CONTROL OF COMPLEX DYNAMICAL SYSTEMS: Optimizing the Dynamics of Instationary Technical Processes

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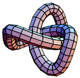

TECHNISCHE UNIVERSITÄT CHEMNITZ

Fakultät für Mathematik
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Overview

Introduction

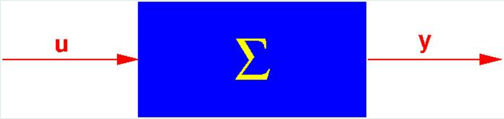
Optimization and control of instationary physical/technical processes require mathematical model:

Dynamical Systems

$$\Sigma(p) : \begin{cases} 0 = f(t, x(t), \partial_t x(t), \partial_{tt} x(t), u(t), p), \quad x(t_0) = x_0, & \text{(a)} \\ y(t) = g(t, x(t), \partial_t x(t), u(t), p) & \text{(b)} \end{cases}$$

with

- (generalized) states $x(t) \equiv x(t;p) \in \mathcal{X}$,
- inputs $u(t) \in \mathcal{U}$,
- outputs $y(t) \equiv y(t;p) \in \mathcal{Y}$, (b) is called output equation,
- $p \in \mathbb{R}^d$ is a parameter vector.



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(a) may represent

- system of ordinary differential equations (ODEs);
- system of differential-algebraic equations (DAEs);
- system of partial differential equations (PDEs);
- system of integro-differential equations,
- a mixture thereof.

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Optimization and control of instationary technical processes require:

- Mathematical Modeling
- Analysis of Dynamical Systems / Systems Theory
- Numerical Simulation
- Optimization / Optimal Control
- Control Theory
- Mathematical Software

Optimization and control of instationary technical processes require:

- Mathematical Modeling
- Analysis of Dynamical Systems / Systems Theory
  - robustness and stability analysis/margins,
  - infinite-dimensional systems and semigroups,
  - system norms,
  - descriptor systems.
- Numerical Simulation
- Optimization / Optimal Control
- Control Theory
- Mathematical Software

Optimization and control of instationary technical processes require:

- Mathematical Modeling
- Analysis of Dynamical Systems / Systems Theory
- Numerical Simulation
  - adaptive FEM,
  - hierarchical matrices,
  - methods for stiff ODEs and DAEs,
  - numerical linear algebra (preconditioning, eigenvalue problems),
  - parallel algorithms.
- Optimization / Optimal Control
- Control Theory
- Mathematical Software

Optimization and control of instationary technical processes require:

- Mathematical Modeling
- Analysis of Dynamical Systems / Systems Theory
- Numerical Simulation
- Optimization / Optimal Control
  - dynamic linear-quadratic optimization,
  - shape optimization.
- Control Theory
- Mathematical Software

Optimization and control of instationary technical processes require:

- Mathematical Modeling
- Analysis of Dynamical Systems / Systems Theory
- Numerical Simulation
- Optimization / Optimal Control
- Control Theory
  - LQR/LQG design,
  - robust stabilization,
  - model predictive control (MPC),
  - H_∞-control.
- Mathematical Software

Introduction

Mathematical ingredients / own research fields

Optimization and control of instationary technical processes require:

- Mathematical Modeling
- Analysis of Dynamical Systems / Systems Theory
- Numerical Simulation
- Optimization / Optimal Control
- Control Theory
- Mathematical Software
  - SLICOT (Subroutine Library in Control Theory), www.slicot.org;
  - M.E.S.S. (Matrix Equations Sparse Solvers), www.tu-chemnitz.de/mathematik/industrie_technik;
  - several control-related software packages for MATLAB and distributed-memory computing.

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- Numerical Simulation
- Optimization / Optimal Control
- Control Theory
- Mathematical Software

and, all-embracing and linking the above,

- **System Approximation / Model (Order) Reduction,**
  i.e., replacing the dynamical model by one of substantially lower dimensions in order to facilitate or even enable simulation, optimization, and control.

Feedback Control

Important observation

Optimized trajectory $x_*(t; u_*)$ and control $u_*(t)$ computed using optimization techniques ("open-loop") are not achieved in practice due to

- external disturbances,
- model uncertainties,
- modeling errors/unmodeled dynamics,
- measurement errors.

