

Gene Golub SIAM Summer School 2013  
Matrix Functions and Matrix Equations  
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# Matrix Equations and Model Reduction

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g<sup>2</sup>s<sup>3</sup> 2013  
SIAM Summer School









# Introduction

## Model Reduction — Abstract Definition

### 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*).



# Model Reduction for Dynamical Systems

## Original System

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

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



## Reduced-Order Model (ROM)

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

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

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



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## Goal:

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

Secondary goal: reconstruct approximation of  $x$  from  $\hat{x}$ .

# Model Reduction for Dynamical Systems

## Parameter-Dependent Dynamical Systems

### Dynamical Systems

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

with

- (generalized) **states**  $x(t; p) \in \mathbb{R}^n$  ( $E \in \mathbb{R}^{n \times n}$ ),
- **inputs**  $u(t) \in \mathbb{R}^m$ ,
- **outputs**  $y(t; p) \in \mathbb{R}^q$ , (b) is called **output equation**,
- $p \in \Omega \subset \mathbb{R}^d$  is a **parameter vector**,  $\Omega$  is bounded.

### Applications:

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

**Requirement:** keep parameters as symbolic quantities in ROM.

# Model Reduction for Dynamical Systems

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# Model Reduction for Dynamical Systems

## Linear Systems

### Linear, Time-Invariant (LTI) Systems

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

### Linear, Time-Invariant Parametric Systems

$$\begin{aligned} E(p)\dot{x}(t; p) &= A(p)x(t; p) + B(p)u(t), \\ y(t; p) &= C(p)x(t; p) + D(p)u(t), \end{aligned}$$

where  $A(p), E(p) \in \mathbb{R}^{n \times n}$ ,  $B(p) \in \mathbb{R}^{n \times m}$ ,  $C(p) \in \mathbb{R}^{q \times n}$ ,  $D(p) \in \mathbb{R}^{q \times m}$ .





# Application Areas

(Optimal) Control

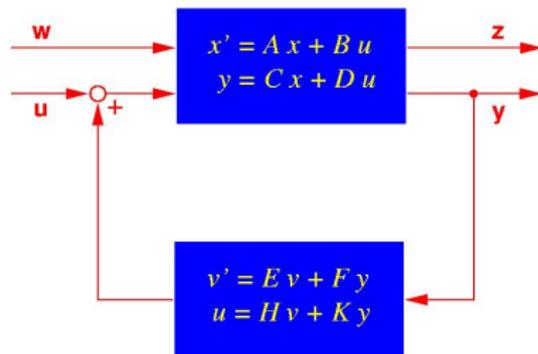
since ~1980ies

## 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-/ $\mathcal{H}_2$ -/ $\mathcal{H}_\infty$ -) control design:  $N \geq n$ .



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

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

$\implies$  reduce order of plant ( $n$ ) and/or controller ( $N$ ).

Standard MOR techniques in systems and control: balanced truncation and related methods.

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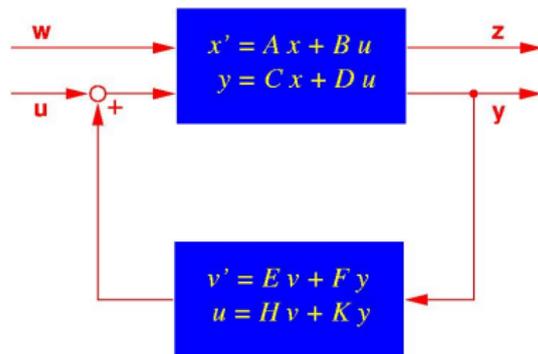
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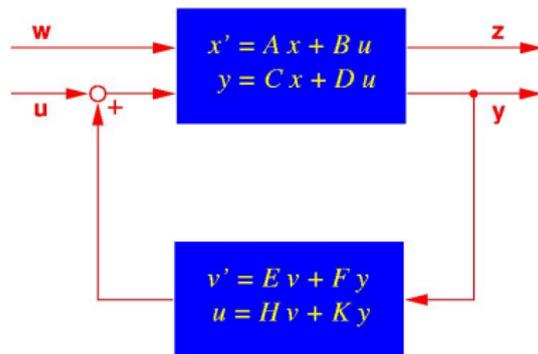
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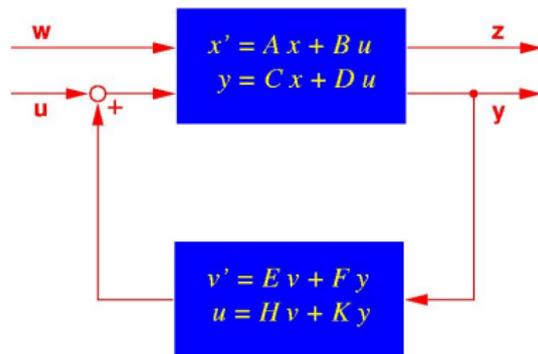
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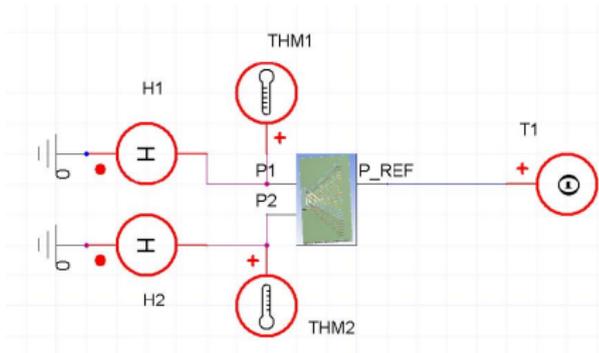


# Motivating Examples

## Electro-Thermic Simulation of Integrated Circuit (IC)

[Source: Evgenii Rudnyi, CADFEM GmbH]

- SIMPLORER<sup>®</sup> test circuit with 2 transistors.



- Conservative thermic sub-system in SIMPLORER: voltage  $\rightsquigarrow$  temperature, current  $\rightsquigarrow$  heat flow.
- Original model:  $n = 270.593$ ,  $m = q = 2 \Rightarrow$   
 Computing time (on Intel Xeon dualcore 3GHz, 1 Thread):
  - Main computational cost for set-up data  $\approx 22min$ .
  - Computation of reduced models from set-up data: 44–49sec. ( $r = 20-70$ ).
  - Bode plot (MATLAB on Intel Core i7, 2,67GHz, 12GB):  
 7.5h for original system,  $< 1min$  for reduced system.
  - Speed-up factor: 18 including /  $\geq 450$  excluding reduced model generation!











# Motivating Examples

## A Nonlinear Model from Computational Neurosciences: the FitzHugh-Nagumo System

# Motivating Examples

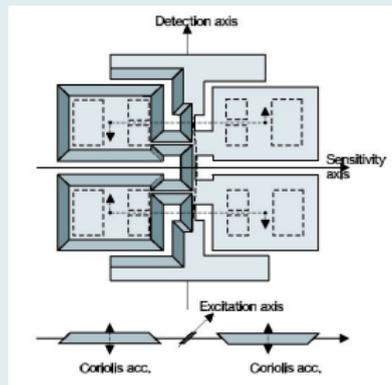
## Parametric MOR: Applications in Microsystems/MEMS Design

### Microgyroscope (butterfly gyro)



- Application: inertial navigation.

- Voltage applied to electrodes induces vibration of wings, resulting rotation due to Coriolis force yields sensor data.
- FE model of second order:  
 $N = 17.361 \rightsquigarrow n = 34.722, m = 1, q = 12.$
- Sensor for position control based on acceleration and rotation.



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









# Numerical Linear Algebra

## 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 (in single precision):  $4 \cdot n_x \cdot n_y$  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:

$$\hat{X} = \sum_{j=1}^r \sigma_j u_j v_j^T,$$

where  $X = U\Sigma V^T$  is the singular value decomposition (SVD) of  $X$ .

The approximation error is  $\|X - \hat{X}\|_2 = \sigma_{r+1}$ .

### Idea for dimension reduction

Instead of  $X$  save  $u_1, \dots, u_r, \sigma_1 v_1, \dots, \sigma_r v_r$ .

$\rightsquigarrow$  memory =  $4r \times (n_x + n_y)$  bytes.



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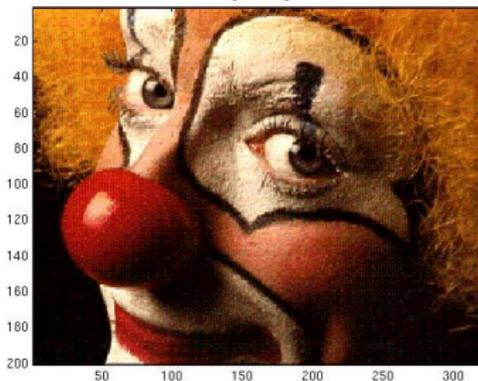
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# Example: Image Compression by Truncated SVD

## Example: Clown

Original image



$320 \times 200$  pixel

$\rightsquigarrow \approx 256$  kB











# Systems and Control Theory

## The Laplace transform

### Definition

The Laplace transform of a time domain function  $f \in L_{1,loc}$  with  $\text{dom}(f) = \mathbb{R}_0^+$  is

$$\mathcal{L} : f(t) \mapsto f(s) := \mathcal{L}\{f(t)\}(s) := \int_0^{\infty} e^{-st} f(t) dt, \quad s \in \mathbb{C}.$$

$F$  is a function in the (Laplace or) frequency domain.

**Note:** for frequency domain evaluations ("frequency response analysis"), one takes  $\text{re } s = 0$  and  $\text{im } s \geq 0$ . Then  $\omega := \text{im } s$  takes the role of a frequency (in [rad/s], i.e.,  $\omega = 2\pi\nu$  with  $\nu$  measured in [Hz]).

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### Lemma

$$\mathcal{L}\{\dot{f}(t)\}(s) = sF(s).$$

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Note: for ease of notation, in the following we will use lower-case letters for both, a function and its Laplace transform!

# Systems and Control Theory

## The Model Reduction Problem as Approximation Problem in Frequency Domain

### Linear Systems in Frequency Domain

Application of Laplace transform  $(x(t) \mapsto x(s), \dot{x}(t) \mapsto sx(s))$  to linear system

$$E\dot{x}(t) = Ax(t) + Bu(t), \quad y(t) = Cx(t) + Du(t)$$

with  $x(0) = 0$  yields:

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

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$\implies$  I/O-relation in frequency domain:

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

$G(s)$  is the **transfer function** of  $\Sigma$ .

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Example.

# Systems and Control Theory

## The Model Reduction Problem as Approximation Problem in Frequency Domain

### Formulating model reduction in frequency domain

Approximate the dynamical system

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

by reduced-order system

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

of order  $r \ll n$ , such that

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of order  $r \ll n$ , such that

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

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

# Systems and Control Theory

## Properties of linear systems

### Definition

A linear system

$$E\dot{x}(t) = Ax(t) + Bu(t), \quad y(t) = Cx(t) + Du(t)$$

is **stable** if its transfer function  $G(s)$  has all its poles in the left half plane and it is **asymptotically (or Lyapunov or exponentially) stable** if all poles are in the open left half plane  $\mathbb{C}^- := \{z \in \mathbb{C} \mid \Re(z) < 0\}$ .

### Lemma

Sufficient for asymptotic stability is that  $A$  is **asymptotically stable (or Hurwitz)**, i.e., the spectrum of  $A - \lambda E$ , denoted by  $\Lambda(A, E)$ , satisfies  $\Lambda(A, E) \subset \mathbb{C}^-$ .

Note that by abuse of notation, often *stable system* is used for asymptotically stable systems.

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# Systems and Control Theory

## Realizations of Linear Systems (with $E = I_n$ for simplicity)

### Definition

For a linear (time-invariant) system

$$\Sigma : \begin{cases} \dot{x}(t) &= Ax(t) + Bu(t), \\ y(t) &= Cx(t) + Du(t), \end{cases} \quad \begin{array}{l} \text{with transfer function} \\ G(s) = C(sI - A)^{-1}B + D, \end{array}$$

the quadruple  $(A, B, C, D) \in \mathbb{R}^{n \times n} \times \mathbb{R}^{n \times m} \times \mathbb{R}^{q \times n} \times \mathbb{R}^{q \times m}$  is called a **realization** of  $\Sigma$ .

### Realizations are not unique!

Transfer function is invariant under **state-space transformations**,

$$\mathcal{T} : \begin{cases} x & \rightarrow Tx, \\ (A, B, C, D) & \rightarrow (TAT^{-1}, TB, CT^{-1}, D), \end{cases}$$



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Hence,

$$(A, B, C, D), \quad \left( \begin{bmatrix} A & 0 \\ 0 & A_1 \end{bmatrix}, \begin{bmatrix} B \\ B_1 \end{bmatrix}, [C \ 0], D \right),$$

$$(TAT^{-1}, TB, CT^{-1}, D), \quad \left( \begin{bmatrix} A & 0 \\ 0 & A_2 \end{bmatrix}, \begin{bmatrix} B \\ 0 \end{bmatrix}, [C \ C_2], D \right),$$

are all realizations of  $\Sigma$ !

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the quadruple  $(A, B, C, D) \in \mathbb{R}^{n \times n} \times \mathbb{R}^{n \times m} \times \mathbb{R}^{q \times n} \times \mathbb{R}^{q \times m}$  is called a **realization** of  $\Sigma$ .

### Definition

The **McMillan degree** of  $\Sigma$  is the unique minimal number  $\hat{n} \geq 0$  of states necessary to describe the input-output behavior completely.

A **minimal realization** is a realization  $(\hat{A}, \hat{B}, \hat{C}, \hat{D})$  of  $\Sigma$  with order  $\hat{n}$ .

