Relative Error Model Reduction For Distributed Parameter Systems

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MS51 – Model Reduction of Large-Scale Systems

Overview

- Distributed parameter systems
- Relative error model reduction
- Balanced stochastic truncation (BST)
- Computing the Gramians
  - Solving large, sparse Lyapunov equations
  - Solving large, sparse algebraic Riccati equations
- Performance results
- Conclusions

Distributed Parameter Systems

Given Hilbert spaces

$\mathbb{X}$ – state space,

$\mathbb{U}$ – control space,

$\mathbb{Y}$ – output space,

and operators

$$\begin{array}{ll} \mathcal{A}: & \text{dom}(\mathcal{A}) \subset \mathbb{X} \to \mathbb{X}, \\ \mathcal{B}: & \mathbb{U} \to \mathbb{X}, \\ \mathcal{C}: & \mathbb{X} \to \mathbb{Y}. \end{array}$$

Then, a linear distributed parameter system in abstract form is given by

$$\begin{aligned} \dot{x} &= \mathcal{A}x + \mathcal{B}u, \qquad x(0) = x_0 \in \mathbb{X}, \\ y &= \mathcal{C}x. \end{aligned}$$

Example

Parabolic PDE in domain $\Omega \in \mathbb{R}^d$

(heat equation, convection-diffusion equation)

$$\frac{\partial x}{\partial t} = \sum_{i,j=1}^{d} \frac{\partial x}{\partial \xi_i} \left(a_{ij}(\xi) \frac{\partial x}{\partial \xi_j} \right) + \sum_{i=1}^{d} b_i(\xi) \frac{\partial x}{\partial \xi_i} + cx + Bu(t),$$

$$\xi \in \Omega, \;\; t > 0$$

with initial and boundary conditions ($\partial\Omega = \Gamma_1 \cup \Gamma_2 \cup \Gamma_3$)

$$\begin{aligned} x(\xi, t) &= B_1 u_1(t), & \xi \in \Gamma_1, \\ \frac{\partial}{\partial \eta} x(\xi, t) &= B_2 u_2(t), & \xi \in \Gamma_2, \\ x(\xi, t) + \frac{\partial}{\partial \eta} x(\xi, t) &= B_3 u_3(t), & \xi \in \Gamma_3, \\ x(\xi, 0) &= x_0(\xi), & \xi \in \Omega, \\ y &= Cx, & t \geq 0 \end{aligned}$$

- $B = 0$ $\Longrightarrow$ boundary control problem
- $B_j = 0 \; \forall j$ $\Longrightarrow$ point control problem

Weak formulation, use test functions $v \in \mathbb{V} = \mathbb{H}_0^1(\Omega)$
$\Longrightarrow$ distributed parameter system.

Discretization

Consider sequence of subspaces $\mathbb{X}_n \subset \mathbb{X}$ with $\dim(\mathbb{X}_n) = n < \infty$, such that $\forall \varphi \in \mathbb{X}$ there exists $\varphi_n \in \mathbb{X}_n$ with

$$\lim_{n\to\infty} \|\varphi_n - \varphi\|_{\mathbb{X}} = 0.$$

Define orthogonal projection $\Pi_n : \mathbb{X} \to \mathbb{X}_n$ and

$$\begin{aligned} < A_n\varphi_n, \psi_n >_{\mathbb{X}} &:= - < \mathcal{A}\varphi_n, \psi_n >_{\mathbb{X}} \quad \forall \varphi_n, \psi_n \in \mathbb{X}_n, \\ B_n &:= \Pi_n B, \\ C_n &:= C|_{\mathbb{X}_n}, \end{aligned}$$

$\Longrightarrow$ finite dimensional linear system

$$\begin{aligned} \dot{x}_n &= A_n x_n + B_n u_n, \qquad x(0) = \Pi_n x_0, \\ y_n &= C_n x_n. \end{aligned}$$

Matrix Representation

Galerkin approach, space discretization by finite element method (FEM) $\Longrightarrow$

$$\begin{aligned} M\dot{x} &= -Kx + Bu, \qquad x(0) = x_0, \\ y &= Cx, \end{aligned}$$

with

- stiffness matrix $K \in \mathbb{R}^{n \times n}$,
- mass matrix $M \in \mathbb{R}^{n \times n}$,
- $B \in \mathbb{R}^{n \times m}$,
- $C \in \mathbb{R}^{p \times n}$,

where

$$\begin{aligned} A &:= -M^{-1}K, \\ B &:= M^{-1}B. \end{aligned}$$

Linear Dynamical Systems

Consider continuous time-invariant system

$$\begin{aligned}\dot{x}(t) &= Ax(t) + Bu(t), \quad t > 0, \qquad x(0) = x_0,\\ y(t) &= Cx(t) + Du(t),\end{aligned}$$

not necessarily minimal.

Assume

- n state variables, i.e., $x(t) \in \mathbb{R}^n$, $n =$ order of the system;
- m inputs, i.e., $u(t) \in \mathbb{R}^m$;
- $p \leq m$ outputs, i.e., $y(t) \in \mathbb{R}^p$;
- n large, A sparse, $m, p \ll n$;
- A stable, i.e., $\lambda(A) \subset \mathbb{C}^- \implies$ system is stable;
- D has full (row) rank, i.e., DD^T is non-singular. ($D = 0 \implies$ set $D = \gamma \begin{bmatrix} I_p & 0 \end{bmatrix}$.)