Consequence: Need feedback control ("closed-loop control")

$$u(t) = u_*(t) + U(t, x(t) - x_*(t)).$$

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Feedback Control

Example: optimal control of Burgers equation

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\begin{aligned}
\partial_t x(t,\xi) &= \nu\,\partial_{\xi\xi} x(t,\xi) - x(t,\xi)\,\partial_\xi x(t,\xi) + B(\xi)u(t) + F(\xi)v(t),\\
x(t,0) &= x(t,1) = 0, \quad x(0,\xi) = x_0(\xi) + \eta(\xi), \quad \xi \in (0,1),\\
y(t,\xi) &= C\,x(t,\xi) + w(t,\xi).
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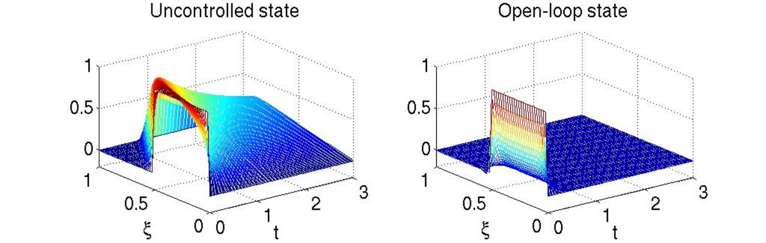

Supported by DFG grant BE3715/1-1 *Numerical Solution of Optimal Control Problems with Instationary Diffusion-Convection and Diffusion-Reaction Equations*.

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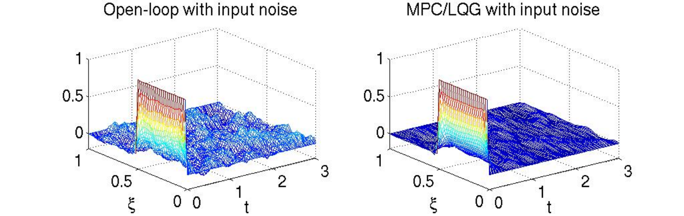
Feedback control using MPC-LQG scheme:



Reduction of tracking error $\int_0^T \|x(t) - x_*(t)\|_2^2\, dt$ by factor > 10.

[Benner/Görner, PAMM 2006]; [Benner/Görner/Saak, Springer LNCSE 2006].

Feedback Control

Computation of feedback operators requires (locally) the numerical solution of large-scale matrix equations:

- algebraic/differential Riccati equation (ARE/DRE) for $A \in \mathbb{R}^{n \times n}$, $B \in \mathbb{R}^{n \times m}$, $C \in \mathbb{R}^{p \times n}$ given and $X \in \mathbb{R}^{n \times n}$ unknown:

$$\left.\begin{array}{c} 0 \\ \dot{X} \end{array}\right\} = \mathcal{R}(X) := A^T X + XA - XBB^T X + C^T C.$$

- Lyapunov equation:

$$0 = \mathcal{L}(X) := A^T X + XA + W.$$

Feedback Control

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- algebraic/differential Riccati equation (ARE/DRE)
- Lyapunov equation:

Nowadays, can solve large-scale equations with $n = \mathcal{O}(10^6)$ ($\Rightarrow \mathcal{O}(10^{12}$ unknowns) on desktop computers due to sparsity- and structure-exploitation. Selected contributions:

1. Benner/Mehrmann/Xu, JCAM 1997 and NM 1998: invariant subspace method.
2. Benner/Byers, IEEE T-AC 1998: modified Newton's method, line search.
3. Benner/Quintana-Ortí, NA 1999: low-rank solution of Lyapunov equations.
4. Benner, IEEE CSM 2004: solving matrix equations for PDE control and MOR.
5. Benner/Mena, MTNS 2004: BDF methods for RDEs.
6. Baur/Benner, Computing 2006: use $\mathcal{H}$-matrices for solution of Lyapunov equations.
7. Benner/Li/Penzl, NLAA 2008: (Newton-)ADI for large-scale AREs, Lyapunov eqns.
8. Benner/Li/Truhar, submitted to JCAM: Galerkin-ADI for Lyapunov equations.
9. Benner/Mena, in preparation for SINUM: Rosenbrock methods for RDEs, convergence to ∞-dim. Riccati operator.

Model of chemical or biological reaction-diffusion process, here 3 substances or species c_i, $i = 1, 2, 3$ (only forward reaction $S_1 + S_2 \rightarrow S_3$; PDE for S_3 can be solved independently when c_1, c_2 are known):

Coupled system of reaction-diffusion equations:

$$\partial_t c_i(\xi, t) = D_i \Delta c_i(\xi, t) - k c_1(\xi, t) c_2(\xi, t), \quad i = 1, 2 \text{ on } \Omega \times (0, T).$$

Boundary conditions:

$$\begin{aligned} \frac{\partial}{\partial n} c_1(\xi, t) &= 0 \text{ on } \delta\Omega \times (0, T), \\ \frac{\partial}{\partial n} c_2(\xi, t) &= \begin{cases} 0 & \text{on} \quad (\delta\Omega \setminus \Omega_u) \times (0, T), \\ \alpha(\xi, t) u(t) & \text{on} \quad \Omega_u \times (0, T). \end{cases} \end{aligned}$$

Initial conditions: $c_1(\xi, 0) = c_{1,0}(\xi), \quad c_2(\xi, 0) = c_{2,0}(\xi).$

Goal: Complete reaction of S_1 in specified time with control constraint.

Supported by DFG grant BE3715/1-1 *Numerical Solution of Optimal Control Problems with Instationary Diffusion-Convection and Diffusion-Reaction Equations*.

