ADI-based Galerkin-Methods for Algebraic Lyapunov and Riccati Equations

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joint work with Jens Saak (TU Chemnitz)

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- Low-Rank ADI for Lyapunov equations
- Factored Galerkin-ADI Iteration



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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:

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

 $G = 0 \Longrightarrow$ Lyapunov equation:

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

- $n = 10^3 10^6 \iff 10^6 10^{12}$ 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 $B \in \mathbb{R}^{n \times m}$, $m \ll n$, $C \in \mathbb{R}^{p \times n}$, $p \ll n$.
- Standard (eigenproblem-based) $O(n^3)$ methods are not applicable!



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Low-Rank Approximation

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

Example:

- Linear 1D heat equation with point control,
- $\Omega = [0, 1],$
- FEM discretization using linear B-splines,

•
$$h = 1/100 \implies n = 101.$$

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



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

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



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Numerical solution of linear-quadratic optimal control problem for parabolic PDEs via Galerkin approach, spatial FEM discretization \rightsquigarrow

LQR Problem (finite-dimensional)

$$\begin{array}{ll} \operatorname{Min} \ \mathcal{J}(u) &= \ \frac{1}{2} \int_{0}^{\infty} \left(y^{T} Q y + u^{T} R u \right) dt \quad \text{for} \quad u \in \mathcal{L}_{2}(0,\infty;\mathbb{R}^{m}), \\ \text{subject to} \quad M\dot{x} = -Sx + Bu, \quad x(0) = x_{0}, \quad y = Cx, \\ \text{with stiffness } S \in \mathbb{R}^{n \times n}, \text{ mass } M \in \mathbb{R}^{n \times n}, B \in \mathbb{R}^{n \times m}, \ C \in \mathbb{R}^{p \times n}. \end{array}$$

Solution of finite-dimensional LQR problem: feedback control

$$u_*(t) = -B^T X_* x(t) =: -K_* x(t),$$

where $X_* = X_*^T \ge 0$ is the unique stabilizing¹ solution of the ARE

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

with $A := -M^{-1}S$, $B := M^{-1}BR^{-\frac{1}{2}}$, $C := CQ^{-\frac{1}{2}}$.

¹X is stabilizing $\Leftrightarrow \Lambda (A - BB^T X) \subset \mathbb{C}^-$.



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Linear, Time-Invariant (LTI) Systems



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



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Linear, Time-Invariant (LTI) Systems

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

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

Model Reduction Based on Balancing

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

$$TPT^{T} = T^{-T}QT^{-1} = \operatorname{diag}(\sigma_{1}, \ldots, \sigma_{n}), \quad \sigma_{1} \geq \ldots \geq \sigma_{n} \geq 0.$$

Balancing Σ w.r.t. P, Q:

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



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For Balanced Truncation: P/Q = controllability/observabilityGramian of Σ , i.e., for asymptotically stable systems, P, Q solve dual Lyapunov equations

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



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Basic Model Reduction Procedure

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

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

2 Truncation ~> reduced-order model:

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



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Implementation: SR Method

Given Cholesky (square) or (low-rank approximation to) full-rank (maybe rectangular, "thin") factors of P, Q
 P = S^TS, Q = R^TR.

Compute SVD

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

Set

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

Reduced-order model is

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



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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

(H + pI)v = r(V + pI)w = t

can be solved easily/efficiently.

DI Iteration

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

$$u_{0} = 0$$

(H+p_{k}l)u_{k-\frac{1}{2}} = (p_{k}l - V)u_{k-1} + s
(V+p_{k}l)u_{k} = (p_{k}l - H)u_{k-\frac{1}{2}} + s

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



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The Lyapunov operator

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

can be decomposed into the linear operators

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

In analogy to the standard ADI method we find the

ADI iteration for the Lyapunov equation			[Wachspress 1988
P ₀	=	0	
$(A+p_kI)X_{k-\frac{1}{2}}$	=	$-W-P_{k-1}(x)$	$(A^T - p_k I)$
$(A + p_k I)X_k^{\dagger}$	=	$-W - X_{k-\frac{1}{2}}^{T}$	$A^T - p_k I$)



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• For $A \in \mathbb{R}^{n \times n}$ stable, $B \in \mathbb{R}^{n \times m}$ ($w \ll n$), consider Lyapunov equation

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

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[Wachspress 1988]

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

$$(A + \overline{p_k}I)X_k^T = -BB^T - X_{k-\frac{1}{2}}(A^T - \overline{p_k}I)$$

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

• For $X_0 = 0$ and proper choice of p_k : $\lim_{k \to \infty} X_k = X$ superlinear.