Corresponding transfer function is

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

Relative Error Model Reduction

Want reduced-order model

$$\begin{aligned}\dot{\tilde{x}}(t) &= \tilde{A}\tilde{x}(t) + \tilde{B}\tilde{u}(t), \qquad k = 0, 1, 2, \ldots, \\ \tilde{y}(t) &= \tilde{C}\tilde{x}(t) + \tilde{D}\tilde{u}(t),\end{aligned}$$

of order $\ell \ll n$ with $\tilde{u}(t) \in \mathbb{R}^m$, $\tilde{y}(t) \in \mathbb{R}^p$ such that

$$\|\Delta_{\mathrm{rel}}\|_\infty \text{ is "small"},$$

where the relative error Δ_{rel} is defined by

$$\tilde{G}(s) = G(s)(I + \Delta_{\mathrm{rel}}).$$

If $G(s)$ is square ($p = m$), then relative error model reduction problem can be formulated as

$$\min_{\mathrm{order}(\tilde{G}) \leq \ell} \|G^{-1}(G - \tilde{G})\|_\infty,$$

where approximation quality measured by H_∞-norm

$$\|G\|_\infty = \operatorname*{ess\,sup}_{\omega \in \mathbb{R}} \sigma_{\max}(G(\jmath\omega)).$$

Stochastic Realization

[Desai/Pal '84, Green '88]

For system $G(s) = C(sI - A)^{-1}B + D$ consider power spectrum

$$\Phi(s) := G(s)G^T(-s).$$

Square minimum-phase right spectral factor of $\Phi(s)$:

$$W(s) = \hat{C}(sI - \hat{A})^{-1}\hat{B} + \hat{D},$$

where minimal state-space realization is given by [*Anderson '67*]

$$\begin{aligned}
\hat{A} &= A, \\
\hat{B} &= BD^T + PC^T \in \mathbb{R}^{n\times p}, \\
\hat{C} &= \hat{D}^{-1}(C - \hat{B}^T Q) \in \mathbb{R}^{p\times n}, \\
\hat{D} &= R \in \mathbb{R}^{p\times p} \quad \text{for } R^T R = DD^T.
\end{aligned}$$

and

$$\begin{aligned}
P &= \text{controllability Gramian of } G, \\
Q &= \text{observability Gramian of } W.
\end{aligned}$$

Definition:

minimum-phase system $\Leftrightarrow$ transfer function has no $\overline{\mathbb{C}^+}$-zeros.

Definition

A minimal realization (A, B, C, D) of a linear system $G(s)$ is a balanced stochastic realization (BSR) iff

$$P = Q = \Sigma = \mathrm{diag}(\sigma_1, \sigma_2, \ldots, \sigma_n)$$

with

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

Note:

- for non-minimal system can achieve

$$\begin{aligned} P &= \mathrm{diag}(\Sigma_1, \Sigma_2, 0, 0) \geq 0, \\ Q &= \mathrm{diag}(\Sigma_1, 0, \Sigma_3, 0) \geq 0, \\ \Sigma_1 &= \mathrm{diag}(\sigma_1, \sigma_2, \ldots, \sigma_t) > 0 \end{aligned}$$

- σ_j are Hankel singular values of $W^T(-s)G(s)$.

Theorem *[Desai/Pal '84]*

There exists $T \in \mathbb{R}^{n \times n}$ nonsingular such that

$$(A, B, C, D) = (T^{-1}AT, T^{-1}B, CT, D)$$

is a BSR.

Balanced Stochastic Truncation (BST)

For state-space transformation by nonsingular T let

$$\begin{aligned} T^{-1}AT &= \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}, \quad T^{-1}B = \begin{bmatrix} B_1 \\ B_2 \end{bmatrix}, \\ CT &= \begin{bmatrix} C_1 & C_2 \end{bmatrix}. \end{aligned}$$

Theorem *[Desai/Pal '84, Green '88/90]*

If $(T^{-1}AT, T^{-1}B, CT, D)$ is a BSR, then

$$(\tilde{A}, \tilde{B}, \tilde{C}, \tilde{D}) := (A_{11}, B_1, C_1, D)$$

is a stable, minimal BSR with properties

a) $\tilde{G}(s) = \tilde{C}(sI_\ell - \tilde{A})^{-1}\tilde{B} + \tilde{D}$ satisfies relative error bound

$$\|\Delta_{\mathrm{rel}}\|_\infty \leq \prod_{j=\ell+1}^{t} \frac{1+\sigma_j}{1-\sigma_j} - 1.$$

b) $G(s)$ minimum-phase $\Rightarrow \tilde{G}(s)$ minimum-phase.