# Systems and Control Theory

## Realizations of Linear Systems (with $E = I_n$ for simplicity)

### Definition

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### Theorem

A realization  $(A, B, C, D)$  of a linear system is minimal  $\iff$   
 $(A, B)$  is controllable and  $(A, C)$  is observable.

# Systems and Control Theory

## Balanced Realizations

### Definition

A realization  $(A, B, C, D)$  of a linear system  $\Sigma$  is **balanced** if its infinite controllability/observability Gramians  $P/Q$  satisfy

$$P = Q = \text{diag} \{ \sigma_1, \dots, \sigma_n \} \quad (\text{w.l.o.g. } \sigma_j \geq \sigma_{j+1}, j = 1, \dots, n-1).$$

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When does a balanced realization exist?

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When does a balanced realization exist?

Assume  $A$  to be Hurwitz, i.e.  $\Lambda(A) \subset \mathbb{C}^-$ . Then:

### Theorem

Given a **stable** minimal linear system  $\Sigma : (A, B, C, D)$ , a balanced realization is obtained by the state-space transformation with

$$T_b := \Sigma^{-\frac{1}{2}} V^T R,$$

where  $P = S^T S$ ,  $Q = R^T R$  (e.g., Cholesky decompositions) and  $SR^T = U \Sigma V^T$  is the SVD of  $SR^T$ .

**Proof.** Exercise!

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$\sigma_1, \dots, \sigma_n$  are the **Hankel singular values** of  $\Sigma$ .

**Note:**  $\sigma_1, \dots, \sigma_n \geq 0$  as  $P, Q \geq 0$  by definition, and  $\sigma_1, \dots, \sigma_n > 0$  in case of minimality!

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The infinite controllability/observability Gramians  $P/Q$  satisfy the **Lyapunov equations**

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

# Systems and Control Theory

## Balanced Realizations

### Theorem

The infinite controllability/observability Gramians  $P/Q$  satisfy the [Lyapunov equations](#)

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

**Proof.** (For controllability Gramian only, observability case is analogous!)

$$\begin{aligned}
 AP + PA^T + BB^T &= A \int_0^\infty e^{At} BB^T e^{A^T t} dt + \int_0^\infty e^{At} BB^T e^{A^T t} dt A^T + BB^T \\
 &= \int_0^\infty \underbrace{Ae^{At} BB^T e^{A^T t} + e^{At} BB^T e^{A^T t} A^T}_{= \frac{d}{dt} e^{At} BB^T e^{A^T t}} dt + BB^T \\
 &= \underbrace{\lim_{t \rightarrow \infty} e^{At} BB^T e^{A^T t}}_{= 0} - \underbrace{e^{A \cdot 0} BB^T}_{= I_n} \underbrace{e^{A^T \cdot 0}}_{= I_n} + BB^T \\
 &= 0.
 \end{aligned}$$

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The Hankel singular values (HSVs) of a stable minimal linear system are system invariants, i.e. they are unaltered by state-space transformations!

# Systems and Control Theory

## Balanced Realizations

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**Proof.** In balanced coordinates, the HSVs are  $\Lambda(PQ)^{\frac{1}{2}}$ . Now let

$$(\hat{A}, \hat{B}, \hat{C}, D) = (TAT^{-1}, TB, CT^{-1}, D)$$

be any transformed realization with associated controllability Lyapunov equation

$$0 = \hat{A}\hat{P} + \hat{P}\hat{A}^T + \hat{B}\hat{B}^T = TAT^{-1}\hat{P} + \hat{P}T^{-T}A^T T^T + TBB^T T^T.$$

This is equivalent to

$$0 = A(T^{-1}\hat{P}T^{-T}) + (T^{-1}\hat{P}T^{-T})A^T + BB^T.$$

The uniqueness of the solution of the Lyapunov equation implies that  $\hat{P} = TPT^T$  and, analogously,  $\hat{Q} = T^{-T}QT^{-1}$ . Therefore,

$$\hat{P}\hat{Q} = TPQT^{-1},$$

showing that  $\Lambda(\hat{P}\hat{Q}) = \Lambda(PQ) = \{\sigma_1^2, \dots, \sigma_n^2\}$ .

# Systems and Control Theory

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**Note:**  $\sigma_1, \dots, \sigma_n \geq 0$  as  $P, Q \geq 0$  by definition, and  $\sigma_1, \dots, \sigma_n > 0$  in case of minimality!

### Remark

For non-minimal systems, the Gramians can also be transformed into diagonal matrices with the leading  $\hat{n} \times \hat{n}$  submatrices equal to  $\text{diag}(\sigma_1, \dots, \sigma_{\hat{n}})$ , and

$$\hat{P}\hat{Q} = \text{diag}(\sigma_1^2, \dots, \sigma_{\hat{n}}^2, 0, \dots, 0).$$

see [LAUB/HEATH/PAIGE/WARD 1987, TOMBS/POSTLETHWAITE 1987].



## Qualitative and Quantitative Study of the Approximation Error System Norms

Consider transfer function

$$G(s) = C(sI - A)^{-1}B + D$$

and input functions  $u \in \mathcal{L}_2^m \cong L_2^m(-\infty, \infty)$ , with the  $L_2$ -norm

$$\|u\|_2^2 := \frac{1}{2\pi} \int_{-\infty}^{\infty} u(j\omega)^H u(j\omega) d\omega.$$

Assume  $A$  (asymptotically) stable:  $\Lambda(A) \subset \mathbb{C}^- := \{z \in \mathbb{C} : \operatorname{re} z < 0\}$ .  
Then for all  $s \in \mathbb{C}^+ \cup j\mathbb{R}$ ,  $\|G(s)\| \leq M < \infty \Rightarrow$

$$\int_{-\infty}^{\infty} y(j\omega)^H y(j\omega) d\omega = \int_{-\infty}^{\infty} u(j\omega)^H G(j\omega)^H G(j\omega) u(j\omega) d\omega$$

(Here,  $\|\cdot\|$  denotes the Euclidian vector or spectral matrix norm.)

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$$\Rightarrow y \in \mathcal{L}_2^q \cong L_2^q(-\infty, \infty).$$

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Consequently, the 2-induced operator norm

$$\|G\|_\infty := \sup_{\|u\|_2 \neq 0} \frac{\|Gu\|_2}{\|u\|_2}$$

is well defined. It can be shown that

$$\|G\|_\infty = \sup_{\omega \in \mathbb{R}} \|G(j\omega)\| = \sup_{\omega \in \mathbb{R}} \sigma_{\max}(G(j\omega)).$$

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*Sketch of proof:*

$$\|G(j\omega)u(j\omega)\| \leq \|G(j\omega)\| \|u(j\omega)\| \Rightarrow "\leq".$$

$$\text{Construct } u \text{ with } \|Gu\|_2 = \sup_{\omega \in \mathbb{R}} \|G(j\omega)\| \|u\|_2.$$

# Qualitative and Quantitative Study of the Approximation Error

## System Norms

Consider transfer function

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

### Hardy space $\mathcal{H}_\infty$

Function space of matrix-/scalar-valued functions that are analytic and bounded in  $\mathbb{C}^+$ .

The  $\mathcal{H}_\infty$ -norm is

$$\|F\|_\infty := \sup_{\operatorname{re} s > 0} \sigma_{\max}(F(s)) = \sup_{\omega \in \mathbb{R}} \sigma_{\max}(F(j\omega)).$$

Stable transfer functions are in the Hardy spaces

- $\mathcal{H}_\infty$  in the SISO case (single-input, single-output,  $m = q = 1$ );
- $\mathcal{H}_\infty^{q \times m}$  in the MIMO case (multi-input, multi-output,  $m > 1, q > 1$ ).

## Qualitative and Quantitative Study of the Approximation Error System Norms

Consider transfer function

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Paley-Wiener Theorem (Parseval's equation/Plancherel Theorem)

$$L_2(-\infty, \infty) \cong \mathcal{L}_2, \quad L_2(0, \infty) \cong \mathcal{H}_2$$

Consequently, 2-norms in time and frequency domains coincide!

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$\mathcal{H}_\infty$  approximation error

Reduced-order model  $\Rightarrow$  transfer function  $\hat{G}(s) = \hat{C}(sI_r - \hat{A})^{-1}\hat{B} + \hat{D}$ .

$$\|y - \hat{y}\|_2 = \|Gu - \hat{G}u\|_2 \leq \|G - \hat{G}\|_\infty \|u\|_2.$$

$\Rightarrow$  compute reduced-order model such that  $\|G - \hat{G}\|_\infty < tol!$

Note: error bound holds in time- and frequency domain due to Paley-Wiener!

# Qualitative and Quantitative Study of the Approximation Error System Norms

Consider stable transfer function

$$G(s) = C (sI - A)^{-1} B, \quad \text{i.e. } D = 0.$$

## Hardy space $\mathcal{H}_2$

Function space of matrix-/scalar-valued functions that are analytic  $\mathbb{C}^+$  and bounded w.r.t. the  $\mathcal{H}_2$ -norm

$$\begin{aligned} \|F\|_2 &:= \frac{1}{2\pi} \left( \sup_{\text{re } \sigma > 0} \int_{-\infty}^{\infty} \|F(\sigma + j\omega)\|_F^2 d\omega \right)^{\frac{1}{2}} \\ &= \frac{1}{2\pi} \left( \int_{-\infty}^{\infty} \|F(j\omega)\|_F^2 d\omega \right)^{\frac{1}{2}}. \end{aligned}$$

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- $\mathcal{H}_2$  in the SISO case (single-input, single-output,  $m = q = 1$ );
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$$\|F\|_2 = \frac{1}{2\pi} \left( \int_{-\infty}^{\infty} \|F(j\omega)\|_F^2 d\omega \right)^{\frac{1}{2}}.$$

## $\mathcal{H}_2$ approximation error for impulse response ( $u(t) = u_0\delta(t)$ )

Reduced-order model  $\Rightarrow$  transfer function  $\hat{G}(s) = \hat{C}(sI_r - \hat{A})^{-1}\hat{B}$ .

$$\|y - \hat{y}\|_2 = \|Gu_0\delta - \hat{G}u_0\delta\|_2 \leq \|G - \hat{G}\|_2 \|u_0\|.$$

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### Theorem (Practical Computation of the $\mathcal{H}_2$ -norm)

$$\|F\|_2^2 = \text{tr} \left( B^T Q B \right) = \text{tr} \left( C P C^T \right),$$

where  $P, Q$  are the controllability and observability Gramians of the corresponding LTI system.

# Qualitative and Quantitative Study of the Approximation Error

## Approximation Problems

### Output errors in time-domain

$$\begin{aligned}\|y - \hat{y}\|_2 &\leq \|G - \hat{G}\|_\infty \|u\|_2 &&\implies \|G - \hat{G}\|_\infty < \text{tol} \\ \|y - \hat{y}\|_\infty &\leq \|G - \hat{G}\|_2 \|u\|_2 &&\implies \|G - \hat{G}\|_2 < \text{tol}\end{aligned}$$

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$\mathcal{H}_\infty$ -norm	best approximation problem for given reduced order $r$ in general open; <b>balanced truncation</b> yields suboptimal solution with computable $\mathcal{H}_\infty$ -norm bound.
$\mathcal{H}_2$ -norm	necessary conditions for best approximation known; (local) optimizer computable with <b>iterative rational Krylov algorithm (IRKA)</b>
Hankel-norm $\ G\ _H := \sigma_{\max}$	optimal Hankel norm approximation (AAK theory).

# Qualitative and Quantitative Study of the Approximation Error

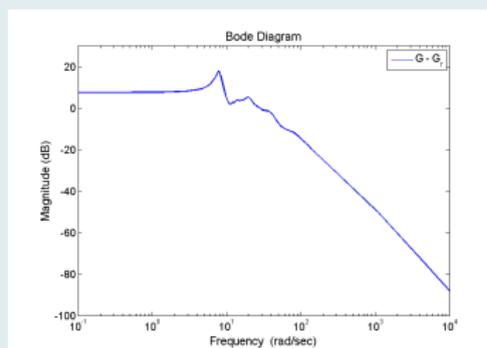
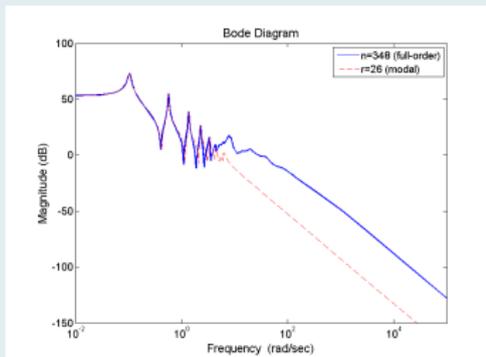
## Computable error measures

Evaluating system norms is computationally very (sometimes too) expensive.

## Other measures

- absolute errors  $\|G(j\omega_j) - \hat{G}(j\omega_j)\|_2$ ,  $\|G(j\omega_j) - \hat{G}(j\omega_j)\|_\infty$  ( $j = 1, \dots, N_\omega$ );
- relative errors  $\frac{\|G(j\omega_j) - \hat{G}(j\omega_j)\|_2}{\|G(j\omega_j)\|_2}$ ,  $\frac{\|G(j\omega_j) - \hat{G}(j\omega_j)\|_\infty}{\|G(j\omega_j)\|_\infty}$ ;
- "eyeball norm", i.e. look at **frequency response/Bode (magnitude) plot**:  
for SISO system, log-log plot frequency vs.  $|G(j\omega)|$  (or  $|G(j\omega) - \hat{G}(j\omega)|$ )  
in decibels,  $1 \text{ dB} \simeq 20 \log_{10}(\text{value})$ .