- Pre-computed optimized control using prima-dual active set method [Griesse/Volkwein '05]; perturbation of plant model and initial states ⇝ optimized trajectory (production rate) is not achieved.
- Design nonlinear feedback, based on MPC-LQG idea [Ito/Kunisch '03/'06], but use time-varying linearizations (convergence proof/suboptimality estimate: [Benner/Hein '10]).

Results

[Benner/Hein, PAMM 2009]; submission to SICON in preparation.

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Goal:

Stabilization to steady-state solutions of flows (with velocity field v and pressure χ), described by Navier-Stokes equations

$$\partial_t v + v \cdot \nabla v - \frac{1}{Re}\Delta v + \nabla \chi = f \tag{1a}$$

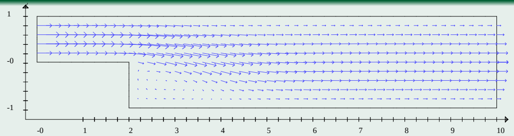
$$\operatorname{div} v = 0, \tag{1b}$$

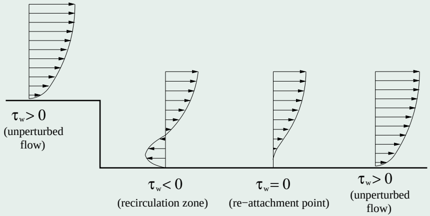
on $Q_\infty := \Omega \times (0, \infty)$, $\Omega \subseteq \mathbb{R}^d$, $d = 2, 3$ with smooth boundary $\Gamma := \partial\Omega$, and boundary and initial conditions

$$\begin{aligned} v &= g \quad \text{on } \Sigma_\infty := \Gamma \times (0, \infty), \\ v(0) &= w + z(0) \quad (w = \text{ given velocity field}). \end{aligned}$$

Supported by DFG SPP1253 grant BE2174/8-1,2 *Optimal Control-Based Feedback Stabilization of Multi-Field Flow Problems*.

Have:





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Motivating Examples from Current Projects
Feedback stabilization of flow problems

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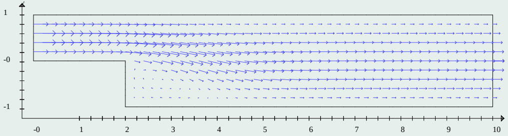

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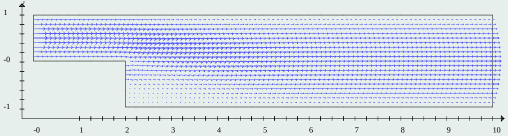

[Benner/Rothaug/Schneider 2008]: optimized trajectory/open-loop control computed with discrete adjoint technique.

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von Kármán vortex street

- $Re = 300$.
- Vortex suppression by blowing in at upper end of cylinder.
- Proportional feedback, not Riccati-optimized yet.

[Bänsch/Benner/Weichelt, in preparation]

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Motivating Examples from Current Projects

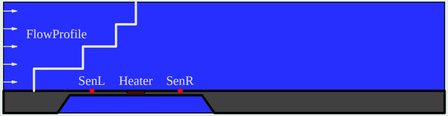
Design optimization for microsystems

Flow sensor (anemometer)

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

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

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



Supported by DFG grant BE2174/7-1 *Automatic, Parameter-Preserving Model Reduction for Applications in Microsystems Technology* with IMTEK, Freiburg.

Flow sensor (anemometer)

Parameter study based on reduced-order model:

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

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

[Baur/Benner, AT 2009]

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- The complexity of simulation and, in particular, control and optimization increases rapidly due to
  - multiphysics applications (e.g., MEMS),
  - parameter uncertainties,
  - network structures (e.g., nanoelectronics, biochemical (metabolic) networks),
  - complicated 3D geometries (e.g., machine tools).
- Particular instance of curse of dimensionality:

  Increase in computing power is often not sufficient to compensate for increased complexity.
- Need reduced-order models!

Model Order Reduction as Key Technology

Key Observation

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Model Order Reduction as Key Technology

Key Observation

Example: algorithmic vs. hardware speed-up

- Parameter studies need to be accessible to design engineers on daily basis on desktop computers.
- In anemometer example, full parameter study reduced

  from 11.3 days to 93 seconds

  using new simulation technique (on dual core processor@2.6 GHz).

  $\Longrightarrow$ *Speed-up:* $\approx 10,500$.
- As clock cycles appear to be limited, the same *hardware* speed-up can only be expected from multi-core technology.
- If ideal parallel speed-up would be achieved, this would require $\approx$ 21,000 cores.
- Also note: real-time parameter study already possible on high-end quadcore machine when using reduced-order model.
- Gain from algorithms even more significant for d-dimensional parameter spaces ($d \geq 2$).

