusions and Outlook

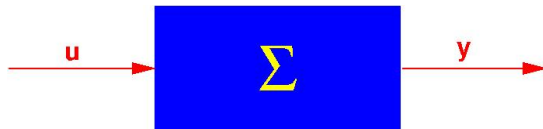
Dynamical Systems

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

with

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

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



Original System

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Reduced-Order System

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

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

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

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Linear, Time-Invariant (LTI) / Descriptor Systems

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

Laplace Transformation / Frequency Domain

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

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

yields I/O-relation in frequency domain:

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

G is the transfer function of Σ .



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G is the **transfer function** of Σ .

Problem

Approximate the dynamical system

$$\begin{aligned} E\dot{x} &= Ax + Bu, & A, E &\in \mathbb{R}^{n \times n}, & B &\in \mathbb{R}^{n \times m}, \\ y &= Cx + Du, & C &\in \mathbb{R}^{p \times n}, & D &\in \mathbb{R}^{p \times m}, \end{aligned}$$

by reduced-order system

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

of order $r \ll n$, such that

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

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

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Here:

- **linear** systems,
- $n \gg m, p$,
- n so large, that $A(, E)$ cannot be stored in main memory (RAM) as $n \times n$ array: $n > 5000$, say, e.g., from
 - semi-discretization of PDEs,
 - finite element modeling of MEMS,
 - VLSI design/circuit simulation, . . .
- $A(, E)$ **sparse or data-sparse**, i.e., $A(, E)$ can be stored in $\mathcal{O}(n)$ or $\mathcal{O}(n \log n)$ memory locations, but matrix manipulations like similarity transformations are too expensive (possible exception: permutations, sparse factorizations).



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Time-domain simulation

Evaluation of **variation-of-constants formula**

$$y(t) = C \exp(At) \left(x^0 + \int_0^t \exp(-A\tau) B u(\tau) d\tau \right),$$

usually too expensive \rightsquigarrow **numerical simulation**, e.g., using backwards Euler

$$y_h(t_{k+1}) = C(E - h_k A)^{-1} (E x_h(t_k) + h_k B u(t_{k+1})) + D u(t_{k+1}),$$

Bottleneck: solution of $(E - h_k A)z = b$, computation time can be significantly reduced by using reduced-order model:

$$\hat{y}_h(t_{k+1}) = \hat{C}(\hat{E} - h_k \hat{A})^{-1} (\hat{E} x_h(t_k) + h_k \hat{B} u(t_{k+1})) + \hat{D} u(t_{k+1}).$$



Frequency-domain simulation

Frequency response analysis, e.g., for Bode, Nyquist or Nichols plots, requires evaluation of transfer function

$$G(j\omega_k) = C(j\omega_k E - A)^{-1}B + D, \quad \omega_k \geq 0, \quad k = 1, \dots, N_f.$$

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But: the cost for solving the linear systems in time/frequency domain simulation may not benefit from smaller order, if efficient sparse direct solver for full-size sparse system matrices is available.

An easy improvement

Significant reduction can be achieved by transforming (\hat{A}, \hat{E}) to Hessenberg-triangular form using QZ algorithm, i.e., compute orthogonal Q, Z such that

$$Q(\lambda \hat{E} - \hat{A})Z = \lambda \begin{bmatrix} \diagdown & & \\ & \diagdown & \\ & & \diagdown \end{bmatrix} - \begin{bmatrix} \diagdown & & \\ & \diagdown & \\ & & \diagdown \end{bmatrix} \equiv \begin{bmatrix} \diagdown & & \\ & \diagdown & \\ & & \diagdown \end{bmatrix}.$$

New reduced-order system: $(Q\hat{E}Z, Q\hat{A}Z, Q\hat{B}, \hat{C}Z)$, linear systems of equations

$$\begin{aligned} (j\omega \hat{E} - \hat{A})x &= b, \\ (\hat{E} - h_k \hat{A})x_{k+1} &= \hat{E}x_k + \dots, \quad \text{etc.} \end{aligned}$$

have Hessenberg form **and can thus be solved using $r - 1$ Givens rotations only!** (Needs Hessenberg solver inside simulator.)

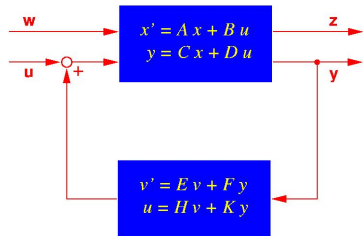
For symmetric systems, further reduction can be achieved.

Feedback Controllers

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

- input = output of plant,
- output = input of plant.

Modern (LQG-/ \mathcal{H}_2 -/ \mathcal{H}_∞ -) control design: $N \geq n$.



Practical controllers require small N ($N \sim 10$, say) due to

- real-time constraints,
- increasing fragility for larger N .