For MIMO systems,  $q \times m$  array of plots  $G_{ij}$ .







# Model Reduction by Projection

## Goals

- 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

$$\int_{-\infty}^t u(\tau)^T y(\tau) d\tau \geq 0 \quad \forall t \in \mathbb{R}, \quad \forall u \in L_2(\mathbb{R}, \mathbb{R}^m).$$

("system does not generate energy").

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$$\int_{-\infty}^t u(\tau)^T y(\tau) d\tau \geq 0 \quad \forall t \in \mathbb{R}, \quad \forall u \in L_2(\mathbb{R}, \mathbb{R}^m).$$

(“system does not generate energy”).

# Model Reduction by Projection

## Goals

- 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:
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# Model Reduction by Projection

## Projection Basics

### Definition 3.1 (Projector)

A projector is a matrix  $P \in \mathbb{R}^{n \times n}$  with  $P^2 = P$ . Let  $\mathcal{V} = \text{range}(P)$ , then  $P$  is **projector onto  $\mathcal{V}$** . On the other hand, if  $\{v_1, \dots, v_r\}$  is a basis of  $\mathcal{V}$  and  $V = [v_1, \dots, v_r]$ , then  $P = V(V^T V)^{-1} V^T$  is a projector onto  $\mathcal{V}$ .

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- Let  $\mathcal{W} \subset \mathbb{R}^n$  be another  $r$ -dimensional subspace and  $W = [w_1, \dots, w_r]$  be a basis matrix for  $\mathcal{W}$ , then  $P = V(W^T V)^{-1} W^T$  is an **oblique projector onto  $\mathcal{V}$  along  $\mathcal{W}$** .

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# Model Reduction by Projection

## Projection and Interpolation

### Methods:

- 1 Modal Truncation
- 2 Rational Interpolation (Padé-Approximation and (rational) Krylov Subspace Methods)
- 3 Balanced Truncation
- 4 many more...

Joint feature of these methods:

computation of reduced-order model (ROM) by projection!

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Assume trajectory  $x(t; u)$  is contained in low-dimensional subspace  $\mathcal{V}$ . Thus, use [Galerkin](#) or [Petrov-Galerkin-type projection](#) of state-space onto  $\mathcal{V}$  along complementary subspace  $\mathcal{W}$ :  $x \approx VW^T x =: \tilde{x}$ , where

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

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

$$\|x - \tilde{x}\| = \|x - V\hat{x}\|,$$

and the reduced-order model is

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

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Important observation:

- The state equation residual satisfies  $\dot{\tilde{x}} - A\tilde{x} - Bu \perp \mathcal{W}$ , since

$$W^T (\dot{\tilde{x}} - A\tilde{x} - Bu) = W^T (VW^T \dot{x} - AVW^T x - Bu)$$

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## Projection and Interpolation

### Projection $\rightsquigarrow$ Rational Interpolation

Given the ROM

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the error transfer function can be written as

$$G(s) - \hat{G}(s) = \left( C(sI_n - A)^{-1} B + D \right) - \left( \hat{C}(sI_r - \hat{A})^{-1} \hat{B} + \hat{D} \right)$$

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$\text{range}(P(s_*)) \subset \text{range}(V)$ , all matrices have full rank  $\Rightarrow$  "=",

$$P(s_*)^2 = V(s_* I_r - \hat{A})^{-1} W^T (s_* I_n - A) V(s_* I_r - \hat{A})^{-1} W^T (s_* I_n - A)$$

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If  $s_* \in \mathbb{C} \setminus (\Lambda(A) \cup \Lambda(\hat{A}))$ , then  $P(s_*)$  is a projector onto  $\mathcal{V} \implies$

$$\text{if } (s_* I_n - A)^{-1} B \in \mathcal{V}, \text{ then } (I_n - P(s_*))(s_* I_n - A)^{-1} B = 0,$$

hence

$$G(s_*) - \hat{G}(s_*) = 0 \implies G(s_*) = \hat{G}(s_*), \text{ i.e., } \hat{G} \text{ interpolates } G \text{ in } s_*!$$

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$$\text{Analogously, } = C(sI_n - A)^{-1} \underbrace{\left( I_n - (sI_n - A) V(sI_r - \hat{A})^{-1} W^T \right)}_{=: Q(s)} B.$$

If  $s_* \in \mathbb{C} \setminus (\Lambda(A) \cup \Lambda(\hat{A}))$ , then  $Q(s)^H$  is a projector onto  $\mathcal{W} \implies$

$$\text{if } (s_* I_n - A)^{-*} C^T \in \mathcal{W}, \text{ then } C(s_* I_n - A)^{-1} (I_n - Q(s_*)) = 0,$$

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# Model Reduction by Projection

## Projection and Interpolation

### Theorem 3.3

[GRIMME '97, VILLEMAGNE/SKELTON '87]

Given the ROM

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and  $s_* \in \mathbb{C} \setminus (\Lambda(A) \cup \Lambda(\hat{A}))$ , if either

- $(s_* I_n - A)^{-1} B \in \text{range}(V)$ , or
- $(s_* I_n - A)^{-*} C^T \in \text{range}(W)$ ,

then the interpolation condition

$$G(s_*) = \hat{G}(s_*).$$

in  $s_*$  holds.

Note: extension to Hermite interpolation conditions later!

# Modal Truncation

## Basic method:

Assume  $A$  is diagonalizable,  $T^{-1}AT = D_A$ , project state-space onto  $A$ -invariant subspace  $\mathcal{V} = \text{span}(t_1, \dots, t_r)$ ,  $t_k =$  eigenvectors corresp. to “dominant” modes / eigenvalues of  $A$ . Then with

$$V = T(:, 1:r) = [t_1, \dots, t_r], \quad \tilde{W}^H = T^{-1}(1:r,:), \quad W = \tilde{W}(V^H \tilde{W})^{-1},$$

reduced-order model is

$$\hat{A} := W^H A V = \text{diag}\{\lambda_1, \dots, \lambda_r\}, \quad \hat{B} := W^H B, \quad \hat{C} = C V$$

Also computable by truncation:

$$T^{-1}AT = \begin{bmatrix} \hat{A} & \\ & A_2 \end{bmatrix}, \quad T^{-1}B = \begin{bmatrix} \hat{B} \\ B_2 \end{bmatrix}, \quad CT = [\hat{C}, C_2], \quad \hat{D} = D.$$



# Modal Truncation

Basic method:

$$T^{-1}AT = \begin{bmatrix} \hat{A} & \\ & A_2 \end{bmatrix}, \quad T^{-1}B = \begin{bmatrix} \hat{B} \\ B_2 \end{bmatrix}, \quad CT = [\hat{C}, C_2], \quad \hat{D} = D.$$

Properties:

Error bound:

$$\|G - \hat{G}\|_{\infty} \leq \|C_2\| \|B_2\| \frac{1}{\min_{\lambda \in \Lambda(A_2)} |\operatorname{Re}(\lambda)|}.$$

Proof:

$$\begin{aligned} G(s) &= C(sI - A)^{-1}B + D = CTT^{-1}(sI - A)^{-1}TT^{-1}B + D \\ &= CT(sI - T^{-1}AT)^{-1}T^{-1}B + D \\ &= [\hat{C}, C_2] \begin{bmatrix} (sI_r - \hat{A})^{-1} & \\ & (sI_{n-r} - A_2)^{-1} \end{bmatrix} \begin{bmatrix} \hat{B} \\ B_2 \end{bmatrix} + D \\ &= \hat{G}(s) + C_2(sI_{n-r} - A_2)^{-1}B_2, \end{aligned}$$



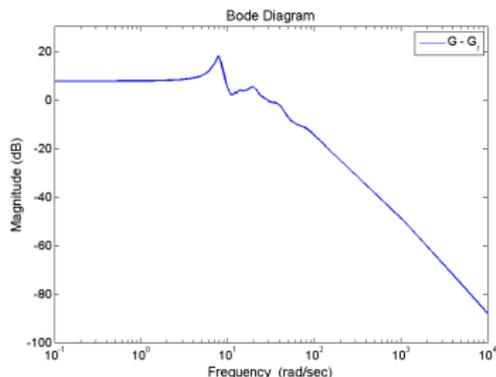
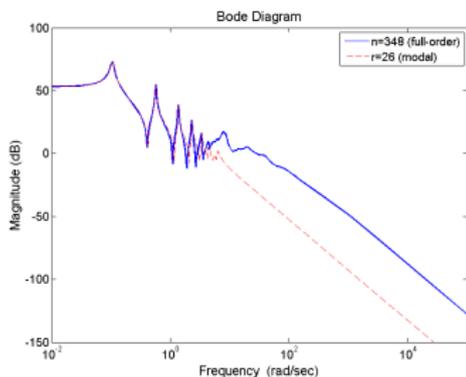


# Modal Truncation

## Example

**BEAM**, SISO system from [SLICOT Benchmark Collection for Model Reduction](#),  $n = 348$ ,  $m = q = 1$ , reduced using 13 dominant complex conjugate eigenpairs, error bound yields  $\|G - \hat{G}\|_{\infty} \leq 1.21 \cdot 10^3$

## Bode plots of transfer functions and error function



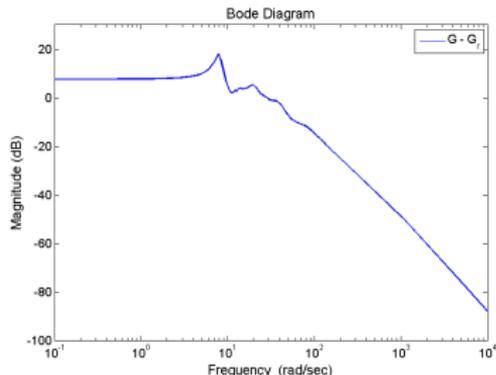
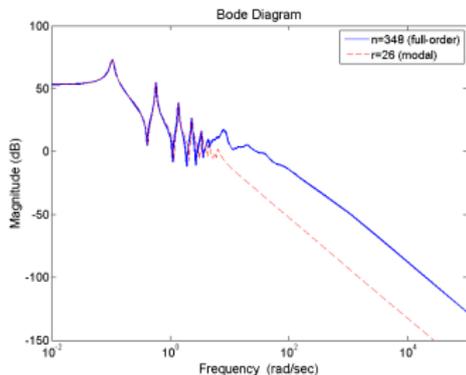
MATLAB® demo.

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## Bode plots of transfer functions and error function



MATLAB<sup>®</sup> demo.

# Modal Truncation

## Extensions

### Base enrichment

**Static modes** are defined by setting  $\dot{x} = 0$  and assuming unit loads, i.e.,  $u(t) \equiv e_j, j = 1, \dots, m$ :

$$0 = Ax(t) + Be_j \implies x(t) \equiv -A^{-1}b_j.$$

Projection subspace  $\mathcal{V}$  is then augmented by  $A^{-1}[b_1, \dots, b_m] = A^{-1}B$ .

**Interpolation-projection framework**  $\implies G(0) = \hat{G}(0)$ !

If two sided projection is used, complimentary subspace can be augmented by  $A^{-T}C^T \implies G'(0) = \hat{G}'(0)$ ! (If  $m \neq q$ , add random vectors or delete some of the columns in  $A^{-T}C^T$ ).







# Modal Truncation

## Dominant Poles

### Pole-Residue Form of Transfer Function

Consider partial fraction expansion of transfer function with  $D = 0$ :

$$G(s) = \sum_{k=1}^n \frac{R_k}{s - \lambda_k}$$

with the **residues**  $R_k := (Cx_k)(y_k^H B) \in \mathbb{C}^{q \times m}$ .

**Note:**  $R_k = (Cx_k)(y_k^H B)$  are the residues of  $G$  in the sense of the residue theorem of complex analysis:

$$\begin{aligned} \operatorname{res}(G, \lambda_\ell) &= \lim_{s \rightarrow \lambda_\ell} (s - \lambda_\ell) G(s) = \sum_{k=1}^n \underbrace{\lim_{s \rightarrow \lambda_\ell} \frac{s - \lambda_\ell}{s - \lambda_k}}_{R_k = R_\ell} \\ &= \begin{cases} 0 & \text{for } k \neq \ell \\ 1 & \text{for } k = \ell \end{cases} \end{aligned}$$



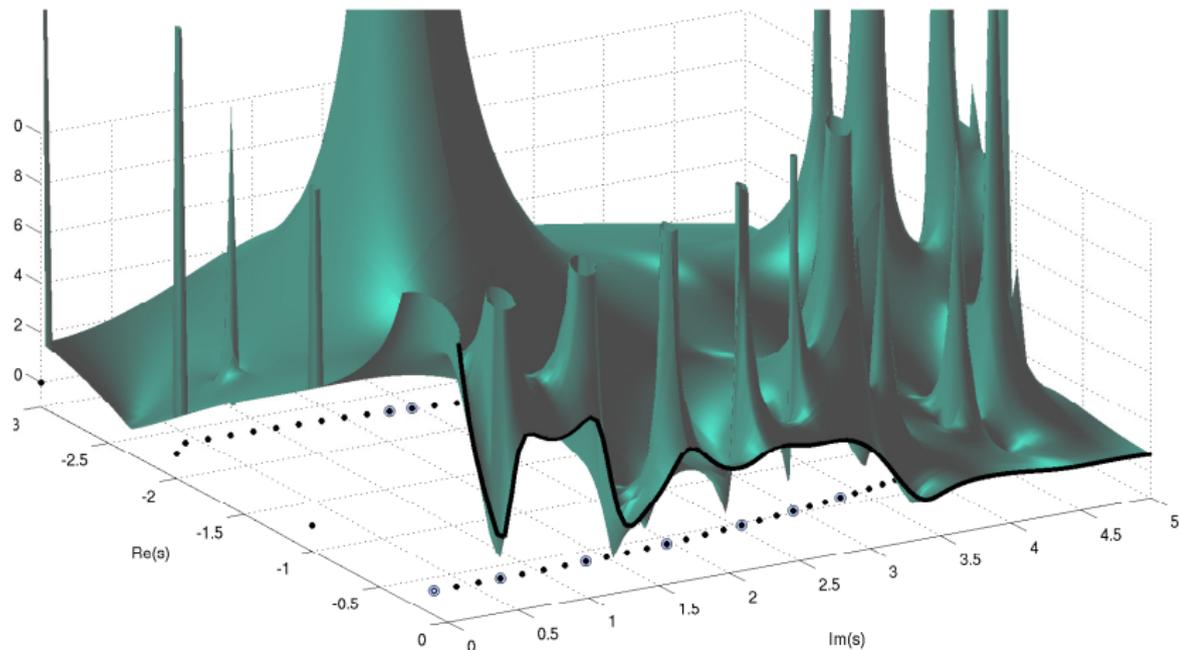






# Dominant Poles

Random SISO Example ( $B, C^T \in \mathbb{R}^n$ )













# Padé Approximation

## Idea:

- Consider (even for possibly singular  $E$  if  $\lambda E - A$  regular):

$$E\dot{x} = Ax + Bu, \quad y = Cx$$

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**Neumann Lemma.**  $\|F\| < 1 \Rightarrow I - F$  invertible,  $(I - F)^{-1} = \sum_{k=0}^{\infty} F^k$ .