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$$\Downarrow$$

KEY TECHNOLOGY:
system approximation / model order reduction (MOR)

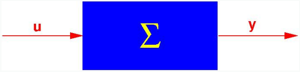
Main idea

Replace differential equation by low-order one while preserving input-output behavior as well as important system invariants and physical properties!

Original System

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

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



Reduced-Order System

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

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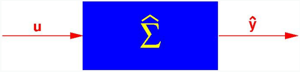

Model Order Reduction
Basic Ideas

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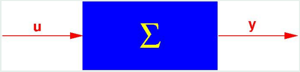

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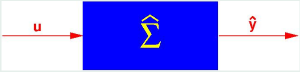

Large-Scale Linear Systems

Linear, time-invariant (LTI) systems

$$\Sigma : \left\{ \begin{array}{rcl} \dot{x}(t) & = & Ax + Bu, \\ y(t) & = & Cx + Du, \end{array} \right. \quad \begin{array}{ll} A \in \mathbb{R}^{n \times n}, & B \in \mathbb{R}^{n \times m}, \\ C \in \mathbb{R}^{q \times n}, & D \in \mathbb{R}^{q \times m}. \end{array}$$

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

Laplace transform: state-space $\rightarrow$ frequency domain yields transfer function of Σ:

$$Y(s) = \underbrace{\left(C(sI_n - A)^{-1}B + D\right)}_{=:G(s)} U(s).$$

Goal: find $\hat{A} \in \mathbb{R}^{r \times r}, \hat{B} \in \mathbb{R}^{r \times q}, \hat{C} \in \mathbb{R}^{q \times r}, D \in \mathbb{R}^{q \times m}$ such that

$$\begin{array}{rcl} \|G - \hat{G}\| & = & \|(C(sI_n - A)^{-1}B + D) - (\hat{C}(sI_r - \hat{A})^{-1}\hat{B} + \hat{D})\| < \mathrm{tol} \\ & \Rightarrow & \|y - \hat{y}\| \leq \mathrm{tol}\|u\|. \end{array}$$

Large-Scale Linear Systems

Linear, time-invariant (LTI) systems

$$\Sigma : \left\{ \begin{array}{rcl} \dot{x}(t) & = & Ax + Bu, \\ y(t) & = & Cx + Du, \end{array} \right. \qquad \begin{array}{ll} A \in \mathbb{R}^{n\times n}, & B \in \mathbb{R}^{n\times m}, \\ C \in \mathbb{R}^{q\times n}, & D \in \mathbb{R}^{q\times m}. \end{array}$$

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

Model order reduction by projection

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

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

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

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

Linear, time-invariant (LTI) systems

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

Balanced Truncation [Moore '81]

Compute (implicitly) balanced realization of Σ, i.e. state-space transformation so that controllability and observability Gramians P, Q satisfy

$$P = Q = \operatorname{diag}(\sigma_1, \ldots, \sigma_n), \quad \sigma_1 \geq \ldots \geq \sigma_n > 0,$$

reduced-order model obtained by truncated realization.

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Properties:

- Eliminates states hard to reach and hard to observe (equal in balanced coordinates).
- Adaptive choice of r based on computable error bound:

$$\|G - \hat{G}\|_{\mathcal{H}_\infty} \leq 2 \sum_{\ell=r+1}^{n} \sigma_j.$$

- Maximizes energy preserved in reduced-order model of order $r \Longrightarrow$ generalizations in several directions using appropriate energy functionals.

Large-Scale Linear Systems

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Bottleneck: based on solving Lyapunov equations

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

(Projection matrices are by-product.)

Thus: until ~ 2000, only used for $n \leq 100$.

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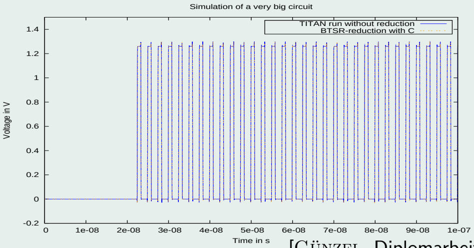
Algorithmic improvements $\Longrightarrow$ application now for $n = \mathcal{O}(10^6)$.

- Benner/Quintana-Ortí, MCMDS 2000 / ParComp 2003.
  (Dense linear algebra, parallel algorithms $\Rightarrow$ $n \gg 1000$.)
- Penzl 1999 (LAA 2006); Li/White, SIMAX 2002; Benner, IEEE CSM 2004 / MCMDS 2010; Benner + co-authors 1999–2009; ...
  (Sparse algorithms $\Rightarrow$ $n \gg 10,000$.)
- Baur/Benner, SISC 2008.
  (Hierarchical matrices + formatted arithmetic, data-sparse systems.)

Application in Microelectronics: VLSI Design

Balanced Truncation was implemented in circuit simulator TITAN (Qimonda AG, Infineon Technologies).

TITAN simulation results for industrial circuit:
14,677 resistors, 15,404 capacitors, 14 voltage sources, 4,800 MOSFETs.
14 linear subcircuits of varying order extracted and reduced.