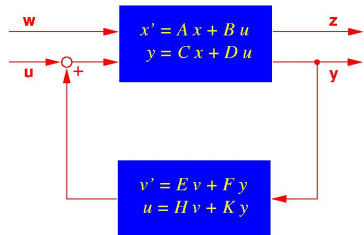
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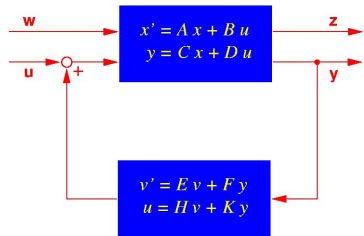
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Inverse Problems

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System inversion

Assume $m = p$, $D \in \mathbb{R}^{m \times m}$ invertible (generalizations possible!), then

$$G^{-1}(s) = -D^{-1}C(sE - (A - BD^{-1}C))^{-1}BD^{-1} + D^{-1}.$$

Some applications like

- inverse-based control,
- identification of source terms,

reconstruct input function from reference trajectory/measured outputs: given $Y(s)$, the Laplace transform of $y(t)$, compute $U(s) = G^{-1}(s)Y(s)$.

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Goal: reduced-order transfer function $\hat{G}(s)$ such that

$$\hat{U}(s) = \hat{G}^{-1}(s)Y(s)$$

has small error

$$\|U - \hat{U}\| = \|G^{-1}Y - \hat{G}^{-1}Y\| \leq \|G^{-1} - \hat{G}^{-1}\| \|Y\| \leq \text{tolerance} \cdot \|Y\|.$$

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

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

⇒ 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”),

All this can be achieved by system-theoretic methods based on balancing!



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Balancing Basics

($E = I_n$ for ease of notation)

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(A, B, C, D) is a realization of Σ (**nonunique**).

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Model Reduction Based on Balancing

Given $P, Q \in \mathbb{R}^{n \times n}$ symmetric positive definite (spd), and a **contragredient transformation** $T: \mathbb{R}^n \rightarrow \mathbb{R}^n$,

$$TPT^T = T^{-T}QT^{-1} = \text{diag}(\sigma_1, \dots, \sigma_n), \quad \sigma_1 \geq \dots \geq \sigma_n \geq 0.$$

Balancing Σ w.r.t. P, Q :

$$\Sigma \equiv (A, B, C, D) \mapsto (TAT^{-1}, TB, CT^{-1}, D) \equiv \Sigma.$$

Generalization to $P, Q \geq 0$ possible: if \hat{n} is McMillan degree of Σ , then

$$T(PQ)T^{-1} = \text{diag}(\sigma_1, \dots, \sigma_{\hat{n}}, 0, \dots, 0).$$

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Basic Model Reduction Procedure

- 1 Given $\Sigma \equiv (A, B, C, D)$ and balancing (w.r.t. given P, Q spd) transformation $T \in \mathbb{R}^{n \times n}$ nonsingular, compute

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

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Implementation: SR Method

- 1 Compute **Cholesky** (square) or **full-rank** (maybe rectangular, "thin") factors of P, Q

$$P = S^T S, \quad Q = R^T R.$$

- 2 Compute SVD

$$SR^T = [U_1, U_2] \begin{bmatrix} \Sigma_1 & \\ & \Sigma_2 \end{bmatrix} \begin{bmatrix} V_1^T \\ V_2^T \end{bmatrix}.$$

- 3 Set

$$W = R^T V_1 \Sigma_1^{-1/2}, \quad V = S^T U_1 \Sigma_1^{-1/2}.$$

- 4 Reduced-order model is

$$(\hat{A}, \hat{B}, \hat{C}, \hat{D}) := (W^T A V, W^T B, C V, D) \quad (\equiv (A_{11}, B_1, C_1, D).)$$

Implementation: SR Method

- 1 Compute **Cholesky** (square) or **full-rank** (maybe rectangular, "thin") factors of P, Q

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- 2 Compute SVD

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Balancing for Simulation, Control

Truncate realization, balanced w.r.t. $P = Q = \text{diag}(\sigma_1, \dots, \sigma_n) = \Sigma$,
 $\sigma_1 \geq \dots \geq \sigma_r > \sigma_{r+1} \geq \dots \sigma_n \geq 0$ at size r .

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Classical Balanced Truncation (BT)

MULLIS/ROBERTS '76, MOORE '81

- P/Q = controllability/observability Gramian of $\Sigma \equiv (A, B, C, D)$.
- For asymptotically stable systems, P, Q solve dual **Lyapunov equations**

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

- $\{\sigma_1^{\text{BT}}, \dots, \sigma_n^{\text{BT}}\}$ are the Hankel singular values (HSVs) of Σ .
- Preserves stability, extends to unstable systems w/o purely imaginary poles using frequency domain definition of the Gramians [ZHOU/SALOMON/WU '99].
- Preserves passivity for certain symmetric systems.
- Computable error bound comes for free:

$$\|G - \hat{G}^{\text{BT}}\|_{H_\infty} \leq 2 \sum_{j=r+1}^n \sigma_j^{\text{BT}},$$

allows adaptive choice of r !