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- As reduced-order model use **rth Padé approximant**  $\hat{G}$  to  $G$ :

$$G(s) = \hat{G}(s) + \mathcal{O}((s - s_0)^{2r}),$$

i.e.,  $m_k = \hat{m}_k$  for  $k = 0, \dots, 2r - 1$

$\rightsquigarrow$  **moment matching** if  $s_0 < \infty$ ,

$\rightsquigarrow$  **partial realization** if  $s_0 = \infty$ .

















# Padé Approximation

The Padé-Lanczos Connection [Gallivan/Grimme/Van Dooren 1994, Freund/Feldmann 1994]

## Padé-via-Lanczos Method (PVL)

### Difficulties:

- Computable error estimates/bounds for  $\|y - \hat{y}\|_2$  often very pessimistic or expensive to evaluate.
- Mostly heuristic criteria for choice of expansion points.  
Optimal choice for second-order systems with proportional/Rayleigh damping (BEATTIE/GUGERCIN '05).
- Good approximation quality only locally.
- Preservation of physical properties only in special cases (e.g. PRIMA/Arnoldi:  $V^T A V$  is stable if  $A$  is negative definite or dissipative  $\rightsquigarrow$  exercises); usually requires post processing which (partially) destroys moment matching properties.



# Interpolatory Model Reduction

## A Change of Perspective: Rational Interpolation

### Computation of reduced-order model by projection

Given an LTI system  $\dot{x} = Ax + Bu, y = Cx$  with transfer function  $G(s) = C(sI_n - A)^{-1}B$ , a reduced-order model is obtained using projection approach with  $V, W \in \mathbb{R}^{n \times r}$  and  $W^T V = I_r$  by computing

$$\hat{A} = W^T A V, \quad \hat{B} = W^T B, \quad \hat{C} = C V.$$

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

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



# Interpolatory Model Reduction

## A Change of Perspective: Rational Interpolation

Theorem (simplified) [GRIMME '97, VILLEMAGNE/SKELTON '87]

If

$$\begin{aligned} \text{span} \{ (s_1 I_n - A)^{-1} B, \dots, (s_k I_n - A)^{-1} B \} &\subset \text{Ran}(V), \\ \text{span} \{ (s_1 I_n - A)^{-T} C^T, \dots, (s_k I_n - A)^{-T} C^T \} &\subset \text{Ran}(W), \end{aligned}$$

then

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

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Remarks:

using Galerkin/one-sided projection yields  $G(s_j) = \hat{G}(s_j)$ , but in general

$$\frac{d}{ds} G(s_j) \neq \frac{d}{ds} \hat{G}(s_j).$$

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Remarks:

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

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

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Remarks:

computation of  $V, W$  from [rational Krylov subspaces](#), e.g.,

- dual rational Arnoldi/Lanczos [GRIMME '97],
- Iterative Rational Krylov-[Algo.](#) [ANTOULAS/BEATTIE/GUGERCIN '07].

# $\mathcal{H}_2$ -Optimal Model Reduction

Best  $\mathcal{H}_2$ -norm approximation problem

$$\text{Find } \arg \min_{\hat{G} \in \mathcal{H}_2 \text{ of order } \leq r} \|G - \hat{G}\|_2.$$

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$\rightsquigarrow$  First-order necessary  $\mathcal{H}_2$ -optimality conditions:

For SISO systems

$$\begin{aligned} G(-\mu_i) &= \hat{G}(-\mu_i), \\ G'(-\mu_i) &= \hat{G}'(-\mu_i), \end{aligned}$$

where  $\mu_i$  are the poles of the reduced transfer function  $\hat{G}$ .

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For MIMO systems

$$\begin{aligned} G(-\mu_i)\tilde{B}_i &= \hat{G}(-\mu_i)\tilde{B}_i, & \text{for } i = 1, \dots, r, \\ \tilde{C}_i^T G(-\mu_i) &= \tilde{C}_i^T \hat{G}(-\mu_i), & \text{for } i = 1, \dots, r, \\ \tilde{C}_i^T G'(-\mu_i)\tilde{B}_i &= \tilde{C}_i^T \hat{G}'(-\mu_i)\tilde{B}_i, & \text{for } i = 1, \dots, r, \end{aligned}$$

where  $T^{-1}\hat{A}T = \text{diag}\{\mu_1, \dots, \mu_r\} = \text{spectral decomposition}$  and

$$\tilde{B} = \hat{B}^T T^{-T}, \quad \tilde{C} = \hat{C}T.$$

$\rightsquigarrow$  [tangential interpolation conditions](#).

# Interpolatory Model Reduction

## Interpolation of the Transfer Function by Projection

Construct reduced transfer function by **Petrov-Galerkin** projection

$\mathcal{P} = VW^T$ , i.e.

$$\hat{G}(s) = CV (sI - W^T AV)^{-1} W^T B,$$

where  $V$  and  $W$  are given as the **rational Krylov subspaces**

$$V = [(-\mu_1 I - A)^{-1} B, \dots, (-\mu_r I - A)^{-1} B],$$

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Then

$$G(-\mu_i) = \hat{G}(-\mu_i) \quad \text{and} \quad G'(-\mu_i) = \hat{G}'(-\mu_i),$$

for  $i = 1, \dots, r$  as desired.

$\rightsquigarrow$  iterative algorithms (IRKA/MIRIAM) that yield  $\mathcal{H}_2$ -optimal models.

[GUGERCIN ET AL. '06], [BUNSE-GERSTNER ET AL. '07],  
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# $\mathcal{H}_2$ -Optimal Model Reduction

## The Basic IRKA Algorithm

---

### Algorithm 1 IRKA (MIMO version/MIRIAm)

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**Input:**  $A$  stable,  $B$ ,  $C$ ,  $\hat{A}$  stable,  $\hat{B}$ ,  $\hat{C}$ ,  $\delta > 0$ .

**Output:**  $A^{opt}$ ,  $B^{opt}$ ,  $C^{opt}$

- 1: **while**  $(\max_{j=1,\dots,r} \left\{ \frac{|\mu_j - \mu_j^{old}|}{|\mu_j|} \right\} > \delta)$  **do**
  - 2:  $\text{diag} \{ \mu_1, \dots, \mu_r \} := T^{-1} \hat{A} T = \text{spectral decomposition,}$   
 $\tilde{B} = \hat{B}^H T^{-T}, \tilde{C} = \hat{C} T.$
  - 3:  $V = \left[ (-\mu_1 I - A)^{-1} B \tilde{B}_1, \dots, (-\mu_r I - A)^{-1} B \tilde{B}_r \right]$
  - 4:  $W = \left[ (-\mu_1 I - A^T)^{-1} C^T \tilde{C}_1, \dots, (-\mu_r I - A^T)^{-1} C^T \tilde{C}_r \right]$
  - 5:  $V = \text{orth}(V), W = \text{orth}(W), W = W(V^H W)^{-1}$
  - 6:  $\hat{A} = W^H A V, \hat{B} = W^H B, \hat{C} = C V$
  - 7: **end while**
  - 8:  $A^{opt} = \hat{A}, B^{opt} = \hat{B}, C^{opt} = \hat{C}$
-



# Balanced Truncation

## Basic principle:

- Recall: a stable system  $\Sigma$ , realized by  $(A, B, C, D)$ , is called **balanced**, if the **Gramians**, i.e., solutions  $P, Q$  of the **Lyapunov equations**

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

satisfy:  $P = Q = \text{diag}(\sigma_1, \dots, \sigma_n)$  with  $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_n > 0$ .

- $\Lambda(PQ)^{\frac{1}{2}} = \{\sigma_1, \dots, \sigma_n\}$  are the Hankel singular values (HSVs) of  $\Sigma$ .

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- $\Lambda(PQ)^{\frac{1}{2}} = \{\sigma_1, \dots, \sigma_n\}$  are the **Hankel singular values (HSVs)** of  $\Sigma$ .
- Compute balanced realization of the system via **state-space transformation**

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

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

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# Balanced Truncation

## Motivation:

The HSVs  $\Lambda(PQ)^{\frac{1}{2}} = \{\sigma_1, \dots, \sigma_n\}$  are **system invariants**: they are preserved under

$$\mathcal{T} : (A, B, C, D) \mapsto (TAT^{-1}, TB, CT^{-1}, D)$$



# Balanced Truncation

## Implementation: SR Method

- 1 Compute (Cholesky) factors of the Gramians,  $P = S^T S$ ,  $Q = R^T R$ .
- 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 ROM is  $(W^T A V, W^T B, C V, D)$ , where

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## Properties:

- Reduced-order model is stable with HSVs  $\sigma_1, \dots, \sigma_r$ .
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### Linear, Time-Invariant (LTI) Systems

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

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Assumptions (for now):  $t_0 = 0$ ,  $x_0 = x(0) = 0$ ,  $D = 0$ .

















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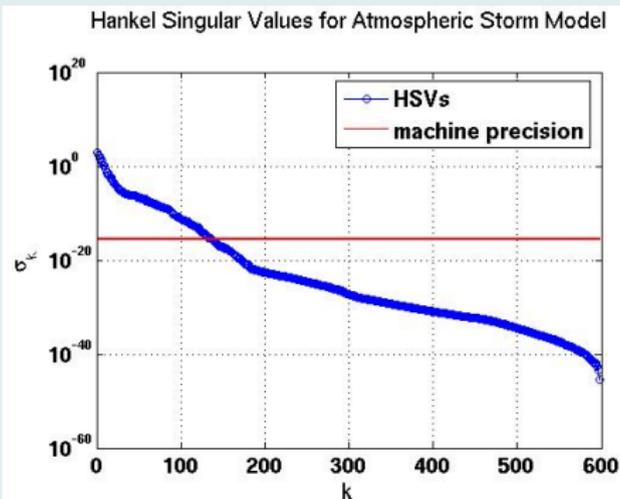
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Let  $P, Q$  be the controllability and observability Gramians of an LTI system  $\Sigma$ . Then the Hankel singular values  $\Lambda(PQ)^{\frac{1}{2}} = \{\sigma_1, \dots, \sigma_n\}$  are the singular values of the Hankel operator associated to  $\Sigma$ .

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## Singular Perturbation Approximation (aka Balanced Residualization)

Assume the system

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \end{bmatrix} = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \begin{bmatrix} B_1 \\ B_2 \end{bmatrix} u, \quad y = [C_1, C_2] \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + Du$$

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Particularly, if  $G(0) = \hat{G}(0)$  ("**zero steady-state error**") is required, one can apply the same condensation technique as in Guyan reduction: instead of  $x_2 = 0$ , set  $\dot{x}_2 = 0$ . This yields the reduced-order model

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with

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**Note:**

- $A_{22}$  invertible as in balanced coordinates,  $A_{22}\Sigma_2 + \Sigma_2A_{22}^T + B_2B_2^T = 0$  and  $(A_{22}, B_2)$  controllable,  $\Sigma_2 > 0 \Rightarrow A_{22}$  stable.
- If the original system is not balanced, first compute a minimal realization by applying balanced truncation with  $r = \hat{n}$ .

# Balancing-Related Methods

## Basic Principle

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

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

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## Classical Balanced Truncation (BT) [MULLIS/ROBERTS '76, MOORE '81]

- $P$  = controllability Gramian of system given by  $(A, B, C, D)$ .
- $Q$  = observability Gramian of system given by  $(A, B, C, D)$ .
- $P, Q$  solve dual [Lyapunov equations](#)

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

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## LQG 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)**

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

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







# Balancing-Related Methods

## Properties

- Guaranteed preservation of physical properties like
  - stability (all),
  - passivity (PRBT),
  - minimum phase (BST).
- Computable error bounds, e.g.,

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

$$\text{LQGBT: } \|G - G_r\|_\infty \leq 2 \sum_{j=r+1}^n \frac{\sigma_j^{LQG}}{\sqrt{1+(\sigma_j^{LQG})^2}}$$

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

- Can be combined with singular perturbation approximation for steady-state performance.
- Computations can be modularized.

