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Solving large-scale differential matrix equations

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MAX PLANCK INSTITUTE FOR DYNAMICS OF COMPLEX TECHNICAL SYSTEMS MAGDEBURG

Motivation

The differential Riccati equation (DRE)

$$-\dot{X} = C^T C + A^T X + XA - XBB^T X =: \mathcal{R}(X), \qquad X(t_f) = M$$

is a non-linear, matrix-valued, and highly stiff ordinary differential equation.

Implicit time integrators [MENA '07, BENNER/MENA '12]

- Backward differentiation formula (BDF)
- linear implicit Runge-Kutta (Rosenbrock) methods
- Midpoint and Trapezoidal rule

Numerical issues

- Methods are fairly time and storage consuming.
- High accuracy requires small time steps or high order methods.
- Time steps need a number of solutions of algebraic matrix equations.

Motivation

Rosenbrock methods

The s-stage Rosenbrock method applied to a matrix differential equation of the form $\dot{X} = F(X)$ is given as

$$X_{k+1} = X_k + \tau \sum_{\ell=1}^{s} \beta_\ell K_\ell^{(k)},$$

$$K_i^{(k)} - \tau \mathcal{J}_k \sum_{\ell=1}^{i} \gamma_{i,\ell} K_\ell^{(k)} = F(X_k + \tau \sum_{\ell=1}^{i-1} \alpha_{i,\ell} K_\ell^{(k)}), \quad \forall i = 1, \dots, s.$$

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- s : order of the Rosenbrock method
- τ : time step
- $\mathcal{J}_k$: Fréchet derivative of F at X_k
- $\alpha_{i,\ell}, \gamma_{i,\ell}, \beta_\ell$: determining coefficients

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- $\alpha_{i,\ell}, \gamma_{i,\ell}, \beta_\ell$: determining coefficients

Example: 2-stage scheme
[DEKKER/VERWER '84]

$$x_{k+1} = x_k + \frac{3}{2}\tau k_1 + \frac{1}{2}\tau k_2,$$
$$(I - \tau \mathcal{J}_k) k_1 = f(x_k),$$
$$(I - \tau \mathcal{J}_k) k_2 = f(x_k + \tau k_1) - 2k_1$$

Motivation

Rosenbrock methods [Mena '07, Benner/Mena '12]

Again, consider the DRE, i.e., $F(X) = \mathcal{R}(X)$.

One-stage Rosenbrock scheme (Ros1) $(\gamma_{i,i} = 1)$

$$X_{k+1} = X_k + \tau \mathcal{K}_1^{(k)}$$

$$\mathcal{K}_1^{(k)} - \tau \mathcal{R}'|_{X_k}(\mathcal{K}_1^{(k)}) = \mathcal{R}(X_k)$$

Motivation

Rosenbrock methods

[Mena '07, Benner/Mena '12]

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One-stage Rosenbrock scheme (Ros1) $(\gamma_{i,i} = 1)$

$$X_{k+1} = X_k + \tau \mathcal{K}_1^{(k)}$$

$$\mathcal{K}_1^{(k)} - \tau (A - BB^T X_k)^T \mathcal{K}_1^{(k)} - \tau \mathcal{K}_1^{(k)} (A - BB^T X_k) = \mathcal{R}(X_k)$$

Motivation

Rosenbrock methods

[Mena '07, Benner/Mena '12]

Again, consider the DRE, i.e., $F(X) = \mathcal{R}(X)$.

One-stage Rosenbrock scheme (Ros1) $(\gamma_{i,i} = 1)$

$$X_{k+1} = X_k + \tau \mathcal{K}_1^{(k)}$$

$$(\tau(A - BB^T X_k) - \frac{1}{2}I)^T \mathcal{K}_1^{(k)} + \mathcal{K}_1^{(k)}(\tau(A - BB^T X_k) - \frac{1}{2}I) = -\mathcal{R}(X_k)$$

Motivation

Rosenbrock methods

[Mena '07, Benner/Mena '12]

Again, consider the DRE, i.e., $F(X) = \mathcal{R}(X)$.

One-stage Rosenbrock scheme (Ros1) ($\gamma_{i,i} = 1$)

$$X_{k+1} = X_k + \tau \mathcal{K}_1^{(k)}$$

$$\tilde{A}^T \mathcal{K}_1^{(k)} + \mathcal{K}_1^{(k)} \tilde{A} = -\mathcal{R}(X_k)$$

$$\tilde{A} := \tau(A - BB^T X_k) - \frac{1}{2} I$$

Motivation

Rosenbrock methods

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Again, consider the DRE, i.e., $F(X) = \mathcal{R}(X)$.

One-stage Rosenbrock scheme (Ros1) $(\gamma_{i,i} = 1)$

$$X_{k+1} = X_k + \tau \mathcal{K}_1^{(k)}$$

$$\tilde{A}^T \mathcal{K}_1^{(k)} + \mathcal{K}_1^{(k)} \tilde{A} = -\mathcal{R}(X_k)$$

Solve one Algebraic Lyapunov Equation (ALE) in each time-step of the 1-stage Rosenbrock method.