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Linear-Quadratic Gaussian Balanced Truncation (LQGBT)

JONCKHEERE/SILVERMAN '83

- P/Q = controllability/observability Gramian of closed-loop system based on LQG compensator.

- P, Q solve dual **algebraic Riccati equations (AREs)**

$$0 = AP + PA^T - PC^T CP + B^T B,$$

$$0 = A^T Q + QA - QBB^T Q + C^T C.$$

- Applies to unstable systems!
(Only stabilizability & detectability are required.)
- Computable error bound comes for free: if $G = M^{-1}N$, $\hat{G} = \hat{M}^{-1}\hat{N}$ are left coprime factorizations with stable factors, then

$$\| [N \ M] - [\hat{N} \ \hat{M}] \|_{H_\infty} \leq 2 \sum_{j=r+1}^n \sigma_j^{\text{LQG}} \left(1 + (\sigma_j^{\text{LQG}})^2 \right)^{\frac{1}{2}},$$

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- Yields reduced-order LQR/LQG controller for free!



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Positive-Real Balanced Truncation (PRBT)

GREEN '88

- Based on positive-real equations, related to positive real (Kalman-Yakubovich-Popov-Anderson) lemma.
- For $m = p$, P, Q solve dual AREs

$$\begin{aligned} 0 &= \bar{A}P + P\bar{A}^T + PC^T\bar{R}^{-1}CP + B\bar{R}^{-1}B^T, \\ 0 &= \bar{A}^TQ + Q\bar{A} + QB\bar{R}^{-1}B^TQ + C^T\bar{R}^{-1}C, \end{aligned}$$

where $\bar{R} = D + D^T$, $\bar{A} = A - B\bar{R}^{-1}C$.

- Preserves stability, strict passivity; needs stability of \bar{A} .
- Computable error bound [GUGERCIN/ANTOULAS '03, B. '05]:

$$\|G - \hat{G}^{\text{PR}}\|_{H_\infty} \leq 2\|R\|^2\|\hat{G}_D\|_\infty\|G_D\|_\infty \sum_{k=r+1}^n \sigma_k^{\text{PR}}.$$

$$(G_D(s) := G(s) + D^T, \hat{G}_D(s) := \hat{G}(s) + D^T.)$$



Balancing for Simulation of Passive Systems

Truncate realization, balanced w.r.t. $P = Q = \text{diag}(\sigma_1, \dots, \sigma_n) = \Sigma$,
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Balancing for Control, Simulation, Inverse Problems

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Balanced Stochastic Truncation (BST)

DESAI/PAL '84, GREEN '88

- P = controllability Gramian of $\Sigma \equiv (A, B, C, D)$, i.e., solution of Lyapunov equation $AP + PA^T + BB^T = 0$.
- Q = observability Gramian of right spectral factor of power spectrum of Σ , i.e., solution of ARE

$$A_W^T Q + QA_W + QB_W(DD^T)^{-1}B_W^T Q + C^T(DD^T)^{-1}C = 0,$$

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- **Preserves stability**; needs stability of A_W .
- Computable relative error bound [GREEN '88]:

$$\|\Delta^{\text{BST}}\|_{H_\infty} = \|G^{-1}(G - \hat{G}^{\text{BST}})\|_{H_\infty} \leq \prod_{j=r+1}^n \frac{1 + \sigma_j^{\text{BST}}}{1 - \sigma_j^{\text{BST}}} - 1,$$

\rightsquigarrow uniform approximation quality over full frequency range.

Note: $|\sigma_j^{\text{BST}}| \leq 1$.



Balancing for Control, Simulation, Inverse Problems

Truncate realization, balanced w.r.t. $P = Q = \text{diag}(\sigma_1, \dots, \sigma_n) = \Sigma$,
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- Zeros of $G(s)$ are preserved in $\hat{G}(s)$. \implies
 $G(s)$ minimum-phase $\implies \hat{G}(s)$ minimum-phase.
- Error bound for inverse system [B. '03]
If $G(s)$ is square, minimal, stable, minimum-phase, nonsingular on $j\mathbb{R}$, then

$$\|G^{-1} - \hat{G}^{-1}\|_{H_\infty} \leq \left(\prod_{j=r+1}^n \frac{1 + \sigma_j^{\text{BST}}}{1 - \sigma_j^{\text{BST}}} - 1 \right) \|\hat{G}^{-1}\|_{H_\infty}.$$



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Basic Principle of Balanced Truncation

Given positive semidefinite matrices $P = S^T S$, $Q = R^T R$, compute balancing state-space transformation so that

$$P = Q = \text{diag}(\sigma_1, \dots, \sigma_n) = \Sigma, \quad \sigma_1 \geq \dots \geq \sigma_n \geq 0,$$

and truncate corresponding realization at size r with $\sigma_r > \sigma_{r+1}$.