• Re-formulation using $X_k = Y_k Y_k^T$ yields iteration for $Y_k...$



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Low-Rank ADI for Lyapunov equations Lyapunov equation $0 = AX + XA^T + BB^T$.

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

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

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

FOR $k = 2, 3, ...$
 $V_k \leftarrow \sqrt{\frac{\operatorname{Re}(p_k)}{\operatorname{Re}(p_{k-1})}} (V_{k-1} - (p_k + \overline{p_{k-1}})(A + p_k I)^{-1}V_{k-1})$
 $Y_k \leftarrow [Y_{k-1} \quad V_k]$
 $Y_k \leftarrow \operatorname{rrlq}(Y_k, \tau)$ % column compression

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

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

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

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

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

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

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

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

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



Source: Physical model: courtesy of Mannesmann/Demag.

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



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• Solve dual Lyapunov equations needed for balanced truncation, i.e., $APM^{T} + MPA^{T} + BB^{T} = 0, \qquad A^{T}QM + M^{T}QA + C^{T}C = 0,$

for 79,841. Note: m = 7, p = 6.

- 25 shifts chosen by Penzl's heuristic from 50/25 Ritz values of A of largest/smallest magnitude, no column compression performed.
- New version in MESS (Matrix Equations Sparse Solvers) requires no factorization of mass matrix!
- Computations done on Core2Duo at 2.8GHz with 3GB RAM and 32Bit-MATLAB(R).





Recent Numerical Results Scaling / Mesh Independence Computations by Martin Köhler

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- A ∈ ℝ^{n×n} ≡ FDM matrix for 2D heat equation on [0, 1]² (LYAPACK benchmark demo_l1, m = 1).
- 16 shifts chosen by Penzl's heuristic from 50/25 Ritz values of A of largest/smallest magnitude.
- Computations using 2 dual core Intel Xeon 5160 with 16 GB RAM.



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- Computations using 2 dual core Intel Xeon 5160 with 16 GB RAM.

n	CMESS	Lyapack	MESS
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

CPU Times



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- Computations using 2 dual core Intel Xeon 5160 with 16 GB RAM.



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 $0 = AX + XA^{T} + BB^{T}$

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

- Compute orthonormal basis range (Z), $Z \in \mathbb{R}^{n \times r}$, for subspace $\mathcal{Z} \subset \mathbb{R}^n$, dim $\mathcal{Z} = r$.
- Solve small-size Lyapunov equation $\hat{A}\hat{X} + \hat{X}\hat{A}^{T} + \hat{B}\hat{B}^{T} = 0.$

Use
$$X \approx Z \hat{X} Z^T$$
.

Examples:

• Krylov subspace methods, i.e., for m = 1:

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

[Saad '90, Jaimoukha/Kasenally '94, Jbilou '02-'08].K-PIK [Simoncini '07],

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



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- Use $X \approx Z \hat{X} Z^T$.

Examples:

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

$$\mathcal{Z} = \operatorname{colspan} \left[egin{array}{cc} V_1, & \ldots, & V_r \end{array}
ight].$$

Note:

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



Factored Galerkin-ADI Iteration

Numerical examples

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FEM semi-discretized control problem for parabolic PDE:

optimal cooling of rail profiles,

•
$$n = 20, 209, m = 7, p = 6.$$



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

Computations by Jens Saak.



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FEM semi-discretized control problem for parabolic PDE:

optimal cooling of rail profiles,

•
$$n = 20, 209, m = 7, p = 6$$



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

Computations by Jens Saak.



Factored Galerkin-ADI Iteration

Numerical examples: optimal cooling of rail profiles, n = 79,841, m = 7, p = 6.

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MESS w/o Galerkin projection and column compression



MESS with Galerkin projection and column compression





Rank of solution factors: 269 / 205


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

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

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

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

• 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, ...