[GÜNZEL, Diplomarbeit 2008; BENNER, Proc. SCEE 2008]

Supported by BMBF network *SyreNe* (includes Qimonda, Infineon, NEC), EU Marie Curie grant *O-Moore-Nice!* (includes NXP), industry grants.

- Reduction of large linear substructures, e.g.,
  - interconnect in integrated circuit design,
  - metabolic networks,

  allows to concentrate efforts on more complicated aspects of model and nonlinear components.
- Algorithmic improvements still possible.
- Major challenge: large linear systems with many inputs/outputs, resulting, e.g., from network structure and system coupling.

Parametric Model Order Reduction

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

Multivariate moment-matching

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.

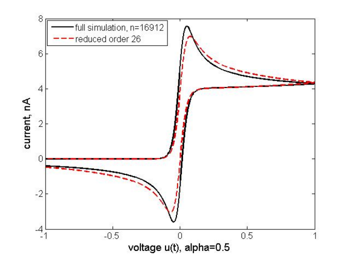
- [Daniel et al. '04]: explicit moment computation, numerically unstable.
- [Farle et al. '06/'07]: Krylov subspace approach, only polynomial parameter-dependance, numerical properties not clear, apparently robust.
- [Feng/Benner '07/'09]: Arnoldi-MGS method, employ recursive dependance of multi-moments, numerically robust, r often larger than necessary.

Electro-chemical SEM: compute cyclic voltammogram based on FEM

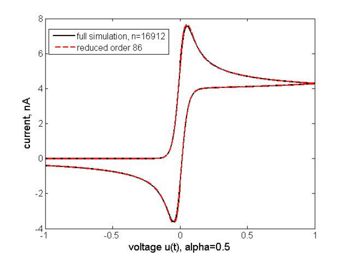
$$E\dot{x}(t) = (A_0 + p_1 A_1 + p_2 A_2)x(t) + Bu(t), \quad y(t) = c^T x(t),$$

where $n = 16,912$, $m = 3$, A_i diagonal.

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



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



[Benner/Feng, PAMM 2007]

Supported by Alexander-von-Humboldt fellowship and DFG grant BE2174/7-1 *Automatic, Parameter-Preserving Model Reduction for Applications in Microsystems Technology*.

Drawbacks of multivariate moment-matching:

- good approximation quality only locally;
- for d-dimensional parameter spaces ($d > 2$), exponentially growing number of moments need to be computed (explicitly or implicitly);
- no error bound or estimate available. (Even not for non-parametric problems!)

New ideas:

- Extend rational (tangential) interpolation (optimal H_2 approximation methods $\rightsquigarrow$ IRKA) to parametric MOR; cooperation with C. Beattie/S. Gugercin (Virginia Tech).
- Combine Balanced Truncation with sparse grid interpolation. First paper [Baur/Benner, AT 2009].

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Rational interpolation [BAUR/BEATTIE/BENNER/GUGERCIN '07/'09]

Under reasonable smoothness assumptions on $G(s,p)$, Hermite interpolation properties of reduced-order model w.r.t. s and p are achieved if projection subspaces are chosen as appropriate rational Krylov subspaces:

$$\begin{aligned}\mathcal{V} &:= \operatorname{span}\left\{\mathcal{A}_{1,1}^{-1}B(\hat{p}^{(1)}),\ldots,\mathcal{A}_{k,\ell}^{-1}B(\hat{p}^{(\ell)})\right\},\\ \mathcal{W} &:= \operatorname{span}\left\{(C(\hat{p}^{(1)})\mathcal{A}_{1,1}^{-1})^T,\ldots,(C(\hat{p}^{(\ell)})\mathcal{A}_{k,\ell}^{-1})^T\right\},\end{aligned}$$

where $\hat{s}^{(i)}$ $(i=1,\ldots,k)$, $\hat{p}^{(j)}$ $(j=1,\ldots,\ell)$ are interpolation points, and

$$\mathcal{A}_{i,j} = \hat{s}^{(i)}\,E(\hat{p}^{(j)}) - A(\hat{p}^{(j)}).$$

Remarks:

- Results extend to MIMO case using tangential interpolation.
- Optimal choice of $\hat{s}^{(j)}$ using H_2-optimal interpolation.
- Optimal choice of $\hat{p}^{(j)}$ for SISO systems $\Sigma(p) = (E, A, B(p), C(p))$.
- Approximation of gradient w.r.t. p allows sensitivity analysis with reduced-order model.