Other Balancing-Based Methods

- Bounded-real balanced truncation (BRBT) – based on bounded real lemma [OPDENACKER/JONCKHEERE '88];
- H_∞ balanced truncation (HinfBT) – closed-loop balancing based on H_∞ compensator [MUSTAFA/GLOVER '91].

Both approaches require solution of dual AREs.

- Frequency-weighted versions of the above approaches.



Balanced Truncation and Relatives

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All balancing-related methods have nice theoretical properties that make them appealing for applications in simulation, control, optimization, inverse problems.

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All balancing-related methods have nice theoretical properties that make them appealing for applications in simulation, control, optimization, inverse problems.

But: computationally demanding w.r.t. to memory and CPU time; need efficient solvers for linear (Lyapunov) and nonlinear (Riccati) matrix equations!

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

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

$$0 = \mathcal{R}(Q) := A^T Q + QA - QGQ + W.$$

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

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

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

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

$$0 = \mathcal{R}(Q) := A^T Q + QA - QGQ + W.$$

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

- $n = 10^3 - 10^6$ ($\implies 10^6 - 10^{12}$ unknowns!),
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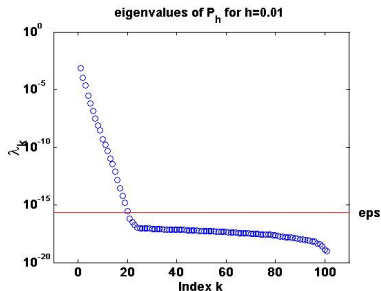
Consider spectrum of ARE solution (analogous for Lyapunov equations).

Example:

- Linear 1D heat equation with point control,
- $\Omega = [0, 1]$,
- FEM discretization using linear B-splines,
- $h = 1/100 \implies n = 101$.

Idea: $Q = Q^T \geq 0 \implies$

$$Q = ZZ^T = \sum_{k=1}^n \lambda_k z_k z_k^T \approx Z^{(r)} (Z^{(r)})^T = \sum_{k=1}^r \lambda_k z_k z_k^T.$$



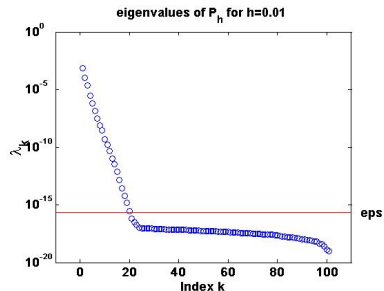
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$$AX + XA^T = -BB^T.$$

- ADI Iteration:** [WACHSPRESS 1988]

$$(A + p_k I)X_{(j-1)/2} = -BB^T - X_{k-1}(A^T - p_k I)$$

$$(A + \bar{p}_k I)X_k^T = -BB^T - X_{(j-1)/2}(A^T - \bar{p}_k I)$$

with parameters $p_k \in \mathbb{C}^-$ and $p_{k+1} = \bar{p}_k$ if $p_k \notin \mathbb{R}$.

- For $X_0 = 0$ and proper choice of p_k : $\lim_{k \rightarrow \infty} X_k = X$ superlinear.
- Re-formulation using $X_k = Y_k Y_k^T$ yields iteration for $Y_k \dots$

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Factored ADI Iteration

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

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

Algorithm [PENZL '97/'00, LI/WHITE '99/'02, B. 04, B./LI/PENZL '99/'08]

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

FOR $j = 2, 3, \dots$

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

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

$$Y_k \leftarrow \operatorname{rrlq}(Y_k, \tau) \quad \% \text{ column compression}$$

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

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

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



Factored ADI Iteration

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

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

- 1 Compute orthonormal basis 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 $m = 1$:

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

[JAIMOUKHA/KASENALLY '94, JBILOU '02-'08].