Solve the Lyapunov equation A_j^T N_j + N_jA_j = -R(X_j).
X_{j+1} ← X_j + t_jN_j.
END FOR *i*



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

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Newton's method (with line search) for AREs

FOR j = 0, 1, ...

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

Solve the Lyapunov equation A_j^TN_j + N_jA_j = -R(X_j).
X_{j+1} ← X_j + t_jN_j.
END FOR j



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

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Newton's method (with line search) for AREs

FOR j = 0, 1, ...

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

Solve the Lyapunov equation A^T_j N_j + N_jA_j = -R(X_j).
X_{j+1} ← X_j + t_jN_j.
END FOR j



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• Convergence for K₀ stabilizing:

- $A_j = A BK_j = A BB^T X_j$ is stable $\forall j \ge 0$.
- $\lim_{j\to\infty} \|\mathcal{R}(X_j)\|_F = 0$ (monotonically).
- $\lim_{j\to\infty} X_j = X_* \ge 0$ (locally quadratic).
- Need large-scale Lyapunov solver; here, ADI iteration: linear systems with dense, but "sparse+low rank" coefficient matrix A_i:

$$A_{j} = A - B \cdot K_{j}$$
$$= sparse - m \cdot$$

m ≪ *n* ⇒ efficient "inversion" using Sherman-Morrison-Woodbury formula:

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



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Re-write Newton's method for AREs

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

$$A_{j}^{T}\underbrace{(X_{j}+N_{j})}_{=X_{j+1}} + \underbrace{(X_{j}+N_{j})}_{=X_{j+1}}A_{j} = \underbrace{-C^{T}C - X_{j}BB^{T}X_{j}}_{=:-W_{j}W_{j}^{T}}$$

Set
$$X_j = Z_j Z_j^T$$
 for rank $(Z_j) \ll n \Longrightarrow$
 $A_i^T (Z_{i+1} Z_{i+1}^T) + (Z_{i+1} Z_{i+1}^T) A_i = -W_i W_i^T$

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_i .



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Optimal feedback

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

can be computed by direct feedback iteration:

• *j*th Newton iteration:

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

 K_j can be updated in ADI iteration, no need to even form Z_j, need only fixed workspace for K_j ∈ ℝ^{m×n}!

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



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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 → fix ADI parameters for all Newton iterations.



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Conclusions and Open Problems

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







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- FDM for 2D heat/convection-diffusion equations on [0, 1]² (LYAPACK benchmarks, m = p = 1) → symmetric/nonsymmetric A ∈ ℝ^{n×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.



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- 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	1.09e-11	23		
CPU time: 76.9 sec.					



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Newto	on-ADI			Newton-Galerkin-ADI			
step	rel. change	rel. residual	ADI	step	rel. change	rel. residual	ADI
1	1	9.99e-01	200	1	1	3.56e-04	20
2	9.99e-01	3.41e+01	23	2	5.25e-01	6.37e+00	10
3	5.25e-01	6.37e+00	20	3	5.37e-01	1.52e+00	6
4	5.37e-01	1.52e+00	20	4	7.03e-01	2.64e-01	10
5	7.03e-01	2.64e-01	23	5	5.57e-01	1.57e-02	10
6	5.57e-01	1.56e-02	23	6	6.59e-02	6.30e-05	10
7	6.59e-02	6.30e-05	23	7	4.03e-04	9.79e-10	10
8	4.02e-04	9.68e-10	23	8	8.45e-09	1.43e-15	10
9	8.45e-09	1.09e-11	23				
10	1.52e-14	1.09e-11	23				
	CPU time:	76.9 sec.			CPU time:	38.0 sec.	



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







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- 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	3.56e+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.				



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- 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				Newton-Galerkin-ADI			
step	rel. change	rel. residual	ADI	step	rel. change	rel. residual	ADI it.
1	1	9.99e-01	200	1	1	1.78e-02	35
2	9.99e-01	3.56e+01	60	2	3.11e-01	3.72e+00	15
3	3.11e-01	3.72e+00	39	3	2.88e-01	9.62e-01	20
4	2.88e-01	9.62e-01	40	4	3.41e-01	1.68e-01	15
5	3.41e-01	1.68e-01	45	5	1.22e-01	5.25e-03	20
6	1.22e-01	5.25e-03	42	6	3.89e-03	2.96e-06	15
7	3.88e-03	2.96e-06	47	7	2.30e-06	6.14e-13	20
8	2.30e-06	6.09e-13	47	'			
	CPU time:	185.9 sec.			CPU time:	75.7 sec.	