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

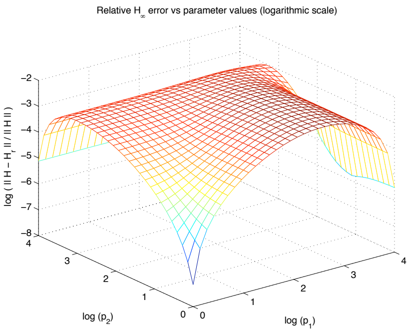
$$E\dot{x}(t) = (A_0 + \sum_{i=1}^{3} p_i A_i)x(t) + bu(t), \quad y(t) = c^T x(t),$$

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

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

Choose 4 interpolation points for parameters ("important" configurations), 6 interpolation frequencies each are picked H_2-optimal by IRKA.
$\Longrightarrow \; k = 6, \ell = 4$, hence $r = 24$.

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



[Baur/Beattie/Benner/Gugercin, submitted to SISC]

Balanced Truncation on sparse grids [Baur/Benner, AT 2009]

- Select interpolation points $\hat{p}^{(0)}, \ldots, \hat{p}^{(\ell)}$, apply Balanced Truncation for fixed $\hat{p}^{(j)}$, and interpolate reduced-order models.
- For 1D case, employ Lagrange-/Hermite-Lagrange-/barycentric interpolation.
- For dD case ($d > 1$), employ sparse grid interpolation [Zenger '91, Griebel '91, Bungartz '92, Klimke/Wohlmuth '05].
- Combination of interpolation and BT error bounds yields L_∞ error bound for parametric system approximation.
- Further advantages:
  - reduced-order models are block-diagonal (i.e., sparse),
  - no structural assumptions on parameter dependance necessary.
- Challenge: approximation of "rough" functions.

Parametric Model Order Reduction

Research directions

- Current program:
  - application to several microsystem models (with IMTEK/FRIAS, Freiburg — DFG grant);
  - use other (non-polynomial) ansatz functions for interpolation;
  - better understanding of sparse grid technology and possible alternatives to escape curse of dimensionality when $d > 3$.
- Medium-term goals:
  - Employ reduced-order parametric models in trajectory optimization.

    Requirements for trust-region methods fulfilled, explore connections to response surface models/Kriging.
  - Application to systems with uncertain parameters: in combination with stochastic MOR ($\rightsquigarrow$ next section), preserve uncertain parameters in reduced-order model together with their statistics.
  - Extension to LPV (linear parameter-varying) systems.
  - Combination of parametric MOR and reduced-basis methods for nonlinear PDEs?

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  - Combination of parametric MOR and reduced-basis methods for nonlinear PDEs?

First idea for model reduction of stochastic systems:
Consider a stochastic linear control system of Itô-type

$$dx = Ax\,dt + \sum_{j=1}^{N} A_j x\,dw_j + Bu\,dt, \quad y = Cx\ .$$

- $w_j = w_j(t)$ are independent zero mean real Wiener processes on probability space $(\Omega, \mathcal{F}, \mu)$ w.r.t. an increasing family $(\mathcal{F}_t)_{t\in\mathbb{R}_+}$ of σ-algebras $\mathcal{F}_t \subset \mathcal{F}$.
- Assume that the homogeneous equation $dx = Ax\,dt + \sum A_j x\,dw_j$ is mean-square-stable, i.e. $\mathcal{E}(\|x(t)\|^2) \stackrel{t\to\infty}{\longrightarrow} 0$, $\forall\ x(0) = x_0$.

In complete analogy to the deterministic case, Balanced Truncation can then be based on the controllability and observability Gramians, given by the solutions of the generalized Lyapunov equations

$$AP + PA^T + \sum_{j=1}^{N} A_j P A_j^T = -BB^T, \quad A^T Q + QA + \sum_{j=1}^{N} A_j^T Q A_j = -C^T C.$$

- Current program:
  - Application to realistic scenarios, e.g., PDEs with uncertain material parameters (diffusion/reaction constants etc.).
  - Investigate theoretical properties (derivation of error bound).
  - Improve numerical methods (need efficient solvers for large-scale generalized Lyapunov equations).
- Medium-term goals:
  - Extend method to unstable problems (find analogy to unstable BT).
  - In combination with parametric MOR, preserve uncertain parameters in reduced-order model together with their statistics.

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Bilinear control system of the form

$$\dot{x} = Ax + \sum_{j=1}^{k} N_j x u_j + Bu, \quad y = Cx,$$

arise, e.g., in

- control of PDEs with mixed boundary conditions,
- approximation of nonlinear systems using Carleman bilinearization.

Nonlinear Model Order Reduction

Balanced Truncation for Bilinear Systems

[Gray/Mesko '98, Condon/Ivanov '05, Benner/Damm '09]

Bilinear control system of the form

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arise, e.g., in

- control of PDEs with mixed boundary conditions,
- approximation of nonlinear systems using Carleman bilinearization.