- K-PIK [SIMONCINI '07],

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Factored Galerkin-ADI Iteration

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

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Examples:

- ADI subspace [B./R.-C. LI/TRUHAR '08]:

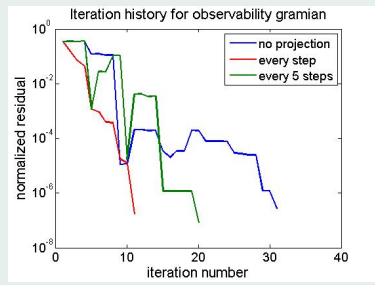
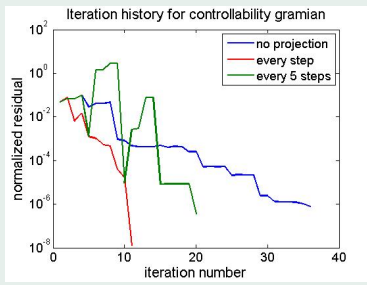
$$\mathcal{Z} = \text{colspan} [V_1, \dots, V_r] .$$

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

FEM semi-discretized control problem for parabolic PDE:

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

Good ADI shifts

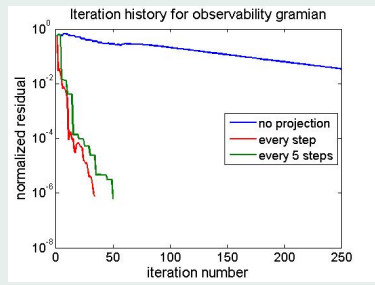
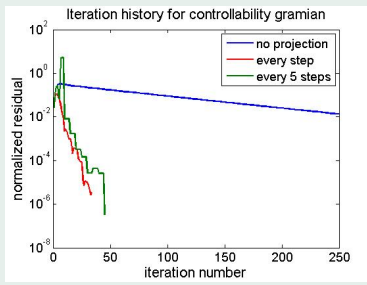


CPU times: 80s (projection every 5th ADI step) vs. 94s (no projection).

FEM semi-discretized control problem for parabolic PDE:

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

Bad ADI shifts



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



Newton's Method for AREs

[KLEINMAN '68, MEHRMANN '91, LANCASTER/RODMAN '95,
B./BYERS '94/'98, B. '97, GUO/LAUB '99]

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- Consider $0 = \mathcal{R}(Q) = C^T C + A^T Q + QA - QBB^T Q$.
- Fréchet derivative of $\mathcal{R}(Q)$ at Q :

$$\mathcal{R}'_Q : Z \rightarrow (A - BB^T Q)^T Z + Z(A - BB^T Q).$$

- Newton-Kantorovich method:

$$Q_{j+1} = Q_j - \left(\mathcal{R}'_{Q_j}\right)^{-1} \mathcal{R}(Q_j), \quad j = 0, 1, 2, \dots$$

Newton's method (with line search) for AREs

FOR $j = 0, 1, \dots$

1 $A_j \leftarrow A - BB^T Q_j =: A - BK_j.$

2 Solve the Lyapunov equation $A_j^T N_j + N_j A_j = -\mathcal{R}(Q_j).$

3 $Q_{j+1} \leftarrow Q_j + t_j N_j.$

END FOR j



Newton's Method for AREs

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Re-write Newton's method for AREs

$$A_j^T N_j + N_j A_j = -\mathcal{R}(Q_j)$$

$$\iff$$

$$A_j^T \underbrace{(Q_j + N_j)}_{=Q_{j+1}} + \underbrace{(Q_j + N_j)}_{=Q_{j+1}} A_j = \underbrace{-C^T C - Q_j B B^T Q_j}_{=: -W_j W_j^T}$$

Set $Q_j = Z_j Z_j^T$ for $\text{rank}(Z_j) \ll n \implies$

$$A_j^T (Z_{j+1} Z_{j+1}^T) + (Z_{j+1} Z_{j+1}^T) A_j = -W_j W_j^T$$

Factored Newton Iteration [B./LI/PENZL '99/'08]

Solve Lyapunov equations for Z_{j+1} directly by factored ADI iteration and use 'sparse + low-rank' structure of A_j .



Low-Rank Newton-ADI for AREs

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Re-write Newton's method for AREs

$$A_j^T N_j + N_j A_j = -\mathcal{R}(Q_j) \\ \iff$$

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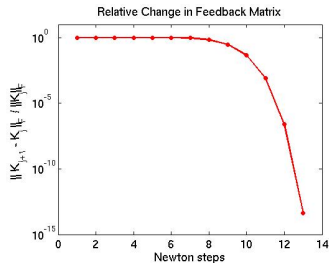
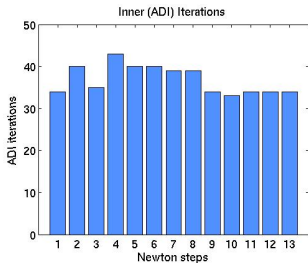
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Solve Lyapunov equations for Z_{j+1} directly by factored ADI iteration and use 'sparse + low-rank' structure of A_j .