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- FDM for 2D heat/convection-diffusion equations on [0, 1]² (LYAPACK benchmarks, m = p = 1) → symmetric/nonsymmetric A ∈ ℝ^{n×n}, n = 10,000.
- 15 shifts chosen by Penzl's heuristic from 50/25 Ritz/harmonic Ritz values of *A*.
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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 $A \in \mathbb{R}^{n imes n}$, $n = 10\,648$

Test system:

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



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> Numerie Results

Numerical Results LQR Problem for 3D Geometry

ov and quations	Newto	on-ADI			NG-ADI	inner= 5, ou	ter = 1
Benner ale quations	NWT 1 2	rel. change $1.0 \cdot 10^{0}$ $3.7 \cdot 10^{-02}$ $1.4 \cdot 10^{-02}$	rel. residual $9.3 \cdot 10^{-01}$ $9.6 \cdot 10^{-02}$ $1.1 \cdot 10^{-03}$	ADI 100 94	NWT rel. char 1 1.0 · CPU	nge rel. residual 10^0 $5.0 \cdot 10^{-11}$ time: 497.6 sec.	ADI 80
yapunov ADI for ADI ADI ADI ADI ADI ADI	3 4 5 6	$\begin{array}{c} 1.4 \cdot 10^{-0.4} \\ 3.5 \cdot 10^{-0.4} \\ 6.4 \cdot 10^{-0.8} \\ 7.5 \cdot 10^{-1.6} \end{array}$	$\begin{array}{c} 1.1 & 10 & 10 \\ 1.0 & 10^{-07} \\ 1.3 & 10^{-10} \\ 1.3 & 10^{-10} \end{array}$	98 97 97 97	NG-ADI	inner= 1, ou nge rel. residual 10^0 7.4 \cdot 10^{-11} time: 856.6 sec.	iter= 1 ADI 71
ADI al ic ADI s nk W	_				NG-ADI NWT rel. chai 1 1.0 · 2 CPU	inner= 0, ou nge rel. residual 10^0 6.5 · 10^{-13} time: 506.6 sec.	iter= 1 ADI 100

Test system:

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

Scaling of CPU times / Mesh Independence

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$$\partial_t x(\xi, t) = \Delta x(\xi, t) \quad \text{in } \Omega$$

$$\partial_\nu x = b(\xi) \cdot \frac{u(t)}{v} - x \quad \text{on } \Gamma_c$$

$$\partial_\nu x = -x \quad \text{on } \partial\Omega \setminus \Gamma_c$$

 $x(\xi,0)=1$

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 $u(t) \in \mathbb{R}$.

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

 $x(\xi,0)=1$

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 $u(t) \in \mathbb{R}$.

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

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 $x(\xi,0)=1$

Consider: output equation y = Cx, where

$$\begin{array}{rl} \mathcal{C}:\mathcal{L}^2(\Omega) & \to \mathbb{R} \\ x(\xi,t) & \mapsto y(t) = \int_{\Omega} x(\xi,t) \, d\xi. \end{array}$$

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

 $x(\xi,0)=1$

Consider: output equation y = Cx, where

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

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

 $x(\xi,0)=1$

Cost Function:

$$\mathcal{J}(u) = \int_0^\infty y^2(t) + u^2(t) \, dt.$$



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Simplified Low Rank Newton-Galerkin ADI

- generalized state space form implementation
- Penzl shifts (16/50/25) with respect to initial matrices
- projection acceleration in every outer iteration step
- projection acceleration in every 5-th inner iteration step

Test system:

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



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ompu	tation Limes			
	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	$1.05\cdot10^{+3}$	
	10	1 050 625	$1.65\cdot10^{+4}$	
	11	4 198 401	$1.35\cdot10^{+5}$	

Test system:

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

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Test system:

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



Quadratic ADI for AREs $0 = \mathcal{R}(X) = A^T X + XA - XBB^T X + W$

Basic QADI iteration

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$$((A - BB^{T}X_{k})^{T} + p_{k}I) X_{k+\frac{1}{2}} = -W - X_{k}((A - p_{k}I)) ((A - BB^{T}X_{k+\frac{1}{2}}^{T})^{T} + p_{k}I) X_{k+1} = -W - X_{k+\frac{1}{2}}^{T}(A - p_{k}I)$$

Derivation of complicated Cholesky factor version, but requires square and invertible Cholesky factors.