# Outline

- 1 Introduction
- 2 Mathematical Basics
- 3 Model Reduction by Projection
- 4 Interpolatory Model Reduction
- 5 Balanced Truncation
- 6 Solving Large-Scale Matrix Equations**
  - Linear Matrix Equations
  - Numerical Methods for Solving Lyapunov Equations
  - Solving Large-Scale Algebraic Riccati Equations
  - Software
- 7 Final Remarks

# Solving Large-Scale Matrix Equations

## Large-Scale Algebraic Lyapunov and Riccati Equations

Algebraic Riccati equation (ARE) for  $A, G = G^T, W = W^T \in \mathbb{R}^{n \times n}$  given and  $X \in \mathbb{R}^{n \times n}$  unknown:

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

$G = 0 \implies$  Lyapunov equation:

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Typical situation in model reduction and optimal control problems for semi-discretized PDEs:

- $n = 10^3 - 10^6$  ( $\implies 10^6 - 10^{12}$  unknowns!),
- $A$  has sparse representation ( $A = -M^{-1}S$  for FEM),
- $G, W$  low-rank with  $G, W \in \{BB^T, C^T C\}$ , where  $B \in \mathbb{R}^{n \times m}, m \ll n, C \in \mathbb{R}^{p \times n}, p \ll n$ .
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Algebraic Riccati equation (ARE) for  $A, G = G^T, W = W^T \in \mathbb{R}^{n \times n}$  given and  $X \in \mathbb{R}^{n \times n}$  unknown:

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

$G = 0 \implies$  Lyapunov equation:

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

Typical situation in model reduction and optimal control problems for semi-discretized PDEs:

- $n = 10^3 - 10^6$  ( $\implies 10^6 - 10^{12}$  unknowns!),
- $A$  has sparse representation ( $A = -M^{-1}S$  for FEM),
- $G, W$  low-rank with  $G, W \in \{BB^T, C^T C\}$ , where  $B \in \mathbb{R}^{n \times m}, m \ll n, C \in \mathbb{R}^{p \times n}, p \ll n$ .
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## Low-Rank Approximation

Consider spectrum of ARE solution (analogous for Lyapunov equations).

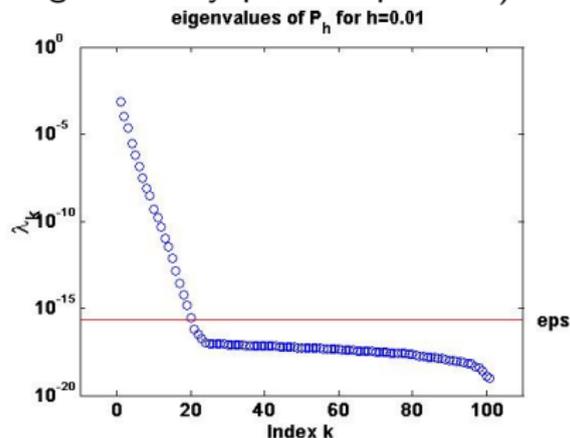
### Example:

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

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

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

$\implies$  Goal: compute  $Z^{(r)} \in \mathbb{R}^{n \times r}$  directly w/o ever forming  $X$ !



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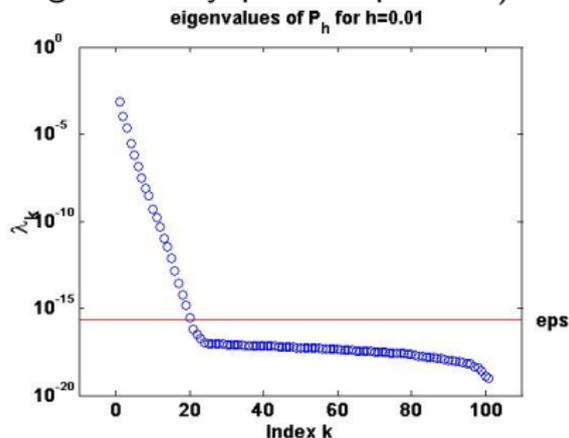
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## Linear Matrix Equations

### Equations without symmetry

Sylvester equation

$$AX + XB = W$$

discrete Sylvester equation

$$AXB - X = W$$

with data  $A \in \mathbb{R}^{n \times n}$ ,  $B \in \mathbb{R}^{m \times m}$ ,  $W \in \mathbb{R}^{n \times m}$  and unknown  $X \in \mathbb{R}^{n \times m}$ .

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# Linear Matrix Equations

## Solvability

Using the **Kronecker (tensor) product**,  $AX + XB = W$  is equivalent to

$$((I_m \otimes A) + (B^T \otimes I_n)) \operatorname{vec}(X) = \operatorname{vec}(W).$$

Hence,

Sylvester equation has a unique solution

$$\iff$$

$M := (I_m \otimes A) + (B^T \otimes I_n)$  is invertible.

$$\iff$$

$$0 \notin \Lambda(M) = \Lambda((I_m \otimes A) + (B^T \otimes I_n)) = \{\lambda_j + \mu_k, \mid \lambda_j \in \Lambda(A), \mu_k \in \Lambda(B)\}.$$

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### Corollary

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Solving the **Sylvester equation**

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via the **equivalent** linear system of equations

$$((I_m \otimes A) + (B^T \otimes I_n)) \operatorname{vec}(X) = \operatorname{vec}(W)$$

requires

- LU factorization of  $nm \times nm$  matrix; for  $n \approx m$ , **complexity is  $\frac{2}{3}n^6$** ;
- storing  $n \cdot m$  unknowns: for  $n \approx m$  we have  **$n^4$  data** for  $X$ .

### Example

$n = m = 1,000 \Rightarrow$  Gaussian elimination on an Intel core i7 (Westmere, 6 cores, 3.46 GHz  $\rightsquigarrow$  83.2 GFLOP peak) would take  $> 94$  DAYS and 7.3 TB of memory!

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## Traditional Methods

Bartels-Stewart method for Sylvester and Lyapunov equation (lyap);  
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All based on the fact that if  $A, B^T$  are in **Schur form**, then

$$M = (I_m \otimes A) + (B^T \otimes I_n)$$

is block-upper triangular. Hence, solve  $Mx = b$  by back-substitution.

- Clever implementation of back-substitution process requires  $nm(n+m)$  flops.
- For Sylvester eqns.,  $B$  in Hessenberg form is enough ( $\rightsquigarrow$  Hessenberg-Schur method).
- Hammarling's method computes Cholesky factor  $Y$  of  $X$  directly.
- All methods require **Schur decomposition** of  $A$  and **Schur or Hessenberg decomposition** of  $B \Rightarrow$  need QR algorithm which requires  $25n^3$  flops for Schur decomposition.

Not feasible for large-scale problems ( $n > 10,000$ ).

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# Numerical Methods for Solving Lyapunov Equations

## The Sign Function Method

### Definition

For  $Z \in \mathbb{R}^{n \times n}$  with  $\Lambda(Z) \cap i\mathbb{R} = \emptyset$  and Jordan canonical form

$$Z = S \begin{bmatrix} J^+ & 0 \\ 0 & J^- \end{bmatrix} S^{-1}$$

the **matrix sign function** is

$$\text{sign}(Z) := S \begin{bmatrix} I_k & 0 \\ 0 & -I_{n-k} \end{bmatrix} S^{-1}.$$

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### Lemma

Let  $T \in \mathbb{R}^{n \times n}$  be nonsingular and  $Z$  as before, then

$$\text{sign}(TZT^{-1}) = T \text{sign}(Z) T^{-1}$$

# Numerical Methods for Solving Lyapunov Equations

## The Sign Function Method

### Computation of $\text{sign}(Z)$

$\text{sign}(Z)$  is root of  $I_n \implies$  use Newton's method to compute it:

$$Z_0 \leftarrow Z, \quad Z_{j+1} \leftarrow \frac{1}{2} \left( c_j Z_j + \frac{1}{c_j} Z_j^{-1} \right), \quad j = 1, 2, \dots$$

$$\implies \text{sign}(Z) = \lim_{j \rightarrow \infty} Z_j.$$

$c_j > 0$  is scaling parameter for convergence acceleration and rounding error minimization, e.g.

$$c_j = \sqrt{\frac{\|Z_j^{-1}\|_F}{\|Z_j\|_F}},$$

based on “equilibrating” the norms of the two summands [HIGHAM '86].

# Solving Lyapunov Equations with the Matrix Sign Function Method

## Key observation:

If  $X \in \mathbb{R}^{n \times n}$  is a solution of  $AX + XA^T + W = 0$ , then

$$\underbrace{\begin{bmatrix} I_n & -X \\ 0 & I_n \end{bmatrix}}_{=:T^{-1}} \underbrace{\begin{bmatrix} A & W \\ 0 & -A^T \end{bmatrix}}_{=:H} \underbrace{\begin{bmatrix} I_n & X \\ 0 & I_n \end{bmatrix}}_{=:T} = \begin{bmatrix} A & 0 \\ 0 & -A^T \end{bmatrix}.$$

Hence, if  $A$  is Hurwitz (i.e., asymptotically stable), then

$$\begin{aligned} \text{sign}(H) &= \text{sign} \left( T \begin{bmatrix} A & 0 \\ 0 & -A^T \end{bmatrix} T^{-1} \right) = T \text{sign} \left( \begin{bmatrix} A & 0 \\ 0 & -A^T \end{bmatrix} \right) T^{-1} \\ &= \begin{bmatrix} -I_n & 2X \\ 0 & I_n \end{bmatrix}. \end{aligned}$$

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## Solving Lyapunov Equations with the Matrix Sign Function Method

Apply sign function iteration  $Z \leftarrow \frac{1}{2}(Z + Z^{-1})$  to  $H = \begin{bmatrix} A & W \\ 0 & -A^T \end{bmatrix}$ :

$$H + H^{-1} = \begin{bmatrix} A & W \\ 0 & -A^T \end{bmatrix} + \begin{bmatrix} A^{-1} & A^{-1}WA^{-T} \\ 0 & -A^{-T} \end{bmatrix}$$

$\implies$  Sign function iteration for Lyapunov equation:

$$\begin{aligned} A_0 &\leftarrow A, & A_{j+1} &\leftarrow \frac{1}{2} \left( A_j + A_j^{-1} \right), \\ W_0 &\leftarrow G, & W_{j+1} &\leftarrow \frac{1}{2} \left( W_j + A_j^{-1} W_j A_j^{-T} \right), \end{aligned} \quad j = 0, 1, 2, \dots$$

Define  $A_\infty := \lim_{j \rightarrow \infty} A_j$ ,  $W_\infty := \lim_{j \rightarrow \infty} W_j$ .

### Theorem

If  $A$  is Hurwitz, then

$$A_\infty = -I_n \quad \text{and} \quad X = \frac{1}{2} W_\infty.$$

# Solving Lyapunov Equations with the Matrix Sign Function Method

## Factored form

Recall sign function iteration for  $AX + XA^T + W = 0$ :

$$\begin{aligned} A_0 &\leftarrow A, & A_{j+1} &\leftarrow \frac{1}{2} (A_j + A_j^{-1}), \\ W_0 &\leftarrow G, & W_{j+1} &\leftarrow \frac{1}{2} (W_j + A_j^{-1} W_j A_j^{-T}), \end{aligned} \quad j = 0, 1, 2, \dots$$

Now consider the second iteration for  $W = BB^T$ , starting with  $W_0 = BB^T =: B_0 B_0^T$ :

$$\begin{aligned} \frac{1}{2} (W_j + A_j^{-1} W_j A_j^{-T}) &= \frac{1}{2} (B_j B_j^T + A_j^{-1} B_j B_j^T A_j^{-T}) \\ &= \frac{1}{2} [B_j \quad A_j^{-1} B_j] [B_j \quad A_j^{-1} B_j]^T. \end{aligned}$$

Hence, obtain factored iteration

$$B_{j+1} \leftarrow \frac{1}{\sqrt{2}} [B_j \quad A_j^{-1} B_j]$$

with  $S := \frac{1}{\sqrt{2}} \lim_{j \rightarrow \infty} B_j$  and  $X = SS^T$ .

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## Solving Lyapunov Equations with the Matrix Sign Function Method

Factored form

[B./Quintana-Ortí '97]

Factored sign function iteration for  $A(SS^T) + (SS^T)A^T + BB^T = 0$ 

$$A_0 \leftarrow A, \quad A_{j+1} \leftarrow \frac{1}{2} (A_j + A_j^{-1}),$$

$$B_0 \leftarrow B, \quad B_{j+1} \leftarrow \frac{1}{\sqrt{2}} [B_j \quad A_j^{-1} B_j], \quad j = 0, 1, 2, \dots$$

## Remarks:

- To get both Gramians, run in parallel

$$C_{j+1} \leftarrow \frac{1}{\sqrt{2}} \begin{bmatrix} C_j \\ C_j A_j^{-1} \end{bmatrix}.$$

- To avoid growth in numbers of columns of  $B_j$  (or rows of  $C_j$ ): column compression by RRLQ or truncated SVD.
- Several options to incorporate scaling, e.g., scale "A"-iteration only.
- Simple stopping criterion:  $\|A_j + I_n\|_F \leq \text{tol}$ .

# Numerical Methods for Solving Lyapunov Equations

## The ADI Method

Recall Peaceman Rachford ADI:

Consider  $Au = s$  where  $A \in \mathbb{R}^{n \times n}$  spd,  $s \in \mathbb{R}^n$ . ADI Iteration Idea:  
Decompose  $A = H + V$  with  $H, V \in \mathbb{R}^{n \times n}$  such that

$$\begin{aligned}(H + pI)v &= r \\ (V + pI)w &= t\end{aligned}$$

can be solved easily/efficiently.