- Linear 2D heat equation with homogeneous Dirichlet boundary and point control/observation.
- FD discretization on uniform 150×150 grid.
- $n = 22,500$, $m = p = 1$, 10 shifts for ADI iterations.
- Convergence of large-scale matrix equation solvers:



Performance of Newton's method for accuracy $\sim 1/n$

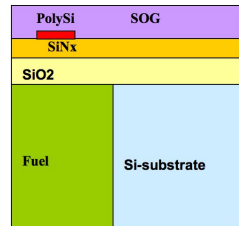
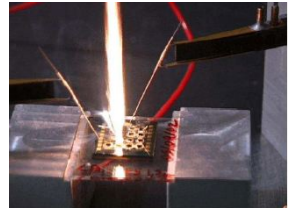
| grid | unknowns | $\frac{\ \mathcal{R}(P)\ _F}{\ P\ _F}$ | it. (ADI it.) | CPU (sec.) |
|------------------|-------------|--|---------------|------------|
| 8×8 | 2,080 | $4.7e-7$ | 2 (8) | 0.47 |
| 16×16 | 32,896 | $1.6e-6$ | 2 (10) | 0.49 |
| 32×32 | 524,800 | $1.8e-5$ | 2 (11) | 0.91 |
| 64×64 | 8,390,656 | $1.8e-5$ | 3 (14) | 7.98 |
| 128×128 | 134,225,920 | $3.7e-6$ | 3 (19) | 79.46 |

Here,

- Convection-diffusion equation,
- $m = 1$ input and $p = 2$ outputs,
- $P = P^T \in \mathbb{R}^{n \times n} \Rightarrow \frac{n(n+1)}{2}$ unknowns.

Confirms mesh independence principle for Newton-Kleinman
[Burns/Sachs/Zietsmann 2006].

- Co-integration of solid fuel with silicon micro-machined 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 neighboring cells.
- Spatial FEM discretization of thermo-dynamical model \rightsquigarrow linear system, $m = 1$, $p = 7$.



Source: The Oberwolfach Benchmark Collection <http://www.intek.de/simulation/benchmark>

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



Numerical Examples: Simulation

Microthruster (MEMS)

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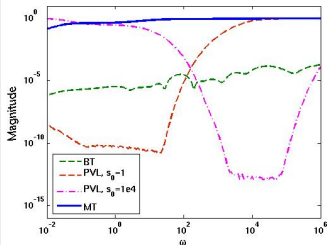
Simulation
Control

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- axial-symmetric 2D model
- FEM discretization using linear (quadratic) elements $\rightsquigarrow n = 4,257$ (11,445) $m = 1$, $p = 7$.
- Reduced model computed using SPARED, modal truncation using ARPACK, and Z. Bai's PVL implementation.

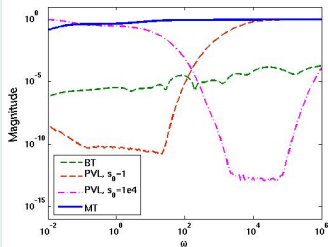
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Relative error $n = 4,257$

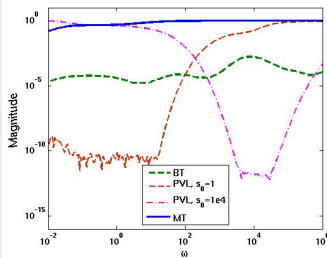


- axial-symmetric 2D model
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Relative error $n = 4, 257$

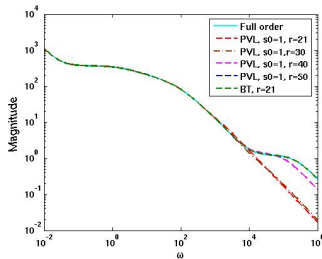


Relative error $n = 11, 445$



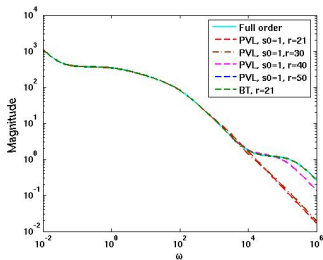
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Frequency Response BT/PVL

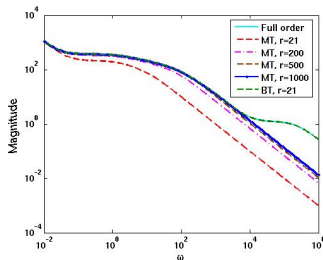


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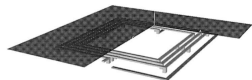
Frequency Response BT/PVL



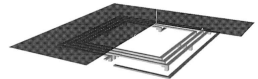
Frequency Response BT/MT



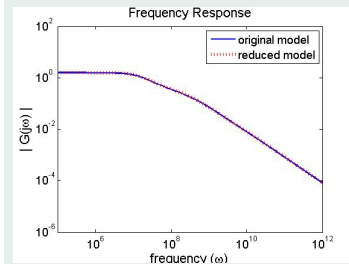
- Passive device used for RF filters etc.
- $n = 1,434$, $m = 1$, $p = 1$.