(Recall: $\tilde{G}(s) = G(s)(I + \Delta_{\mathrm{rel}})$)

Computation of T via Square-Root Methods

[Laub/Heath/Paige/Ward '87, Tombs/Postlethwaite '87]

P, Q are nonnegative semidefinite $\Longrightarrow$

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

Reduced-order model is computed from SVD

$$\begin{aligned} SR^T &= [U_1 \; U_2] \begin{bmatrix} \Sigma_1 & 0 \\ 0 & \Sigma_2 \end{bmatrix} \begin{bmatrix} V_1^T \\ V_2^T \end{bmatrix}, \\ \Sigma_1 &= \operatorname{diag}(\sigma_1^2, \ldots, \sigma_\ell^2), \\ \Sigma_2 &= \operatorname{diag}(\sigma_{\ell+1}^2, \ldots, \sigma_n^2). \end{aligned}$$

Then defining

$$T_l = \Sigma_1^{-1/2} V_1^T R, \qquad T_r = S^T U_1 \Sigma_1^{-1/2},$$

the BST reduced-order model is given by

$$\tilde{A} = T_l A T_r, \quad \tilde{B} = T_l B, \quad \tilde{C} = C T_r, \quad \tilde{D} = D.$$

Balancing-free version possible. [*Varga '91*]

Standard approach:

$S, R = \left[\diagdown\!\!| \right] \in \mathbb{R}^{n \times n}$ – Cholesky factors of P, Q.

Alternative:

$S \in \mathbb{R}^{\text{rank}\,(P) \times n}$
$R \in \mathbb{R}^{\text{rank}\,(Q) \times n}$ – full-rank factors of P, Q.

Idea here:
Find low-rank approximations to full-rank factors!

Computing the Gramians

Controllability Gramian P of

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

given by solution of stable, nonnegative Lyapunov equation

$$AP + PA^T + BB^T = 0,$$

Observability Gramian Q of

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

is stabilizing solution of algebraic Riccati equation (ARE)

$$\begin{aligned} 0 \;=\; & C^T(DD^T)^{-1}C + (A - \hat{B}(DD^T)^{-1}C)^T Q \; + \\ & + \; Q(A - \hat{B}(DD^T)^{-1}C) + Q\hat{B}(DD^T)^{-1}\hat{B}^T Q. \end{aligned}$$

$\Longrightarrow$ Need to solve one Lyapunov equation and one ARE!

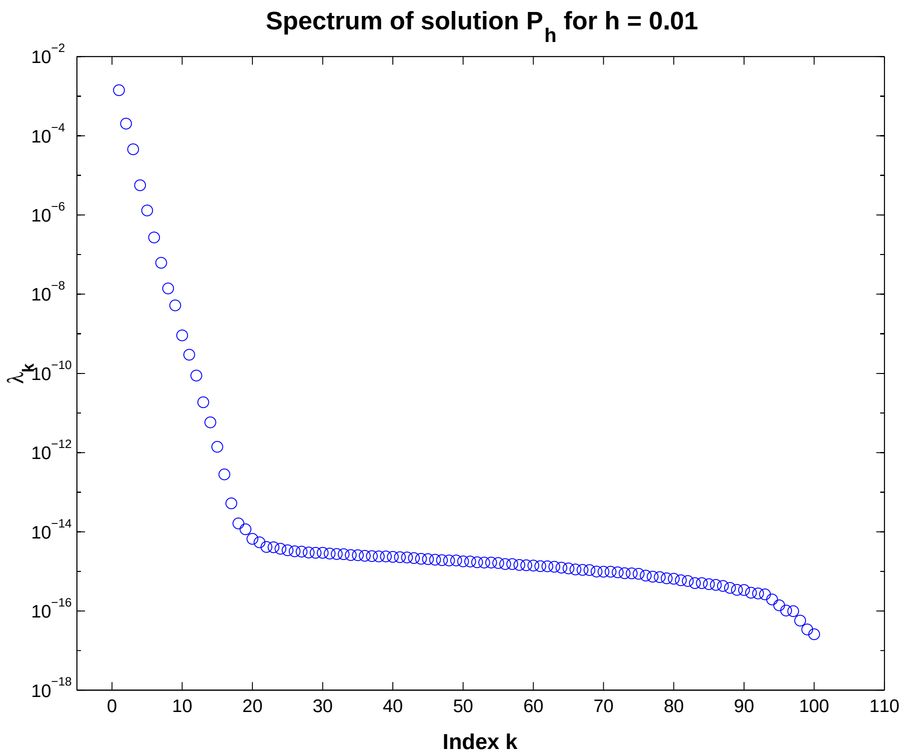
Goal:
get low-rank approximations to factors of P, Q directly.

Low-rank approximation

Consider spectrum of controllability Gramian P.

Example:

Linear 1D heat equation on $[0,1]$ with point control,
finite element discretization using linear B-splines, $n = 100$.



Idea:

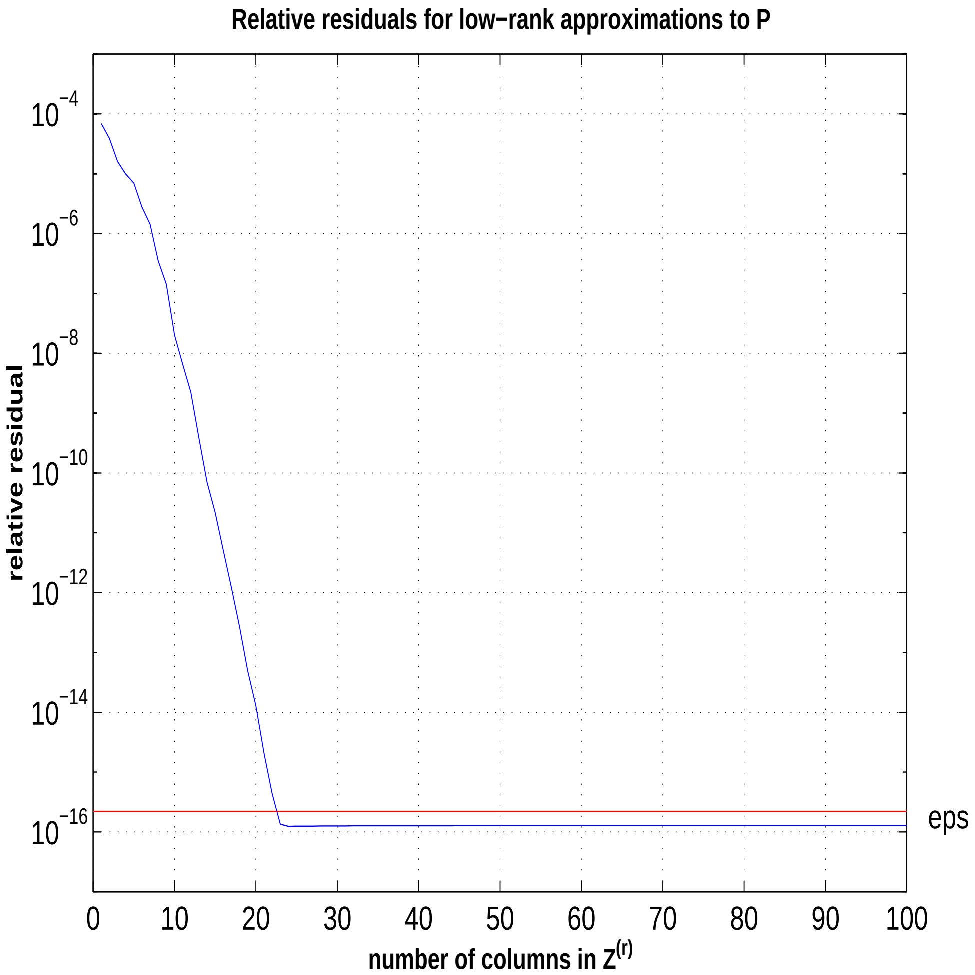
$$P = P^T \geq 0 \quad \Longrightarrow \quad P = ZZ^T = \sum_{k=1}^{n} \lambda_k z_k z_k^T$$

$$\lambda_k \approx 0, \; k > r \quad \Longrightarrow \quad P \approx Z^{(r)}(Z^{(r)})^T = \sum_{k=1}^{r} \lambda_k z_k z_k^T.$$

Approximation quality:

Example as before, check relative residuals of Lyapunov equation for

$$P \approx Z^{(r)}(Z^{(r)})^T, \qquad r = 1, \ldots, 100.$$



ADI Method for Lyapunov Equations

- For $A \in \mathbb{R}^{n\times n}$ stable ($\lambda(A) \in \mathbb{C}^-$), $W \in \mathbb{R}^{n\times w}$ ($w \ll n$), consider Lyapunov equation

$$A^T P + PA = -WW^T.$$

- ADI-Iteration: [*Wachspress '88*]

$$\begin{aligned} (A^T + p_j I) P_{(j-1)/2} &= -WW^T - P_{j-1}(A - p_j I) \\ (A^T + \overline{p_j} I) P_j{}^T &= -WW^T - P_{(j-1)/2}(A - \overline{p_j} I) \end{aligned}$$

  with parameters $p_j \in \mathbb{C}^-$ and $p_{j+1} = \overline{p_j}$ if $p_j \notin \mathbb{R}$.

- For $P_0 = 0$ and proper choice of p_j:

$$\lim_{j\to\infty} P_j = P \text{ superlinear.}$$

- Re-formulation using $P_j = Z_j Z_j^T$ yields iteration for Z_j, after convergence:

$$Z_{j_{\max}} = \left[\; V_1 \quad \ldots \quad V_{j_{\max}} \;\right], \quad V_j = \Big[\;\Big] \in \mathbb{C}^{n\times w}.$$

Newton's Method for AREs

Consider

$$0 = \mathcal{R}(Q) = C^T C + A^T Q + QA - QBB^T Q,$$

with stable A.

Frechét derivative of $\mathcal{R}(Q)$ at Q:

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

Newton-Kantorovich method :

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

$\Longrightarrow$ Newton's method for AREs
[*Kleinman '68, Mehrmann '91, Lancaster/Rodman '95*]

1. $Q_0 \;=\; 0.$
2. FOR $j = 0,\, 1,\, 2,\, \ldots$
   - 2.1 $A_j \leftarrow A - BB^T Q_j =: A - BK_j.$
   - 2.2 Solve Lyapunov equation
     $$A_j^T N_j + N_j A_j \;=\; -\mathcal{R}(Q_j).$$
   - 2.3 $Q_{j+1} \leftarrow Q_j + N_j.$

   END FOR j

Properties

- Convergence:
  - A_j is stable $\forall\ j \geq 0$.
  - $\lim_{j\to\infty} \|\mathcal{R}(Q_j)\|_F = 0$.
  - $0 \leq Q_\infty \leq \ldots \leq Q_{j+1} \leq Q_j \leq \ldots \leq Q_1$.
  - $\lim_{j\to\infty} Q_j = Q_\infty \geq 0$.
  - Quadratic convergence rate.
- Problem: need efficient Lyapunov solver!
- But: $Q = Q^T \in \mathbb{R}^{n\times n} \Longrightarrow n(n+1)/2$ unknowns!
  In general not feasible for very large problems.