Motivation

Rosenbrock methods

[Mena '07, Benner/Mena '12]

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One-stage Rosenbrock scheme (Ros1) ($\gamma_{i,i} = 1$)

$$X_{k+1} = X_k + \tau \mathcal{K}_1^{(k)}$$

$$\tilde{A}^T \mathcal{K}_1^{(k)} + \mathcal{K}_1^{(k)} \tilde{A} = -\mathcal{R}(X_k)$$

Two-stage Rosenbrock scheme (Ros2) following [Dekker, Verwer '84]

$$X_{k+1} = X_k + \frac{3}{2}\tau \mathcal{K}_1^{(k)} + \frac{1}{2}\tau \mathcal{K}_2^{(k)}$$

$$\tilde{A}^T \mathcal{K}_1^{(k)} + \mathcal{K}_1^{(k)} \tilde{A} = -\mathcal{R}(X_k)$$

$$\tilde{A}^T \mathcal{K}_2^{(k)} + \mathcal{K}_2^{(k)} \tilde{A} = -\mathcal{R}(X_k + \tau \mathcal{K}_1^{(k)}) + 2\mathcal{K}_1^{(k)}$$

$$\tilde{A} := \gamma\tau(A - BB^T X_k) - \frac{1}{2} I$$

Motivation

Rosenbrock methods

[Mena '07, Benner/Mena '12]

Again, consider the DRE, i.e., $F(X) = \mathcal{R}(X)$.

One-stage Rosenbrock scheme (Ros1) ($\gamma_{i,i} = 1$)

$$X_{k+1} = X_k + \tau \mathcal{K}_1^{(k)}$$

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Two-stage Rosenbrock scheme (Ros2) following [Dekker, Verwer '84]

$$\begin{aligned} X_{k+1} &= X_k + \frac{3}{2}\tau \mathcal{K}_1^{(k)} + \frac{1}{2}\tau \mathcal{K}_2^{(k)} \\ \tilde{A}^T \mathcal{K}_1^{(k)} + \mathcal{K}_1^{(k)} \tilde{A} &= -\mathcal{R}(X_k) \\ \tilde{A}^T \mathcal{K}_2^{(k)} + \mathcal{K}_2^{(k)} \tilde{A} &= -\mathcal{R}(X_k + \tau \mathcal{K}_1^{(k)}) + 2\mathcal{K}_1^{(k)} \end{aligned}$$

Solve two ALEs in each time-step of the 2-stage Rosenbrock method.

Motivation

Rosenbrock methods

[Mena '07, Benner/Mena '12]

Again, consider the DRE, i.e., $F(X) = \mathcal{R}(X)$.

One-stage Rosenbrock scheme (Ros1) ($\gamma_{i,i} = 1$)

$$X_{k+1} = X_k + \tau \mathcal{K}_1^{(k)}$$

$$\tilde{A}^T \mathcal{K}_1^{(k)} + \mathcal{K}_1^{(k)} \tilde{A} = -\mathcal{R}(X_k)$$

Two-stage Rosenbrock scheme (Ros2) following [Dekker, Verwer '84]

$$X_{k+1} = X_k + \frac{3}{2}\tau \mathcal{K}_1^{(k)} + \frac{1}{2}\tau \mathcal{K}_2^{(k)}$$

$$\tilde{A}^T \mathcal{K}_1^{(k)} + \mathcal{K}_1^{(k)} \tilde{A} = -\mathcal{R}(X_k)$$

$$\tilde{A}^T \mathcal{K}_2^{(k)} + \mathcal{K}_2^{(k)} \tilde{A} = -\mathcal{R}(X_k + \tau \mathcal{K}_1^{(k)}) + 2\mathcal{K}_1^{(k)}$$

Right hand sides become indefinite.

Low-rank vs. indefinite DRE solvers

Right hand side factorization

Consider first stage equation

$$\tilde{A}^T \mathcal{K}_1^{(k)} + \mathcal{K}_1^{(k)} \tilde{A} = -\mathcal{R}(X_k),$$
$$\mathcal{R}(X_k) = C^T C + A^T X_k + X_k A - X_k B B^T X_k \overset{!}{=} G_k G_k^T$$

of 2nd order Rosenbrock method.