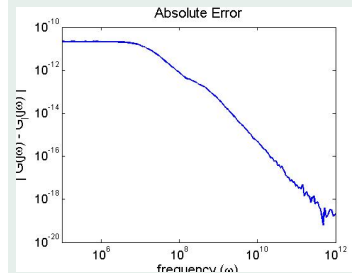
- Passive device used for RF filters etc.
- $n = 1,434$, $m = 1$, $p = 1$.
- Numerical rank of Gramians is 34/41.
- $r = 20$ passive model computed by PRBT (MORLAB).



Frequency Response Analysis



Absolute Error



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

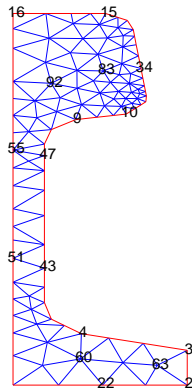
$$c \cdot \rho \frac{\partial}{\partial t} x = \lambda \Delta x, \quad \xi \in \Omega$$

$$\lambda \frac{\partial}{\partial n} x = \kappa (u_k - x), \quad \xi \in \Gamma_k, \quad 1 \leq k \leq 7,$$

$$\frac{\partial}{\partial n} x = 0, \quad \xi \in \Gamma_7.$$

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

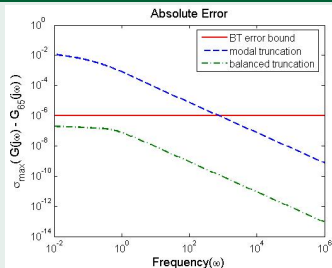
- FEM Discretization, different models for initial mesh ($n = 371$),
1, 2, 3, 4 steps of mesh refinement \implies
 $n = 1357, 5177, 20209, 79841$.



Source: Physical model: courtesy of Mannesmann/Demag.

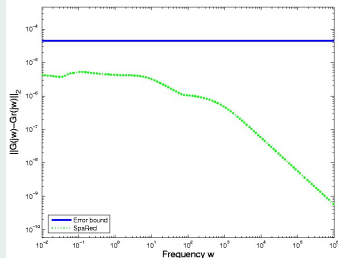
Math. model: TRÖLTZSCH/UNGER '99/'01, PENZL '99, SAAK '03.

$n = 1357$, Absolute Error



- BT model computed with sign function method,
- MT w/o static condensation, same order as BT model.

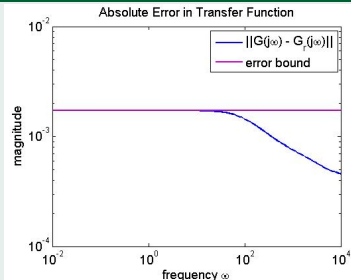
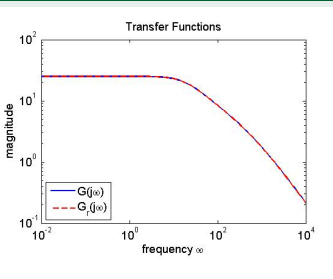
$n = 79841$, Absolute error



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

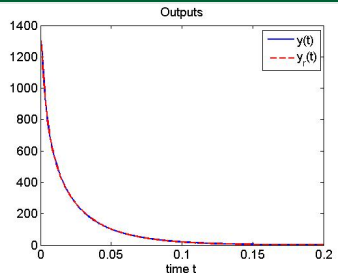
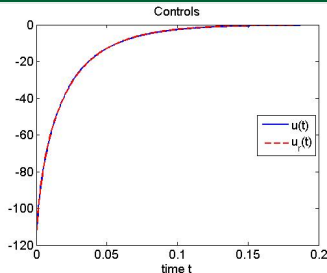
- FD discretized linear 2D heat equation with homogeneous Dirichlet boundary and point control/observation.
- $n = 22.500$, $m = p = 1$.
- Computed reduced-order model (BT): $r = 6$, BT error bound $\delta = 1.7 \cdot 10^{-3}$.
- Solve LQR problem: quadratic cost functional, solution is linear state feedback.

Transfer function approximation



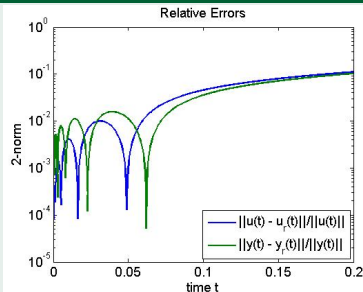
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Computed controls and outputs (implicit Euler)