Factored Newton Iteration

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

$$\Updownarrow$$

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

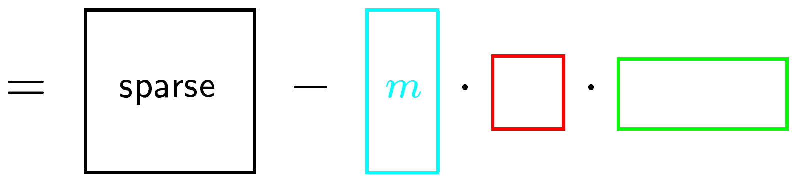
Let $Q_j = Y_j Y_j^T$ for $\mathrm{rank}\,(Y_j) \ll n$:

$$A_j^T \left(Y_{j+1} Y_{j+1}^T\right) + \left(Y_{j+1} Y_{j+1}^T\right) A_j = -W_j W_j^T$$

$$\Downarrow$$

Need method for solving Lyapunov equations which computes Y_{j+1} directly and uses structure of A_j,

$$A_j = A - BK_j = A - B \cdot (B^T Y_j) \cdot Y_j^T,$$



Solution: use factored ADI iteration!

$m \ll n \Rightarrow$ use Sherman-Morrison-Woodbury formula

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

Newton-ADI for ARE

[*B./Li/Penzl '00*]

Solve Lyapunov equation

$$(A - BK_j)^T Y_{j+1} Y_{j+1}^T + Y_{j+1} Y_{j+1}^T (A - BK_j) = -W_j W_j^T$$

with factored ADI iteration.

$$\Downarrow$$

Obtain sequence $Z_0, Z_1, \ldots, Z_{k_{\max}}$ of low-rank approximations to solution of Lyapunov equation.

$$\Downarrow$$

$$Y_{j+1} = Z_{k_{\max}}.$$

$$\Downarrow$$

Newton's method with factored iterates $Q_j = Y_j Y_j^T$.

$$\Downarrow$$

Factored solution of ARE $Q \approx Y_{j_{\max}} Y_{j_{\max}}^T$.

Application to BST

- Approximation of controllability Gramian P with low-rank ADI for Lyapunov equation.

- For solving ARE with Newton's method, need slight modification: right-hand side of Lyapunov equation can not be written as $-W_j W_j^T$.

$$\begin{aligned} \mathrm{RHS} &= -C^T(DD^T)^{-1}C + Q_j\hat{B}(DD^T)^{-1}\hat{B}^T Q_j \\ &=: -\tilde{C}\tilde{C}^T + \tilde{B}_j\tilde{B}_j^T \end{aligned}$$

with $DD^T > 0$.

Lyapunov equation is non-singular linear system

$\Longrightarrow$ write

$$A_j^T Q_{j+1} + Q_{j+1} A_j = -\tilde{C}^T\tilde{C} + \tilde{B}_j^T\tilde{B}_j$$

as

$$\begin{aligned} A_j^T(Q_{j+1} - Q_{j+1}) + (Q_{j+1} - Q_{j+1})A_j \\ = -W_j W_j^T - (-W_j W_j^T). \end{aligned}$$

$\Longrightarrow$ Solve two Lyapunov equations per step.

Problem

need factor of

$$\begin{aligned}\tilde{Q} &:= Q_{j_{\max}} - Q_{j_{\max}} \\ &= Z_{j_{\max}} Z_{j_{\max}}^T - Z_{j_{\max}} Z_{j_{\max}}^T \geq 0.\end{aligned}$$

Solution

[Varga/Fasol '93, Varga '00]

Get full-rank factor from stable, nonnegative Lyapunov equation

$$A^T(R^T R) + (R^T R)A + C^T C = 0$$

where

$$C = \hat{D}^{-T} C - \hat{B}\hat{D}^{-1}\tilde{Q}$$

and

$$D = [\,\hat{D}^T\ 0\,]U$$

is an LQ factorization of D.

Performance Results

MATLAB implementation using the LYAPACK Toolbox (T. Penzl, 1999).