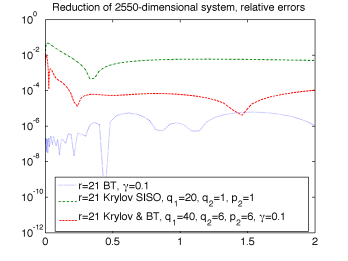
The solutions of the generalized Lyapunov equations

$$AP + PA^T + \sum_{j=1}^{k} N_j P N_j^T = -BB^T, \quad A^T Q + QA + \sum_{j=1}^{k} N_j^T Q N_j = -C^T C$$

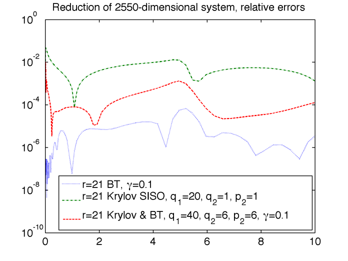
possess certain properties of the controllability and observability Gramians of linear systems, generalized Hankel singular values can be defined, and model reduction analogous to Balanced Truncation can be based upon them.

Numerical Example

- Nonlinear RC circuit [Chen/White '00, Bai/Skoogh '06].
- Carleman bilinearization $\rightsquigarrow$ bilinear system with $n = 2,550$, $k = 1$.
- Compare bilinear Balanced Truncation with Krylov subspace method taken from [Bai/Skoogh '06].



$u(t) = e^{-t}$



$u(t) = (\cos \frac{2\pi t}{10} + 1)/2$

[Benner/Damm, submitted to SICON, 2009]

- Many nonlinear dynamics can be modeled by quadratic bilinear differential algebraic equations (QBDAEs), i.e.

$$E\dot{x} = A_1 x + A_2 x \otimes x + Nxu + bu,$$
$$y = cx,$$

where $E, A_1, N \in \mathbb{R}^{n\times n}, A_2 \in \mathbb{R}^{n\times n^2}, b, c^T \in \mathbb{R}^n$.

- Combination of quadratic and bilinear control systems.
- Variational analysis allows characterization of input-output behavior via generalized transfer functions, e.g.

$$H_1(s) = c\underbrace{(sE - A_1)^{-1} b}_{G(s)},$$

$$H_2(s_1, s_2) = \frac{1}{2} c\left((s_1 + s_2)E - A_1\right)^{-1} \left[A_2(G(s_1) \otimes G(s_2) + G(s_2) \otimes G(s_1)) + N\left(G(s_1) + G(s_2)\right)\right]$$

Which systems can be transformed?

Theorem [Gu '09]

Assume that the state equation of a nonlinear system Σ is given by

$$\dot{x} = a_0 x + a_1 g_1(x) + \ldots + a_k g_k(x) + bu,$$

where $g_i(x) : \mathbb{R}^n \to \mathbb{R}^n$ are compositions of rational, exponential, logarithmic, trigonometric or root functions, respectively.
Then Σ can be transformed into a quadratic bilinear differential algebraic equation of dimension $N > n$.

- transformation is not unique
- original system has to be increased before reduction is possible
- minimal dimension N?

Example

- Consider the following two dimensional nonlinear control system:

$$\dot{x}_1 = \exp(-x_2) \cdot \sqrt{x_1^2 + 1},$$
$$\dot{x}_2 = \sin x_2 + u.$$

- Introduce useful new state variables, e.g.

$$x_3 := \exp(-x_2),\ x_4 := \sqrt{x_1^2 + 1},\ x_5 := \sin x_2,\ x_6 := \cos x_2.$$

- System can be replaced by a QBDAE of dimension 6:

$$\begin{aligned} \dot{x}_1 &= x_3 \cdot x_4, & \dot{x}_2 &= x_5 + u, \\ \dot{x}_3 &= -x_3 \cdot (x_5 + u), & \dot{x}_4 &= \frac{2 \cdot x_1 \cdot x_3 \cdot x_4}{2 \cdot x_4}, \\ \dot{x}_5 &= x_6 \cdot (x_5 + u), & \dot{x}_6 &= -x_5 \cdot (x_5 + u). \end{aligned}$$

Multi-moment-Matching for QBDAEs

- Construct reduced order model by projection:

$$\hat{E} = Z^T E Z, \;\; \hat{A}_1 = Z^T A_1 Z, \;\; \hat{N} = Z^T N Z,$$
$$\hat{A}_2 = Z^T A_2 Z \otimes Z, \;\; \hat{b} = Z^T b, \;\; \hat{c} = cZ$$

- Approximate values and derivatives ("multi-moments") of transfer functions around an expansion point σ using Krylov spaces, e.g.

$$\begin{aligned}
\operatorname{span}\{V\} &= \mathcal{K}_6\left(A_\sigma E, A_\sigma b\right)\\
\operatorname{span}\{W_1\} &= \mathcal{K}_3\left(A_{2\sigma} E, A_{2\sigma}(A_2 V_1 \otimes V_1 - N_1 V_1)\right)\\
\operatorname{span}\{W_2\} &= \mathcal{K}_2\left(A_{2\sigma} E, A_{2\sigma}(A_2(V_2 \otimes V_1 + V_1 \otimes V_2) - N_1 V_2)\right)\\
\operatorname{span}\{W_3\} &= \mathcal{K}_1\left(A_{2\sigma} E, A_{2\sigma}(A_2(V_2 \otimes V_2 + V_2 \otimes V_2))\right)\\
\operatorname{span}\{W_4\} &= \mathcal{K}_1\left(A_{2\sigma} E, A_{2\sigma}(A_2(V_3 \otimes V_1 + V_1 \otimes V_3) - N_1 V_3)\right),
\end{aligned}$$

with $A_\sigma = (A_1 - \sigma E)^{-1}$ and V_i denoting the i-*th* column of V
$\rightarrow$ derivatives match up to order 5 (H_1) and 2 (H_2), respectively.