### ADI Iteration

If  $H, V$  spd  $\Rightarrow \exists p_k, k = 1, 2, \dots$  such that

$$\begin{aligned}u_0 &= 0 \\ (H + p_k I)u_{k-\frac{1}{2}} &= (p_k I - V)u_{k-1} + s \\ (V + p_k I)u_k &= (p_k I - H)u_{k-\frac{1}{2}} + s\end{aligned}$$

converges to  $u \in \mathbb{R}^n$  solving  $Au = s$ .

# Numerical Methods for Solving Lyapunov Equations

## The ADI Method

Recall Peaceman Rachford ADI:

Consider  $Au = s$  where  $A \in \mathbb{R}^{n \times n}$  spd,  $s \in \mathbb{R}^n$ . ADI Iteration Idea:  
Decompose  $A = H + V$  with  $H, V \in \mathbb{R}^{n \times n}$  such that

$$\begin{aligned}(H + pI)v &= r \\ (V + pI)w &= t\end{aligned}$$

can be solved easily/efficiently.

### ADI Iteration

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## Numerical Methods for Solving Lyapunov Equations

The Lyapunov operator

$$\mathcal{L}: P \mapsto AX + XA^T$$

can be decomposed into the linear operators

$$\mathcal{L}_H: X \mapsto AX, \quad \mathcal{L}_V: X \mapsto XA^T.$$

In analogy to the standard ADI method we find the

### ADI iteration for the Lyapunov equation

[WACHSPRESS '88]

$$\begin{aligned} X_0 &= 0 \\ (A + p_k I)X_{k-\frac{1}{2}} &= -W - X_{k-1}(A^T - p_k I) \\ (A + p_k I)X_k^T &= -W - X_{k-\frac{1}{2}}^T(A^T - p_k I). \end{aligned}$$

# Numerical Methods for Solving Lyapunov Equations

## Low-Rank ADI

Consider  $AX + XA^T = -BB^T$  for stable  $A$ ;  $B \in \mathbb{R}^{n \times m}$  with  $m \ll n$ .

### ADI iteration for the Lyapunov equation

[WACHSPRESS '95]

For  $k = 1, \dots, k_{\max}$

$$\begin{aligned} X_0 &= 0 \\ (A + p_k I)X_{k-\frac{1}{2}} &= -BB^T - X_{k-1}(A^T - p_k I) \\ (A + p_k I)X_k^T &= -BB^T - X_{k-\frac{1}{2}}^T(A^T - p_k I) \end{aligned}$$

Rewrite as one step iteration and factorize  $X_k = Z_k Z_k^T$ ,  $k = 0, \dots, k_{\max}$

$$\begin{aligned} Z_0 Z_0^T &= 0 \\ Z_k Z_k^T &= -2p_k (A + p_k I)^{-1} B B^T (A + p_k I)^{-T} \\ &\quad + (A + p_k I)^{-1} (A - p_k I) Z_{k-1} Z_{k-1}^T (A - p_k I)^T (A + p_k I)^{-T} \end{aligned}$$

$\dots \rightsquigarrow$  low-rank Cholesky factor ADI

[PENZL '97/'00, LI/WHITE '99/'02, B./LI/PENZL '99/'08, GUGERCIN/SORENSEN/ANTOULAS '03]

# Numerical Methods for Solving Lyapunov Equations

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[PENZL '97/'00, LI/WHITE '99/'02, B./LI/PENZL '99/'08, GUGERCIN/SORENSEN/ANTOULAS '03]

# Solving Large-Scale Matrix Equations

## Numerical Methods for Solving Lyapunov Equations

$$Z_k = [\sqrt{-2p_k}(A + p_k I)^{-1}B, (A + p_k I)^{-1}(A - p_k I)Z_{k-1}]$$

[PENZL '00]

Observing that  $(A - p_i I)$ ,  $(A + p_k I)^{-1}$  commute, we rewrite  $Z_{k_{\max}}$  as

$$Z_{k_{\max}} = [z_{k_{\max}}, P_{k_{\max}-1}z_{k_{\max}}, P_{k_{\max}-2}(P_{k_{\max}-1}z_{k_{\max}}), \dots, P_1(P_2 \cdots P_{k_{\max}-1}z_{k_{\max}})],$$

[LI/WHITE '02]

where

$$z_{k_{\max}} = \sqrt{-2p_{k_{\max}}}(A + p_{k_{\max}} I)^{-1}B$$

and

$$P_i := \frac{\sqrt{-2p_i}}{\sqrt{-2p_{i+1}}} [I - (p_i + p_{i+1})(A + p_i I)^{-1}].$$

# Solving Large-Scale Matrix Equations

## Numerical Methods for Solving Lyapunov Equations

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# Numerical Methods for Solving Lyapunov Equations

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

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

$$V_1 \leftarrow \sqrt{-2 \operatorname{re} p_1} (A + p_1 I)^{-1} B, \quad Z_1 \leftarrow V_1$$

FOR  $k = 2, 3, \dots$

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

$$Z_k \leftarrow \begin{bmatrix} Z_{k-1} & V_k \end{bmatrix}$$

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

At convergence,  $Z_{k_{\max}} Z_{k_{\max}}^T \approx X$ , where (without column compression)

$$Z_{k_{\max}} = \begin{bmatrix} V_1 & \dots & V_{k_{\max}} \end{bmatrix}, \quad V_k = \begin{bmatrix} \phantom{0} \end{bmatrix} \in \mathbb{C}^{n \times m}.$$

**Note:** Implementation in real arithmetic possible by combining two steps [B./Li/Penzl '99/'08] or using new idea employing the relation of 2 consecutive complex factors [B./Kürschner/Saak '11].

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# Numerical Results for ADI

## Optimal Cooling of Steel Profiles

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

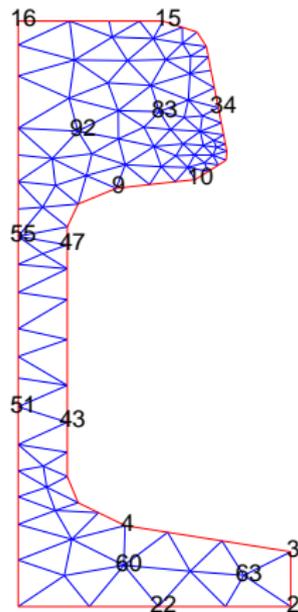
$$c \cdot \rho \frac{\partial}{\partial t} x = \lambda \Delta x, \quad \xi \in \Omega$$

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

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

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

- 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 1999/2001, PENZL 1999, SAAK 2003.

# Numerical Results for ADI

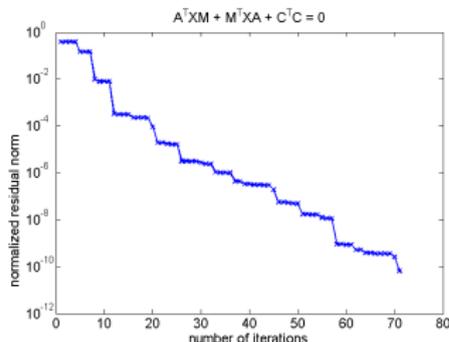
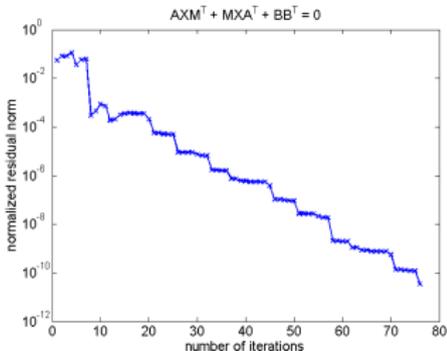
## Optimal Cooling of Steel Profiles

- Solve dual Lyapunov equations needed for balanced truncation, i.e.,

$$APM^T + MPA^T + BB^T = 0, \quad A^TQM + M^TQA + C^TC = 0,$$

for  $n = 79,841$ .

- 25 shifts chosen by Penzl heuristic from 50/25 Ritz values of  $A$  of largest/smallest magnitude, no column compression performed.
- No factorization of mass matrix required.
- Computations done on Core2Duo at 2.8GHz with 3GB RAM and 32Bit-MATLAB.



CPU times: 626 / 356 sec.



# Numerical Results for ADI

Scaling / Mesh Independence

Computations by Martin Köhler '10

- $A \in \mathbb{R}^{n \times n} \equiv$  FDM matrix for 2D heat equation on  $[0, 1]^2$  (LYAPACK benchmark demo\_11,  $m = 1$ ).
- 16 shifts chosen by Penzl heuristic from 50/25 Ritz values of  $A$  of largest/smallest magnitude.
- Computations on 2 dual core Intel Xeon 5160 with 16 GB RAM using M.E.S.S. (<http://svncsc.mpi-magdeburg.mpg.de/trac/messtrac/>).

## CPU Times

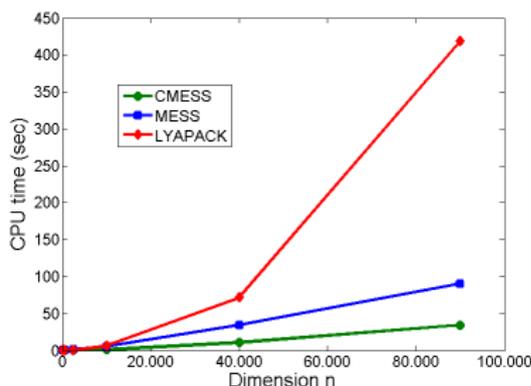
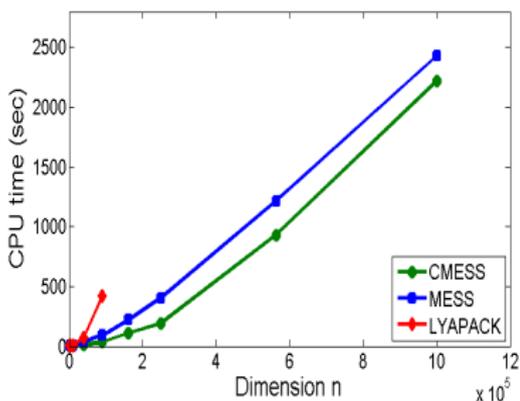
n	M.E.S.S. <sup>1</sup> (C)	LyaPack	M.E.S.S. (MATLAB)
100	0.023	0.124	0.158
625	0.042	0.104	0.227
2,500	0.159	0.702	0.989
10,000	0.965	6.22	5.644
40,000	11.09	71.48	34.55
90,000	34.67	418.5	90.49
160,000	109.3	out of memory	219.9
250,000	193.7	out of memory	403.8
562,500	930.1	out of memory	1216.7
1,000,000	2220.0	out of memory	2428.6

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**Note:** for  $n = 1,000,000$ , **first** sparse LU needs  $\sim 1,100$  sec., using UMFPACK this reduces to 30 sec.

# Factored Galerkin-ADI Iteration

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

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  $m = 1$ :

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

[SAAD '90, JAIMOUKHA/KASENALLY '94, JBILOU '02-'08].

- K-PIK [SIMONCINI '07],

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

- Rational Krylov [DRUSKIN/SIMONCINI '11] ( $\rightsquigarrow$  exercises).

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Examples:

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

$$\mathcal{Z} = \text{colspan} \left[ \begin{array}{c} V_1, \quad \dots, \quad V_r \end{array} \right].$$

Note:

- ① ADI subspace is rational Krylov subspace [J.-R. LI/WHITE '02].
- ② Similar approach: ADI-preconditioned global Arnoldi method [JBILOU '08].

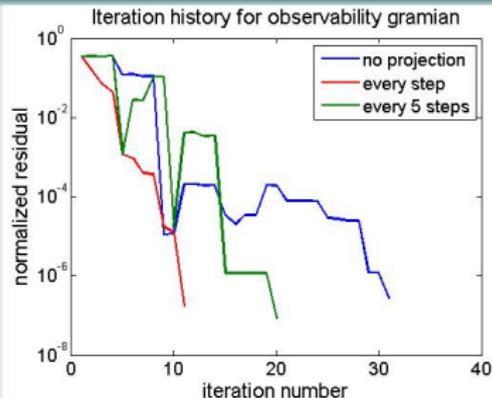
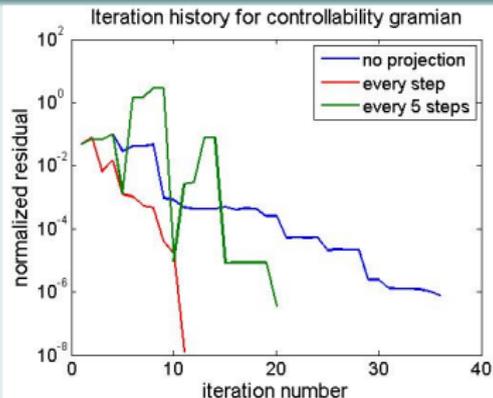
# Numerical Methods for Solving Lyapunov Equations

## Numerical examples for Galerkin-ADI

FEM semi-discretized control problem for parabolic PDE:

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

### Good ADI shifts



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

Computations by Jens Saak '10.