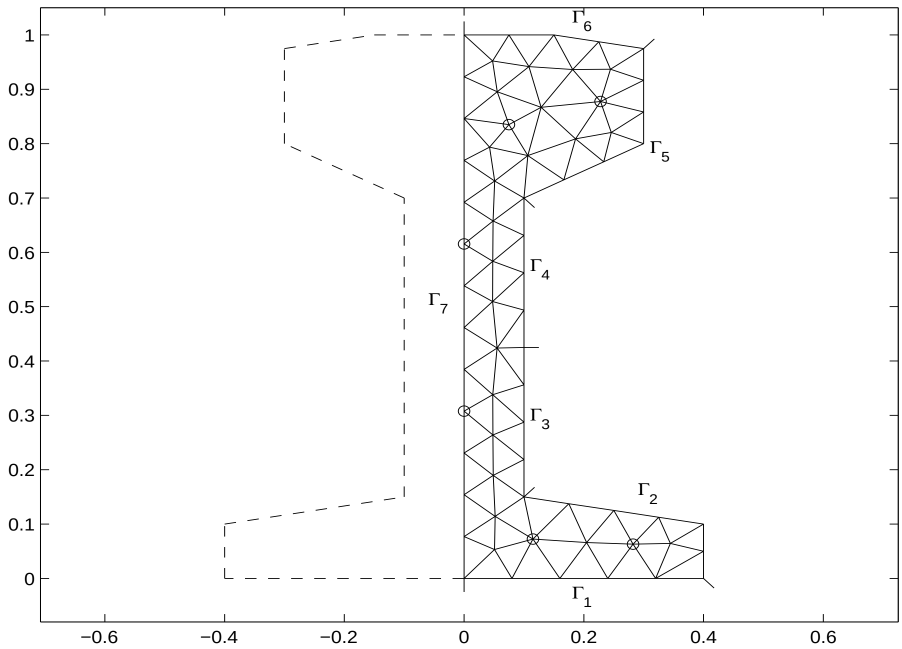
Example 1 [*Tröltzsch/Unger '99, Penzl '99*]

- Optimal cooling of steel profiles.
- Model: boundary control for linear 2D heat equation.

$$\begin{aligned} x_t &= \Delta x, & x \in \Omega \\ x + x_\eta &= u_k, & x \in \Gamma_k,\ k = 1, \ldots, 6, \\ x_\eta &= 0, & x \in \Gamma_7. \end{aligned}$$

$\Longrightarrow n = 821,\ m = p = 6$

- FEM discretization, initial mesh:



Example 1, continued

- Discretization leads to system

$$\begin{aligned} M\dot{x} &= -Kx + Bu, \qquad x(0) = x_0, \\ y &= Cx. \end{aligned}$$

Solution of linear systems of equations:

  - Bandwidth reduction in M, N using reverse Cuthill-McKee algorithm.
  - Instead of $A = -M^{-1}K$ consider