Numerical Example

- FitzHugh-Nagumo system: simple model for neuron (de-)activation.

$$\begin{aligned} \epsilon v_t(x,t) &= \epsilon^2 v_{xx}(x,t) + f(v(x,t)) - w(x,t) + g, \\ w_t(x,t) &= hv(x,t) - \gamma w(x,t) + g, \end{aligned}$$

  with $f(v) = v(v - 0.1)(1 - v)$ and initial and boundary conditions

$$\begin{aligned} v(x,0) &= 0, & w(x,0) &= 0, & x &\in [0,1] \\ v_x(0,t) &= -i_0(t), & v_x(1,t) &= 0, & t &\geq 0, \end{aligned}$$

  where $\epsilon = 0.015, h = 0.5, \gamma = 2, g = 0.05, i_0(t) = 50000t^3 \exp(-15t)$

- parameter g handled as an additional input
- original state dimension $n = 2 \cdot 400$, QBDAE dimension $N = 3 \cdot 400$, reduced QBDAE dimension $r = 26$, chosen expansion point $\sigma = 1$

[Benner/Breiten 2010]

Numerical Example

2d Phase Space

[Benner/Breiten 2010]

Numerical Example

3d Phase Space

[Benner/Breiten 2010]

Nonlinear Model Order Reduction

Research directions

Model reduction for nonlinear systems based on

- Carleman bilinearization and bilinear Balanced Truncation,
- QLDAE transformation and multi-moment matching

has high potential for many classes of nonlinear dynamical systems.

Current program:

- High dimensions can be dealt with using tensor product structures of coefficient matrices — already done for bilinear Krylov subspaces [CONDON/IVANOV '07], for Gramian computation in progress [BENNER/DAMM].
- QLDAE is exact for many nonlinearities, e.g.
  - + reaction-diffusion systems and population balances;
  - + various PDEs with nonlinear convective terms $\mathbf{x}.\nabla\mathbf{x}$: *Burgers, Euler, Navier-Stokes, Kuramoto-Sivashinsky* eqns;

  hence, reduced-order model will have the same nonlinear structure.

  Plan: start program to explore adaptation to various application areas.

Nonlinear Model Order Reduction

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has high potential for many classes of nonlinear dynamical systems.

Medium-term goals:

- Develop error bounds similar to balanced truncation error bound.
- Investigate suitability for further PDEs with polynomial nonlinearities, e.g. *Allen-Cahn*, . . . , . . .

Future Perspectives

Control of Complex Dynamical Systems

Goal

Develop robust control mechanisms for multi-field/-physics applications that are computationally accessible and technically implementable.

Besides model order reduction, this requires robust feedback control operators for

- network structures,
- hierarchical structures,
- coupled processes.

First steps:
DFG SPP1253 grant BE2174/8-1,2 (together with E. Bänsch, FAU Erlangen): *Optimal Control-Based Feedback Stabilization of Multi-Field Flow Problems.*

MOR for dynamical systems has evolved in several areas:

- systems and control theory: Balanced Truncation and related methods, optimal Hankel norm approximation;
- structural mechanics: Modal Truncation, CMS, AMLS;
- circuit simulation: Moment-Matching;
- computational electro-magnetics: Krylov subspace techniques;
- CFD: POD, Reduced Basis methods;
- chemical process engineering: analytical and nonlinear modal methods;
- dynamical systems: Center and Approximate Inertial Manifolds.

$\Longrightarrow$ Challenges:

- identify mathematical cores;
- extract advantageous features;
- derive solid mathematical basis;
- automate reduced-order model extraction $\rightsquigarrow$ need (a posteriori) error estimates;
- feed back optimized/new methods to application areas.

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Model Order Reduction

Ultimate goal

Establish model reduction as a fundamental pillar of numerical simulation for control, optimization, and design of complex dynamical systems.

This requires

- investigation of underlying physics;
- integration of ideas from several application areas;
- efficient numerics by exploiting structures;
- methods for uncertain parameters so that statistical properties are preserved in reduced-order model;
- dedicated methods for classes of nonlinearities.

Future Perspectives

Model Order Reduction

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- methods for uncertain parameters so that statistical properties are preserved in reduced-order model;
- dedicated methods for classes of nonlinearities.

Thank you for your attention!