Idea of Iow-rank Galerkin-QAD

[B./SAAK '09]

[Wong/Balakrishnan et al. '05-'08]

$$V_1 \leftarrow \sqrt{-2\operatorname{Re}(p_1)} (A - B(B^T Y_0) Y_0^T + p_1 I)^{-T} B, \quad Y_1 \leftarrow V_1$$

FOR $k = 2, 3, \dots$

$$V_k \leftarrow V_{k-1} - (p_k + \overline{p_{k-1}})(A - B(B^T Y_{k-1})Y_{k-1}^T + p_k I)^{-T} V_{k-1}$$
$$Y_k \leftarrow \begin{bmatrix} Y_{k-1} & \sqrt{\frac{\operatorname{Re}(p_k)}{2}} V_k \end{bmatrix}$$

 $\begin{array}{l} Y_{k} \leftarrow \left[\begin{array}{c} Y_{k-1} & \sqrt{\operatorname{Re}\left(p_{k-1}\right)} & v_{k} \end{array} \right] \\ Y_{k} \leftarrow \operatorname{rrlq}(Y_{k}, \tau) & \% \text{ column compression} \\ \text{If desired, project ARE onto } \operatorname{range}(Y_{k}), \text{ solve and prolongate.} \end{array}$



Quadratic ADI for AREs $0 = \mathcal{R}(X) = A^T X + XA - XBB^T X + W$

Basic QADI iteration

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$$((A - BB^{T}X_{k})^{T} + p_{k}I) X_{k+\frac{1}{2}} = -W - X_{k}((A - p_{k}I)) ((A - BB^{T}X_{k+\frac{1}{2}}^{T})^{T} + p_{k}I) X_{k+1} = -W - X_{k+\frac{1}{2}}^{T}(A - p_{k}I)$$

Derivation of complicated Cholesky factor version, but requires square and invertible Cholesky factors.

Idea of low-rank Galerkin-QADI

$$V_1 \leftarrow \sqrt{-2\operatorname{Re}(p_1)}(A - B(B^T Y_0)Y_0^T + p_1I)^{-T}B, \quad Y_1 \leftarrow V_1$$

FOR $k = 2, 3, \dots$

$$V_{k} \leftarrow V_{k-1} - (p_{k} + \overline{p_{k-1}})(A - B(B' Y_{k-1})Y'_{k-1} + p_{k}I)^{-1}V_{k-1}$$
$$Y_{k} \leftarrow \begin{bmatrix} Y_{k-1} & \sqrt{\frac{\operatorname{Re}(p_{k})}{\operatorname{Re}(p_{k-1})}}V_{k} \end{bmatrix}$$
$$Y_{k} \leftarrow \operatorname{rrlq}(Y_{k}, \tau) \qquad \% \text{ column compression}$$

If desired, project ARE onto range(Y_k), solve and prolongate.

[B./SAAK '09]

[Wong/Balakrishnan et al. '05-'08]



AREs with High-Rank Constant Term

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Consider ARE

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

with $\operatorname{rank}(W) \not \ll n$, e.g., stabilization of flow problems described by Navier-Stokes eqns. requires solution of

$$0 = \mathcal{R}(X) = M_h - S_h^T X M_h - M_h X S_h - M_h X B_h B_h^T X M_h,$$

where $M_h = \text{mass matrix}$ of FE velocity test functions.





AREs with High-Rank Constant Term Solution: remove *W* from r.h.s. of Lyapunov egns. in Newton-ADI

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One step of Newton-Kleinman iteration for ARE:

$$A_{j}^{T}\underbrace{(X_{j}+N_{j})}_{=X_{j+1}}+X_{j+1}A_{j}=-W-\underbrace{(X_{j}B)}_{=K_{j}^{T}}\underbrace{B^{T}X_{j}}_{=K_{j}} \qquad \text{for } j=1,2,\ldots$$

Subtract two consecutive equations \Longrightarrow

$$A_{j}^{T}N_{j} + N_{j}A_{j} = -N_{j-1}^{T}BB^{T}N_{j-1}$$
 for $j = 1, 2, ...$

See [Banks/Ito '91, B./Hernández/Pastor '03, Morris/Navasca '05] for details and applications of this variant.