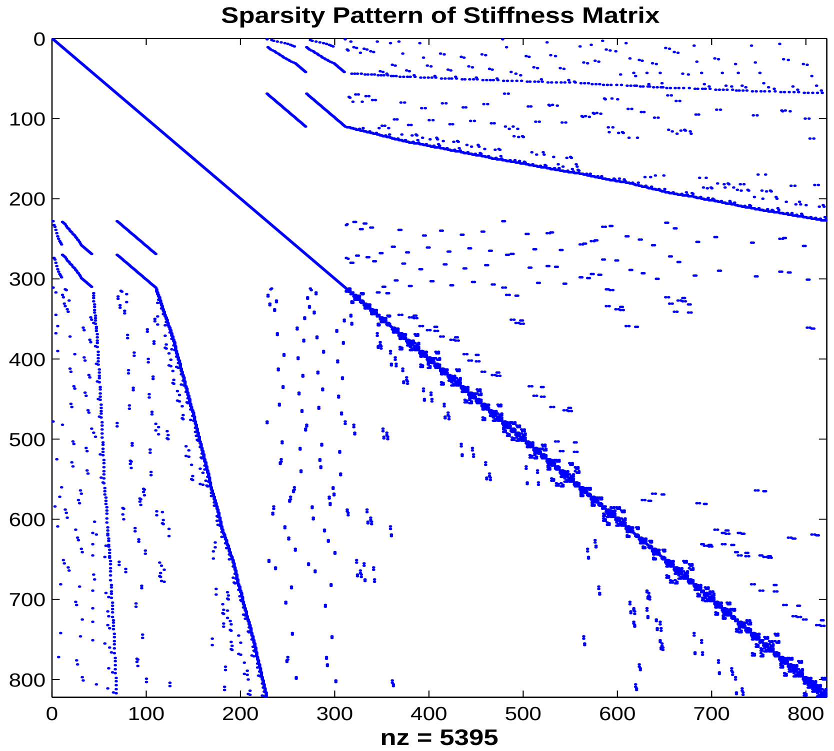
$$A = -M_C^{-1} K M_C^{-T},$$

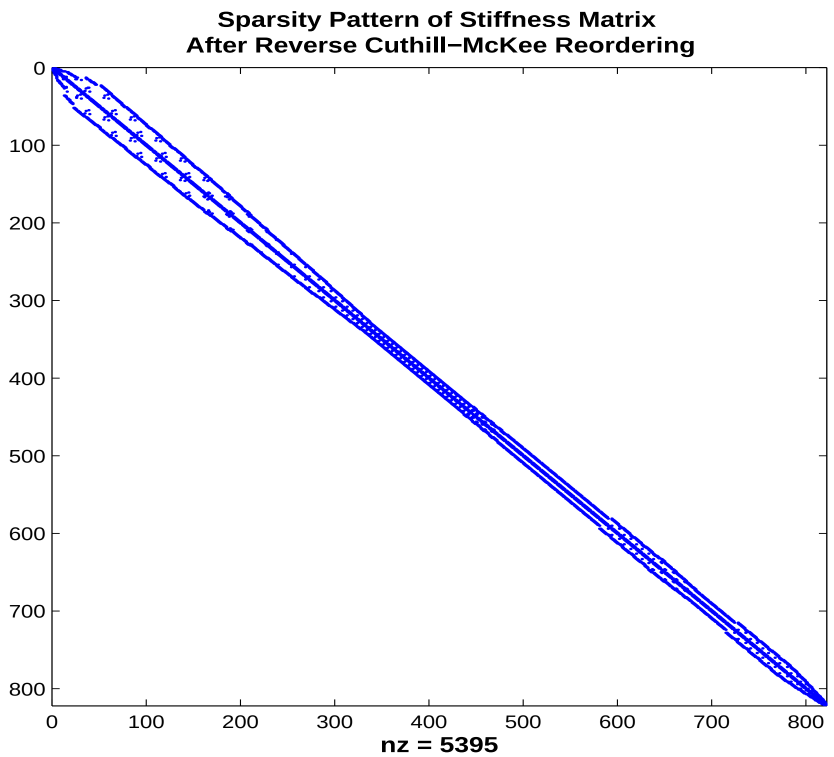
    where M_C = (sparse) Cholesky factor of M.
  - Cholesky factorization and solution of 'shifted' linear systems using sparse direct method.
  - Use ten ADI parameters cyclically.

- Order of reduced-ordel model: $\ell = 50$.

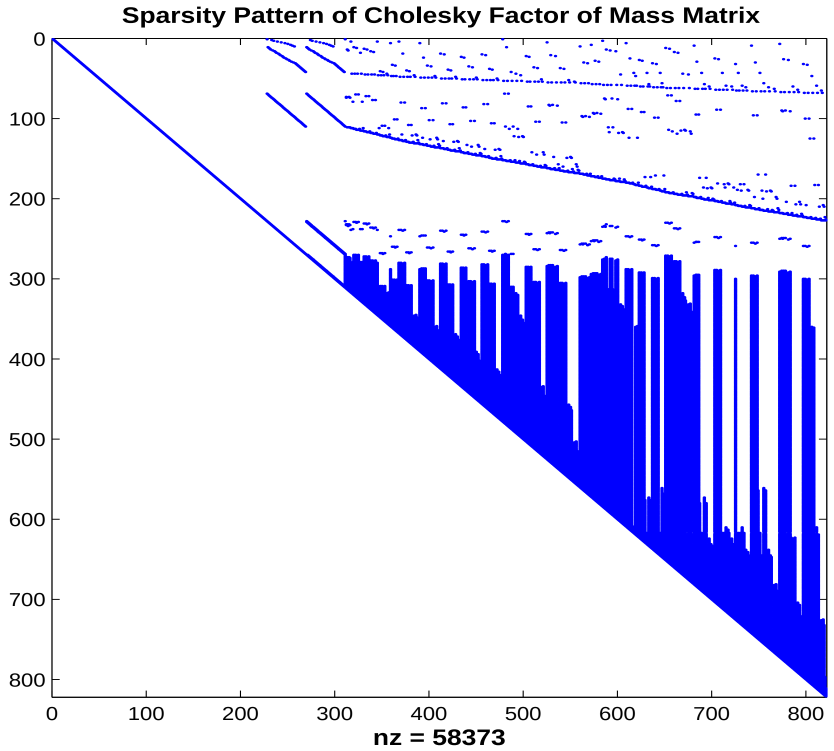
- Error bound:
$\|\Delta_{\mathrm{rel}}\|_\infty \leq \prod_{j=\ell+1}^{t} \frac{1+\sigma_j}{1-\sigma_j} - 1 = 1.75 \cdot 10^{-5}$.