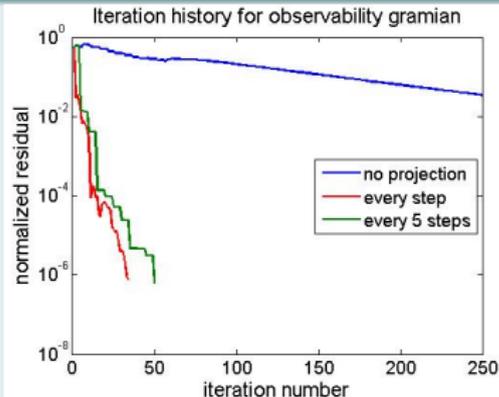
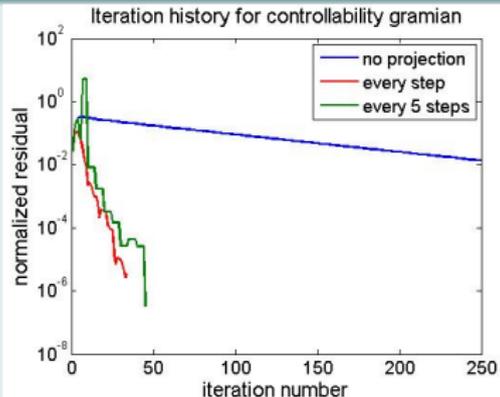
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### Bad ADI shifts



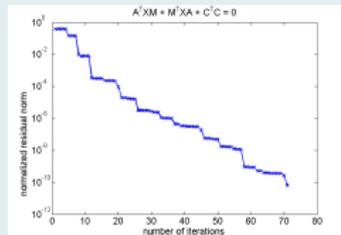
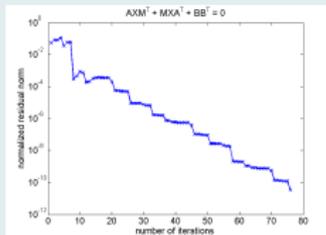
CPU times: 368s (projection every 5th ADI step) vs. 1207s (no projection).

Computations by Jens Saak '10.

# Numerical Methods for Solving Lyapunov Equations

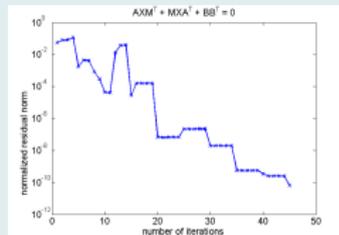
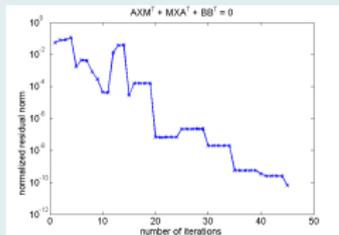
Numerical examples for Galerkin-ADI: optimal cooling of rail profiles,  $n = 79,841$ .

## M.E.S.S. w/o Galerkin projection and column compression



Rank of solution factors: 532 / 426

## M.E.S.S. with Galerkin projection and column compression

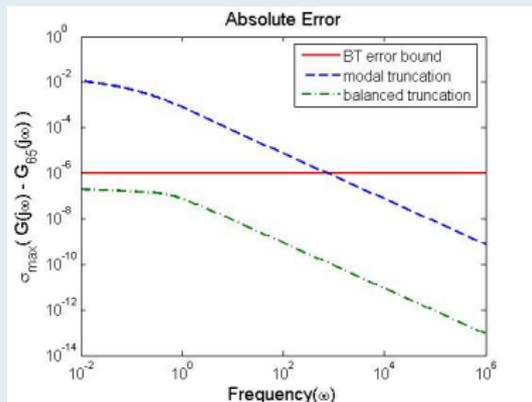


Rank of solution factors: 269 / 205

# Solving Large-Scale Matrix Equations

Numerical example for BT: Optimal Cooling of Steel Profiles

$n = 1,357$ , Absolute Error

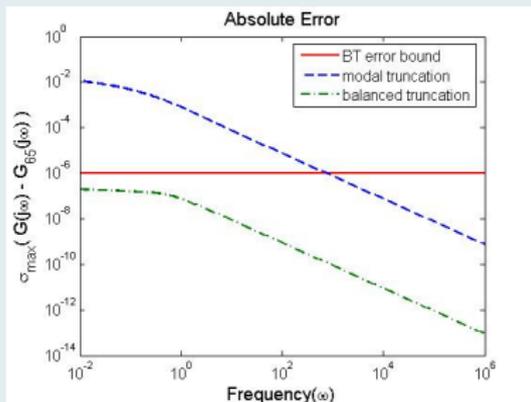


- BT model computed with sign function method,
- MT w/o static condensation, same order as BT model.

# Solving Large-Scale Matrix Equations

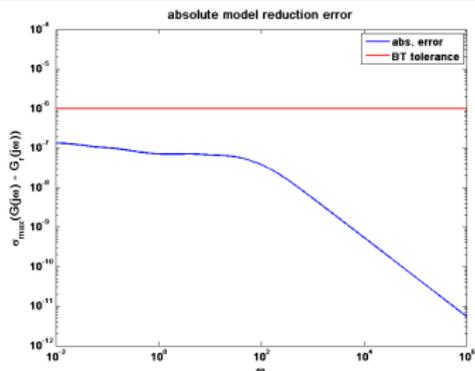
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- MT w/o static condensation, same order as BT model.

$n = 79,841$ , Absolute Error



- BT model computed using M.E.S.S. in MATLAB,
- dualcore, computation time: **<10 min.**

# Solving Large-Scale Matrix Equations

Numerical example for BT: Microgyroscope (Butterfly Gyro)

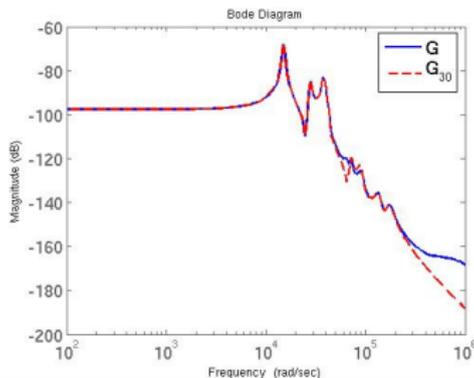
- FEM discretization of structure dynamical model using quadratic tetrahedral elements (ANSYS-SOLID187)  
 $\rightsquigarrow n = 34,722, m = 1, q = 12.$
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## Frequency Response Analysis

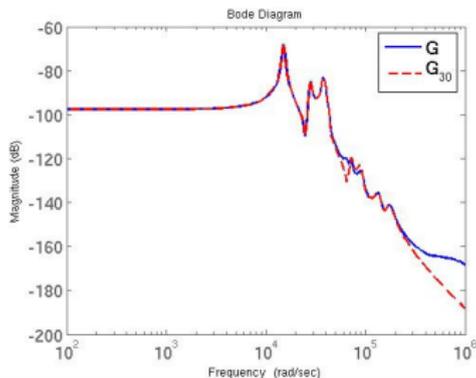


# Solving Large-Scale Matrix Equations

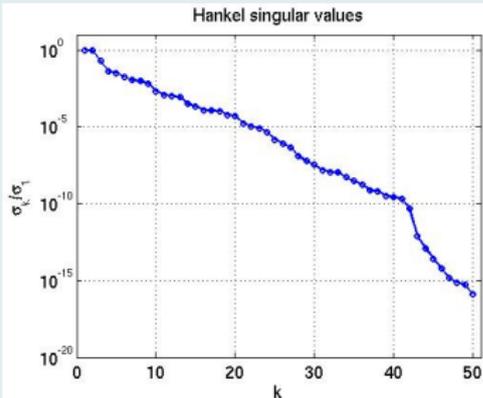
Numerical example for BT: Microgyroscope (Butterfly Gyro)

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

## Frequency Response Analysis



## Hankel Singular Values



# Solving Large-Scale Algebraic Riccati Equations

Theory

[Lancaster/Rodman '95]

## Theorem

Consider the (continuous-time) algebraic Riccati equation (ARE)

$$0 = \mathcal{R}(X) = C^T C + A^T X + XA - XBB^T X,$$

with  $A \in \mathbb{R}^{n \times n}$ ,  $B \in \mathbb{R}^{n \times m}$ ,  $C \in \mathbb{R}^{q \times n}$ ,  $(A, B)$  stabilizable,  $(A, C)$  detectable.

Then:

- (a) There exists a unique stabilizing  $X_* \in \{X \in \mathbb{R}^{n \times n} \mid \mathcal{R}(X) = 0\}$ , i.e.,  $\Lambda(A - BB^T X_*) \in \mathbb{C}^-$ .
- (b)  $X_* = X_*^T \geq 0$  and  $X_* \geq X$  for all  $X \in \{X \in \mathbb{R}^{n \times n} \mid \mathcal{R}(X) = 0\}$ .
- (c) If  $(A, C)$  observable, then  $X_* > 0$ .
- (d)  $\text{span} \left\{ \begin{bmatrix} I_n \\ -X_* \end{bmatrix} \right\}$  is the unique invariant subspace of the Hamiltonian matrix

$$H = \begin{bmatrix} A & BB^T \\ C^T C & -A^T \end{bmatrix}$$

corresponding to  $\Lambda(H) \cap \mathbb{C}^-$ .

# Solving Large-Scale Algebraic Riccati Equations

Numerical Methods

[Bini/Iannazzo/Meini '12]

## Numerical Methods (incomplete list)

- Invariant subspace methods ( $\rightsquigarrow$  eigenproblem for Hamiltonian matrix):
  - Schur vector method (care) [LAUB '79]
  - Hamiltonian SR algorithm [BUNSE-GERSTNER/MEHRMANN '86]
  - Symplectic URV-based method [B./MEHRMANN/XU '97/'98, CHU/LIU/MEHRMANN '07]
- Spectral projection methods
  - Sign function method [ROBERTS '71, BYERS '87]
  - Disk function method [BAI/DEMMELE/GU '94, B. '97]
- (rational, global) Krylov subspace techniques [JAIMOUKHA/KASENALLY '94, JBILOU '03/'06, HEYOUNI/JBILOU '09]
- Newton's method
  - Kleinman iteration [KLEINMAN '68]
  - Line search acceleration [B./BYERS '98]
  - Newton-ADI [B./J.-R. LI/PENZL '99/'08]
  - Inexact Newton [FEITZINGER/HYLLA/SACHS '09]

# Solving Large-Scale Algebraic Riccati Equations

## Newton's Method for AREs

[Kleinman '68, Mehrmann '91, Lancaster/Rodman '95, B./Byers '94/'98, B. '97, Guo/Laub '99]

- Consider  $0 = \mathcal{R}(X) = C^T C + A^T X + XA - XBB^T X$ .
- Fréchet derivative of  $\mathcal{R}(X)$  at  $X$ :

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

- Newton-Kantorovich method:

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

### Newton's method (with line search) for AREs

FOR  $j = 0, 1, \dots$

- 1  $A_j \leftarrow A - BB^T X_j =: A - BK_j$ .
- 2 Solve the Lyapunov equation  $A_j^T N_j + N_j A_j = -\mathcal{R}(X_j)$ .
- 3  $X_{j+1} \leftarrow X_j + t_j N_j$ .

END FOR  $j$

# Solving Large-Scale Algebraic Riccati Equations

## Newton's Method for AREs

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# Newton's Method for AREs

## Properties and Implementation

- Convergence for  $K_0$  stabilizing:

- $A_j = A - BK_j = A - BB^T X_j$  is stable  $\forall j \geq 0$ .
- $\lim_{j \rightarrow \infty} \|\mathcal{R}(X_j)\|_F = 0$  (monotonically).
- $\lim_{j \rightarrow \infty} X_j = X_* \geq 0$  (locally quadratic).

- Need large-scale Lyapunov solver; here, ADI iteration:

linear systems with dense, but “sparse+low rank” coefficient matrix

$A_j$ :

$$\begin{aligned}
 A_j &= A - B \cdot K_j \\
 &= \boxed{\text{sparse}} - \boxed{m} \cdot \boxed{\phantom{K_j}}
 \end{aligned}$$

- $m \ll n \implies$  efficient “inversion” using Sherman-Morrison-Woodbury formula:

$$(A - BK_j + \rho_k^{(j)} I)^{-1} = (I_n + (A + \rho_k^{(j)} I)^{-1} B (I_m - K_j (A + \rho_k^{(j)} I)^{-1} B)^{-1} K_j) (A + \rho_k^{(j)} I)^{-1}.$$

- BUT:  $X = X^T \in \mathbb{R}^{n \times n} \implies n(n+1)/2$  unknowns!

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- BUT:**  $X = X^T \in \mathbb{R}^{n \times n} \implies n(n+1)/2$  unknowns!



# Low-Rank Newton-ADI for AREs

Re-write Newton's method for AREs

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

$$\iff$$

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

Set  $X_j = Z_j Z_j^T$  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 1999/2008]

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

## Feedback Iteration

Optimal feedback

$$K_* = B^T X_* = B^T Z_* Z_*^T$$

can be computed by [direct feedback iteration](#):

- $j$ th Newton iteration:

$$K_j = B^T Z_j Z_j^T = \sum_{k=1}^{k_{\max}} (B^T V_{j,k}) V_{j,k}^T \xrightarrow{j \rightarrow \infty} K_* = B^T Z_* Z_*^T$$

- $K_j$  can be updated in ADI iteration, no need to even form  $Z_j$ , need only fixed workspace for  $K_j \in \mathbb{R}^{m \times n}$ !

Related to earlier work by [BANKS/ITO 1991].

# Solving Large-Scale Matrix Equations

## Galerkin-Newton-ADI

### Basic ideas

- Hybrid method of Galerkin projection methods for AREs [JAIMOUKHA/KASENALLY '94, JBILOU '06, HEYOUNI/JBILOU '09] and Newton-ADI, i.e., use column space of current Newton iterate for projection, solve projected ARE, and prolongate.
- Independence of good parameters observed for Galerkin-ADI applied to Lyapunov equations  $\rightsquigarrow$  fix ADI parameters for all Newton iterations.