But: need $B^T N_0 = K_1 - K_0!$

Assuming K_0 is known, need to compute K_1 .



AREs with High-Rank Constant Term

Solution: remove W from r.h.s. of Lyapunov eqns. in Newton-ADI

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Solution idea:

$$\begin{aligned} & \mathcal{K}_1 &= \mathcal{B}^T \mathcal{X}_1 \\ &= \mathcal{B}^T \int_0^\infty e^{(A - \mathcal{B} \mathcal{K}_0)^T t} (\mathcal{W} + \mathcal{K}_0^T \mathcal{K}_0) e^{(A - \mathcal{B} \mathcal{K}_0) t} dt \\ &= \int_0^\infty g(t) dt \approx \sum_{\ell=0}^N \gamma_\ell g(t_\ell), \end{aligned}$$

where
$$g(t) = \left(\left(e^{(A - BK_0)t} B \right)^T \left(W + K_0^T K_0 \right) \right) e^{(A - BK_0)t}$$

[Borgggaard/Stoyanov '08]:

evaluate $g(t_{\ell})$ using ODE solver applied to $\dot{x} = (A - BK_0)x + adjoint eqn.$


AREs with High-Rank Constant Term

Solution: remove W from r.h.s. of Lyapunov eqns. in Newton-ADI

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Better solution idea:

(related to frequency domain POD [WILLCOX/PERAIRE '02])

$$\begin{split} \mathcal{K}_1 &= \mathcal{B}^T X_1 & (\text{Notation: } A_0 := A - \mathcal{B}\mathcal{K}_0) \\ &= \mathcal{B}^T \cdot \frac{1}{2\pi} \int_{-\infty}^{\infty} (\jmath \omega I_n - A_0)^{-H} (\mathcal{W} + \mathcal{K}_0^T \mathcal{K}_0) (\jmath \omega I_n - A_0)^{-1} \, d\omega \\ &= \int_{-\infty}^{\infty} f(\omega) \, d\omega \approx \sum_{\ell=0}^{N} \gamma_\ell f(\omega_\ell), \end{split}$$

where $f(\omega) = \left(-\left((\jmath\omega I_n + A_0)^{-1}B\right)^T (W + K_0^T K_0)\right) (\jmath\omega I_n - A_0)^{-1}$.

Evaluation of $f(\omega_\ell)$ requires

- 1 sparse LU decmposition (complex!),
- 2m forward/backward solves,
- *m* sparse and 2*m* low-rank matrix-vector products.

Use adaptive quadrature with high accuracy, e.g. Gauß-Kronrod ($\rm MAT-LAB's$ quadgk).



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[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.



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MESS – Matrix Equations Sparse Solvers [Saak/Mena/B. 2008]

[Penzl 2000]

• 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.

C version CMESS under development (Martin Köhler).

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- Galerkin projection can significantly accelerate ADI iteration for Lyapunov equations.
- Low-rank Galerkin-QADI may become a viable alternative to Newton-ADI.
- High-rank constant terms in ARE can be handled using quadrature rules.
- Software is available in MATLAB toolbox LYAPACK and its successor MESS.



Conclusions and Open Problems

ADI for Lyapunov and Riccati Equations

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Conclusions and Open Problems

References

- Galerkin projection can significantly accelerate ADI iteration for Lyapunov equations.
- Low-rank Galerkin-QADI may become a viable alternative to Newton-ADI.
- High-rank constant terms in ARE can be handled using quadrature rules.
- Software is available in MATLAB toolbox LYAPACK and its successor MESS.
- To-Do list:
 - computation of stabilizing initial guess.
 (If hierarchical grid structure is available, a multigrid approach is possible, other approaches based on "cheaper" matrix equations under development.)
 - Implementation of coupled Riccati solvers for LQG controller design and balancing-related model reduction.



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