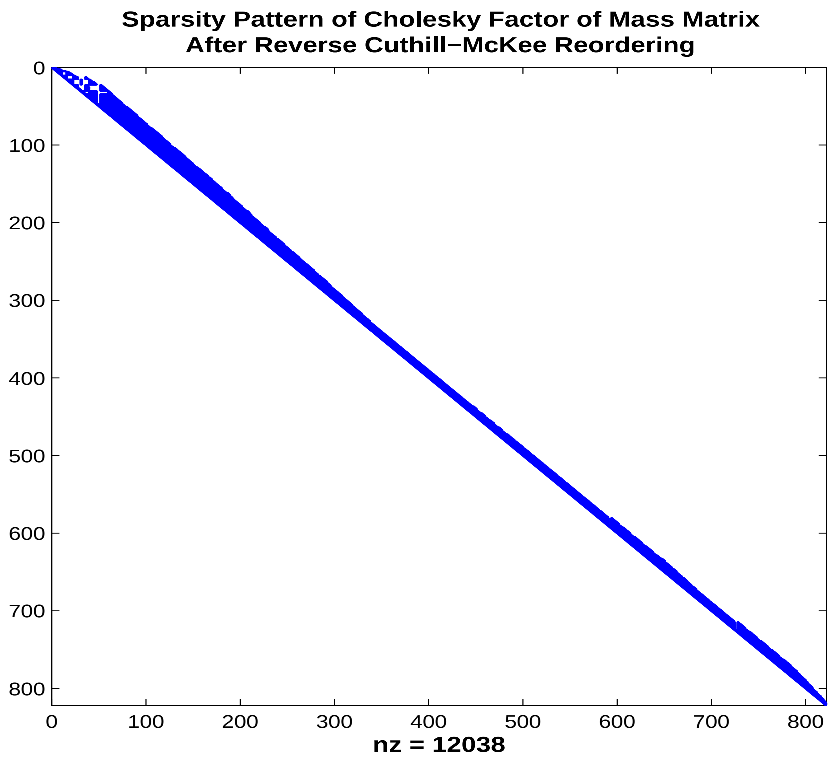
Example 1, Stiffness Matrix





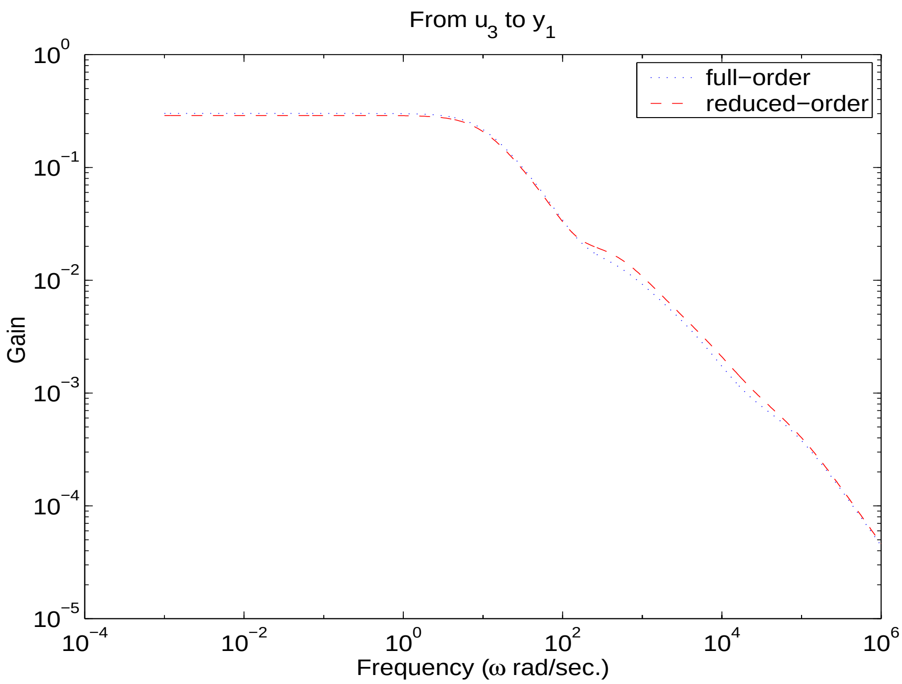
Example 1, Cholesky Factor of Mass Matrix

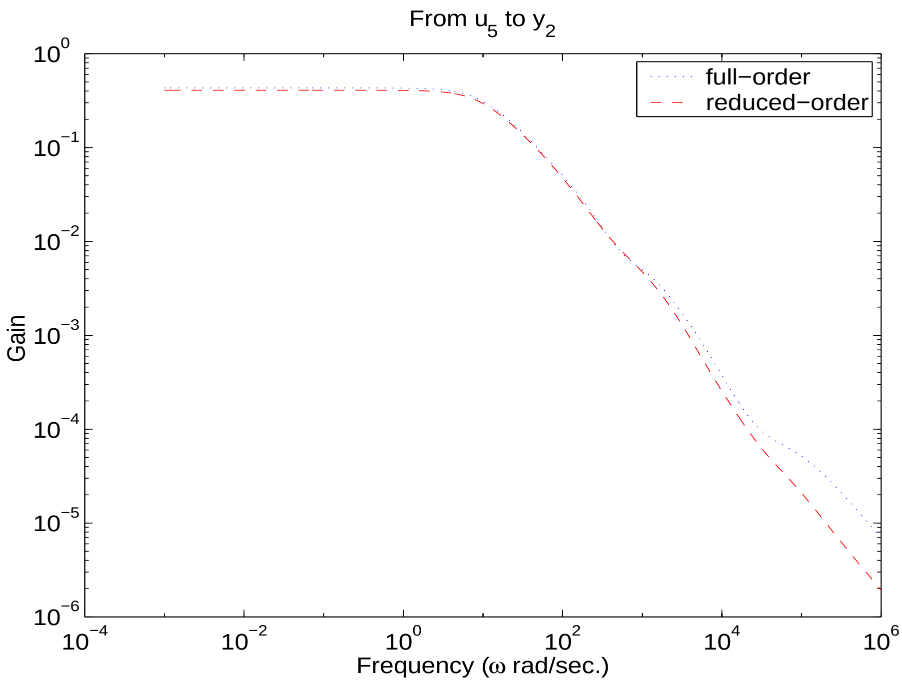




Example 1, Model Reduction Performance

Frequency Response (Magnitude)





Conclusions

- Balanced stochastic truncation model reduction methods
  - with low-rank ADI for solving Lyapunov equations,
  - low-rank ADI based Newton's method for solving AREs,
  - and using low-rank factors of Gramians

  yield efficient method, applicable to large-scale systems.

- Open problems/in progress:
  - Which accuracy for Lyapunov equations needed?
  - Efficient column compression technique to keep number of columns in ADI iterates low.
  - Acceleration of Newton's method using line search or trust region without residual evaluation possible?