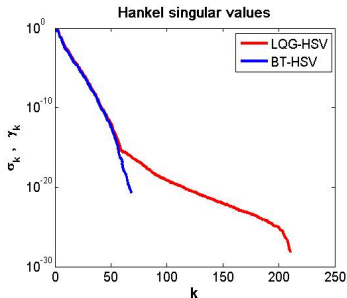


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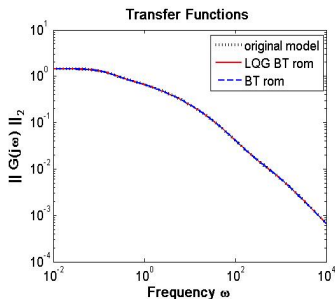
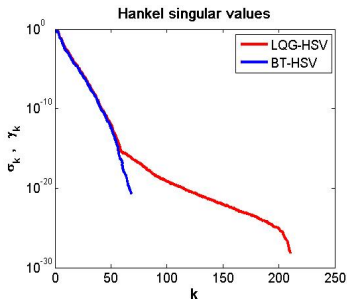
Errors in controls and outputs



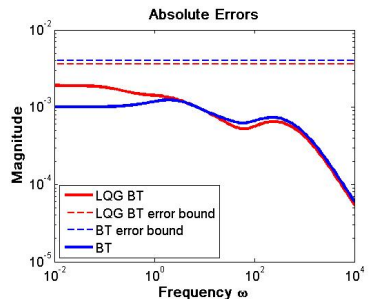
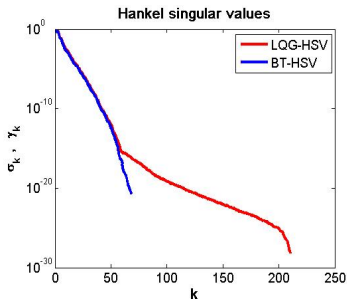
- Boundary control problem for 2D heat flow in copper on rectangular domain; control acts on two sides via Robins BC.
- FDM $\rightsquigarrow n = 4496$, $m = 2$; 4 sensor locations $\rightsquigarrow p = 4$.
- Numerical ranks of BT Gramians are 68 and 124, respectively, for LQG BT both have rank 210.
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- Main message:
Balanced truncation and family are applicable to large-scale systems.
(If efficient numerical algorithms are employed.)
- **Applications:** nanoelectronics, microsystems technology, optimal control, machine tool design, systems biology, ...
- Efficiency of numerical algorithms can be further enhanced, several details require deeper investigation.
- Algorithms for **data-sparse systems** using formatted arithmetic for \mathcal{H} -matrices [BAUR/B. '06/'08].
- Application to **2nd order systems** \rightsquigarrow talk of Jens Saak.
- Extension to **descriptor systems** possible.
[STYKEL SINCE '02, B. 03/'08, FREITAS/MARTINS/ROMMES '08,
HEINKENSCHLOSS/SORENSEN/SUN '06/'08].
- Combination of BT with sparse grid interpolation for **parametric model reduction** [BAUR/B. '08/'09].



Conclusions and Outlook

Model Reduction
of Large-Scale
Systems

Peter Benner

Introduction

System-Theoretic
Model Reduction

Numerical
Examples

Conclusions and
Outlook

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- **Applications:** nanoelectronics, microsystems technology, optimal control, machine tool design, systems biology, ...
- Efficiency of numerical algorithms can be further enhanced, several details require deeper investigation.
- Extension to **nonlinear systems** employing Carleman bilinearization and tensor product structure of Krylov subspaces in combination with **balanced truncation for bilinear systems** [B./Damm '09] quite promising, in particular for **polynomial nonlinearities** as often encountered in biological systems.
- Theory and numerical algorithm for application to **stochastic systems:** [B./Damm '09]; need algorithmic enhancements for really large-scale problems.

BMBF research network **SyreNe**



TU Berlin (*T. Stykel, A. Steinbrecher*)
 TU Braunschweig (*H. Faßbender, J. Amorcho, M. Bollhöfer, A. Eppler*)
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 U Hamburg (*M. Hinze, M. Vierling, M. Kunkel*)
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O-MOORE-NICE!

Operational model order reduction for nanoscale IC electronics

EU support via Marie Curie Host Fellowships for the Transfer of Knowledge (ToK) Industry-Academia Partnership Scheme.



TU Chemnitz (*P. Benner, M. Striebel*)

TU Eindhoven (*W. Schilders, D. Harutyunyan*)

U Antwerpen (*T. Dhaene, L. Di Tommasi*)

NXP Semiconductors (*J. ter Maten, J. Rommes*)



DFG Projects

- Automatic, Parameter-Preserving Model Reduction for Applications in Microsystems Technology.
Jointly with *Jan Gerrit Korvink* (IMTEK/U Freiburg and FRIAS).
- Integrated Simulation of the System "Machine Tool – Drive System – Stock Removal Process" Using Reduced-Order Structural FE Models.
Jointly with *Michael Zäh* (iwb/TU München) and *Heike Faßbender* (ICM/TU Braunschweig).