# Solving Large-Scale Matrix Equations

## Galerkin-Newton-ADI

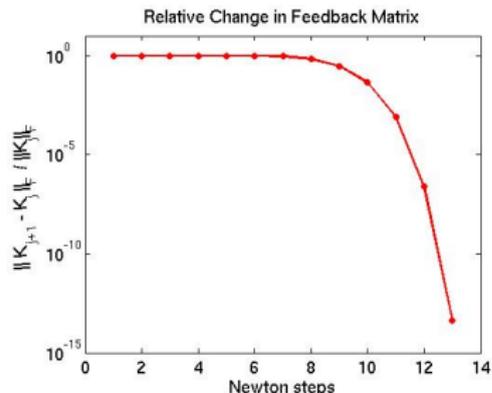
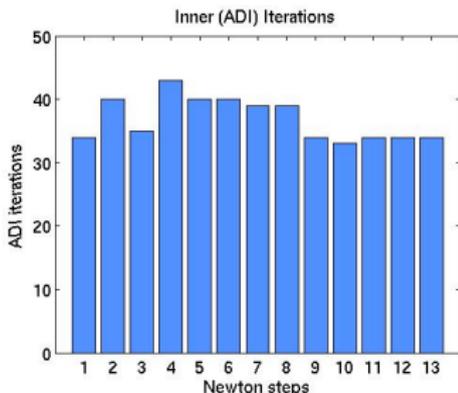
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- Independence of good parameters observed for Galerkin-ADI applied to Lyapunov equations  $\rightsquigarrow$  fix ADI parameters for all Newton iterations.

# Numerical Results

## LQR Problem for 2D Geometry

- Linear 2D heat equation with homogeneous Dirichlet boundary and point control/observation.
- FD discretization on uniform  $150 \times 150$  grid.
- $n = 22.500$ ,  $m = p = 1$ , 10 shifts for ADI iterations.
- Convergence of large-scale matrix equation solvers:





# Numerical Results

## Newton-ADI vs. Newton-ADI-Galerkin

- FDM for 2D **heat**/convection-diffusion equations on  $[0, 1]^2$  (LYAPACK benchmarks,  $m = p = 1$ )  $\rightsquigarrow$  **symmetric**/nonsymmetric  $A \in \mathbb{R}^{n \times n}$ ,  $n = 10,000$ .
- 15 shifts chosen by Penzl's heuristic from 50/25 Ritz/harmonic Ritz values of  $A$ .
- Computations using Intel Core 2 Quad CPU of type Q9400 at 2.66GHz with 4 GB RAM and 64Bit-MATLAB.

### Newton-ADI

step	rel. change	rel. residual	ADI
1	1	9.99e-01	200
2	9.99e-01	3.41e+01	23
3	5.25e-01	6.37e+00	20
4	5.37e-01	1.52e+00	20
5	7.03e-01	2.64e-01	23
6	5.57e-01	1.56e-02	23
7	6.59e-02	6.30e-05	23
8	4.02e-04	9.68e-10	23
9	8.45e-09	1.09e-11	23
10	1.52e-14	<b>1.09e-11</b>	23

CPU time: **76.9 sec.**

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9	8.45e-09	1.09e-11	23
10	1.52e-14	<b>1.09e-11</b>	23

CPU time: **76.9 sec.**

### Newton-Galerkin-ADI

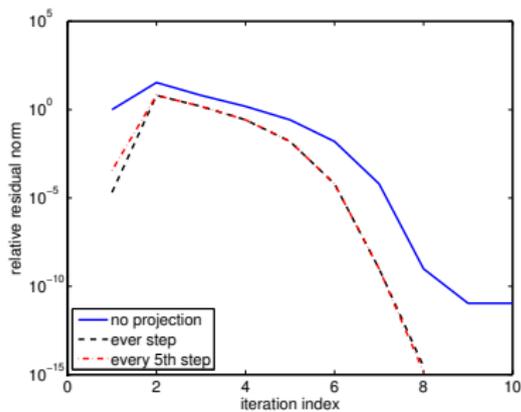
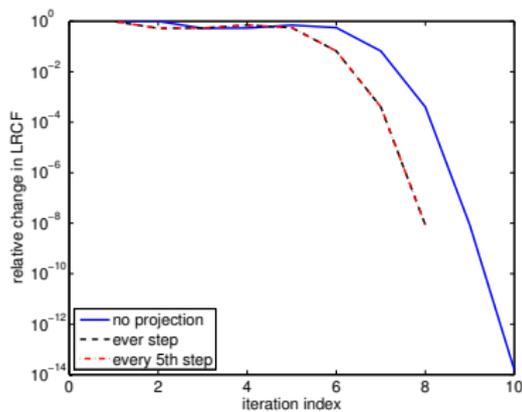
step	rel. change	rel. residual	ADI
1	1	3.56e-04	20
2	5.25e-01	6.37e+00	10
3	5.37e-01	1.52e+00	6
4	7.03e-01	2.64e-01	10
5	5.57e-01	1.57e-02	10
6	6.59e-02	6.30e-05	10
7	4.03e-04	9.79e-10	10
8	8.45e-09	<b>1.43e-15</b>	10

CPU time: 38.0 sec.

# Numerical Results

## Newton-ADI vs. Newton-ADI-Galerkin

- FDM for 2D **heat**/convection-diffusion equations on  $[0, 1]^2$  (LYAPACK benchmarks,  $m = p = 1$ )  $\rightsquigarrow$  **symmetric**/nonsymmetric  $A \in \mathbb{R}^{n \times n}$ ,  $n = 10,000$ .
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### Newton-ADI

step	rel. change	rel. residual	ADI
1	1	9.99e-01	200
2	9.99e-01	3.56e+01	60
3	3.11e-01	3.72e+00	39
4	2.88e-01	9.62e-01	40
5	3.41e-01	1.68e-01	45
6	1.22e-01	5.25e-03	42
7	3.88e-03	2.96e-06	47
8	2.30e-06	6.09e-13	47

CPU time: **185.9 sec.**

# Numerical Results

## Newton-ADI vs. Newton-ADI-Galerkin

- FDM for 2D heat/**convection-diffusion** equations on  $[0, 1]^2$  (LYAPACK benchmarks,  $m = p = 1$ )  $\rightsquigarrow$  symmetric/**nonsymmetric**  $A \in \mathbb{R}^{n \times n}$ ,  $n = 10,000$ .
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6	1.22e-01	5.25e-03	42
7	3.88e-03	2.96e-06	47
8	2.30e-06	6.09e-13	47

CPU time: **185.9 sec.**

### Newton-Galerkin-ADI

step	rel. change	rel. residual	ADI it.
1	1	1.78e-02	35
2	3.11e-01	3.72e+00	15
3	2.88e-01	9.62e-01	20
4	3.41e-01	1.68e-01	15
5	1.22e-01	5.25e-03	20
6	3.89e-03	2.96e-06	15
7	2.30e-06	6.14e-13	20

CPU time: **75.7 sec.**



# Numerical Results

## Example: LQR Problem for 3D Geometry

### Control problem for 3d Convection-Diffusion Equation

- FDM for 3D convection-diffusion equation on  $[0, 1]^3$
- proposed in [SIMONCINI '07],  $q = p = 1$
- non-symmetric  $A \in \mathbb{R}^{n \times n}$ ,  $n = 10\,648$

### Test system:

INTEL Xeon 5160 3.00GHz ; 16 GB RAM; 64Bit-MATLAB (R2010a) using threaded BLAS; stopping tolerance:  $10^{-10}$

# Numerical Results

Example: LQR Problem for 3D Geometry

## Newton-ADI

NWT	rel. change	rel. residual	ADI
1	$1.0 \cdot 10^0$	$9.3 \cdot 10^{-01}$	100
2	$3.7 \cdot 10^{-02}$	$9.6 \cdot 10^{-02}$	94
3	$1.4 \cdot 10^{-02}$	$1.1 \cdot 10^{-03}$	98
4	$3.5 \cdot 10^{-04}$	$1.0 \cdot 10^{-07}$	97
5	$6.4 \cdot 10^{-08}$	$1.3 \cdot 10^{-10}$	97
6	$7.5 \cdot 10^{-16}$	$1.3 \cdot 10^{-10}$	97

CPU time: 4805.8 sec.

## NG-ADI inner= 5, outer= 1

NWT	rel. change	rel. residual	ADI
1	$1.0 \cdot 10^0$	$5.0 \cdot 10^{-11}$	80

CPU time: 497.6 sec.

## NG-ADI inner= 1, outer= 1

NWT	rel. change	rel. residual	ADI
1	$1.0 \cdot 10^0$	$7.4 \cdot 10^{-11}$	71

CPU time: 856.6 sec.

## NG-ADI inner= 0, outer= 1

NWT	rel. change	rel. residual	ADI
1	$1.0 \cdot 10^0$	$6.5 \cdot 10^{-13}$	100

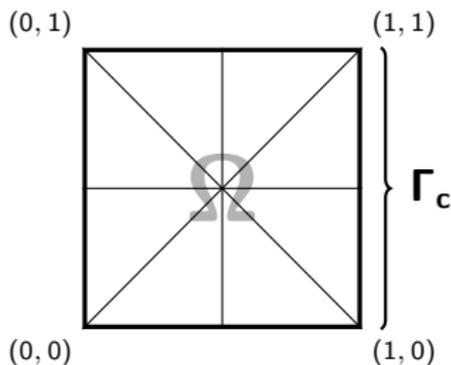
CPU time: 506.6 sec.

## Test system:

INTEL Xeon 5160 3.00GHz ; 16 GB RAM; 64Bit-MATLAB (R2010a) using threaded BLAS; stopping tolerance:  $10^{-10}$

# Numerical Results

## Scaling of CPU times / Mesh Independence



$$\begin{aligned} \partial_t x(\xi, t) &= \Delta x(\xi, t) && \text{in } \Omega \\ \partial_\nu x &= b(\xi) \cdot u(t) - x && \text{on } \Gamma_c \\ \partial_\nu x &= -x && \text{on } \partial\Omega \setminus \Gamma_c \end{aligned}$$

$$x(\xi, 0) = 1$$

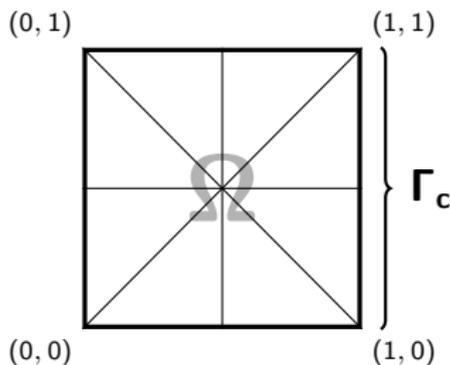
### Note:

Here  $b(\xi) = 4(1 - \xi_2)\xi_2$  for  $\xi \in \Gamma_c$  and 0 otherwise, thus  $\forall t \in \mathbb{R}_{>0}$ , we have  $u(t) \in \mathbb{R}$ .

$$\Rightarrow B_h = M_{\Gamma, h} \cdot b.$$

# Numerical Results

## Scaling of CPU times / Mesh Independence



$$\begin{aligned} \partial_t x(\xi, t) &= \Delta x(\xi, t) && \text{in } \Omega \\ \partial_\nu x &= b(\xi) \cdot u(t) - x && \text{on } \Gamma_c \\ \partial_\nu x &= -x && \text{on } \partial\Omega \setminus \Gamma_c \\ x(\xi, 0) &= 1 \end{aligned}$$

**Consider:** output equation  $y = Cx$ , where

$$\begin{aligned} C : \mathcal{L}^2(\Omega) &\rightarrow \mathbb{R} \\ x(\xi, t) &\mapsto y(t) = \int_{\Omega} x(\xi, t) d\xi \Rightarrow C_h = \underline{1} \cdot M_h. \end{aligned}$$



# Numerical Results

## Scaling of CPU times / Mesh Independence

### Computation Times

discretization level	problem size	time in seconds
3	81	$4.87 \cdot 10^{-2}$
4	289	$2.81 \cdot 10^{-1}$
5	1 089	$5.87 \cdot 10^{-1}$
6	4 225	2.63
7	16 641	$2.03 \cdot 10^{+1}$
8	66 049	$1.22 \cdot 10^{+2}$
9	263 169	$1.05 \cdot 10^{+3}$
10	1 050 625	$1.65 \cdot 10^{+4}$
11	4 198 401	$1.35 \cdot 10^{+5}$

### Test system:

INTEL Xeon 5160 @ 3.00 GHz; 16 GB RAM; 64Bit-MATLAB (R2010a)  
 using threaded BLAS,  
 stopping criterion tolerances:  $10^{-10}$

# Solving Large-Scale Matrix Equations

## Software

### Lyapack

[Penzl 2000]

MATLAB toolbox for solving

- Lyapunov equations and algebraic Riccati equations,
- model reduction and LQR problems.

Main work horse: Low-rank ADI and Newton-ADI iterations.

# Solving Large-Scale Matrix Equations

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### M.E.S.S. – Matrix Equations Sparse Solvers

[B./Köhler/Saak '08–]

- Extended and revised version of LYAPACK.
- Includes solvers for large-scale differential Riccati equations (based on Rosenbrock and BDF methods).
- Many algorithmic improvements:
  - new ADI parameter selection,
  - column compression based on RRQR,
  - more efficient use of direct solvers,
  - treatment of generalized systems without factorization of the mass matrix,
  - new ADI versions avoiding complex arithmetic etc.
- C and MATLAB versions.





# Topics Not Covered

- Extensions to bilinear and stochastic systems.
- Rational interpolation methods for nonlinear systems.
- Other MOR techniques like POD, RB.
- MOR methods for discrete-time systems.
- Extensions to descriptor systems  $E\dot{x} = Ax + Bu$ ,  $E$  singular.
- Parametric model reduction:

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

where  $p \in \mathbb{R}^d$  is a free parameter vector; parameters should be preserved in the reduced-order model.