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Low-rank treatment of the linear term with $X_k = Z_k Z_k^T$, $\mathrm{rank}\,(Z_k) = z_k$

$$A^T Z_k Z_k^T + Z_k Z_k^T A = (A^T Z_k + Z_k)(A^T Z_k + Z_k)^T - A^T Z_k Z_k^T A - Z_k Z_k^T$$

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Low rank representation of $\mathcal{R}(X_k)$ (complex arithmetic)

$$G_k = \left[C^T, \quad A^T Z_k + Z_k, \quad iA^T Z_k, \quad iZ_k, \quad iZ_k Z_k^T B\right] \in \mathbb{C}^{n \times (q + 3z_k + m)}$$

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$$A^T Z_k Z_k^T + Z_k Z_k^T A = (A^T Z_k + Z_k)(A^T Z_k + Z_k)^T - A^T Z_k Z_k^T A - Z_k Z_k^T$$

Low rank representation of $\mathcal{R}(X_k)$ (cancellation)

$$\tilde{A}^T \hat{\mathcal{K}}_1^{(k)} + \hat{\mathcal{K}}_1^{(k)} \tilde{A} = -N_k N_k^T, \quad N_k = \left[C^T, \quad A^T Z_k + Z_k\right] \in \mathbb{R}^{n \times (q+z_k)}$$
$$\tilde{A}^T \tilde{\mathcal{K}}_1^{(k)} + \tilde{\mathcal{K}}_1^{(k)} \tilde{A} = -U_k U_k^T, \quad U_k = \left[A^T Z_k, \quad Z_k, \quad Z_k Z_k^T B\right] \in \mathbb{R}^{n \times (2z_k+m)}$$
$$\mathcal{K}_1^{(k)} := \hat{\mathcal{K}}_1^{(k)} - \tilde{\mathcal{K}}_1^{(k)} \qquad \rightsquigarrow \qquad \text{round off errors}$$

Low-rank vs. indefinite DRE solvers

Right hand side factorization

Consider first stage equation

$$\tilde{A}^T \mathcal{K}_1^{(k)} + \mathcal{K}_1^{(k)} \tilde{A} = -\mathcal{R}(X_k),$$

$$\mathcal{R}(X_k) = C^T C + A^T X_k + X_k A - X_k B B^T X_k \stackrel{!}{=} G_k S_k G_k^T$$

of 2nd order Rosenbrock method.

Low-rank vs. indefinite DRE solvers

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of 2nd order Rosenbrock method.

Low-rank treatment of the linear term with $X_k = L_k D_k L_k^T$, $\mathrm{rank}\,(L_k) = \ell_k$

$$A^T L_k D_k L_k^T + L_k D_k L_k^T A = \begin{bmatrix} A^T L_k, & L_k \end{bmatrix} \begin{bmatrix} 0 & D_k \\ D_k & 0 \end{bmatrix} \begin{bmatrix} A^T L_k, & L_k \end{bmatrix}^T$$

Low-rank vs. indefinite DRE solvers

Right hand side factorization

Consider first stage equation

$$\tilde{A}^T \mathcal{K}_1^{(k)} + \mathcal{K}_1^{(k)} \tilde{A} = -\mathcal{R}(X_k),$$

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of 2nd order Rosenbrock method.

Low-rank treatment of the linear term with $X_k = L_k D_k L_k^T$, $\mathrm{rank}\,(L_k) = \ell_k$

$$A^T L_k D_k L_k^T + L_k D_k L_k^T A = \left[A^T L_k, \quad L_k\right] \begin{bmatrix} 0 & D_k \\ D_k & 0 \end{bmatrix} \left[A^T L_k, \quad L_k\right]^T$$

LDL^T-type splitting of $\mathcal{R}(X_k)$ with $X_k = L_k D_k L_k^T$

$$G_k = \left[C^T, \quad A^T L_k, \quad L_k\right] \in \mathbb{R}^{n \times (q+2\ell_k)},$$

$$S_k = \begin{bmatrix} I_q & 0 & 0 \\ 0 & 0 & D_k \\ 0 & D_k & -D_k L_k^T B B^T L_k D_k \end{bmatrix} \in \mathbb{R}^{(q+2\ell_k) \times (q+2\ell_k)}$$

Low-rank vs. indefinite DRE solvers

Right hand side factorization

Low rank representation of $\mathcal{R}(X_k)$ (complex arithmetic)

$$G_k = \left[C^T,\quad A^TZ_k + Z_k,\quad iA^TZ_k,\quad iZ_k,\quad iZ_kZ_k^TB\right] \in \mathbb{C}^{n\times(q+3z_k+m)}$$

Low rank representation of $\mathcal{R}(X_k)$ (cancellation)

$$\tilde{A}^T\hat{\mathcal{K}}_1^{(k)} + \hat{\mathcal{K}}_1^{(k)}\tilde{A} = -N_kN_k^T,\quad N_k = \left[C^T,\quad A^TZ_k + Z_k\right] \in \mathbb{R}^{n\times(q+z_k)}$$

$$\tilde{A}^T\tilde{\mathcal{K}}_1^{(k)} + \tilde{\mathcal{K}}_1^{(k)}\tilde{A} = -U_kU_k^T,\quad U_k = \left[A^TZ_k,\quad Z_k,\quad Z_kZ_k^TB\right] \in \mathbb{R}^{n\times(2z_k+m)}$$

$$\mathcal{K}_1^{(k)} := \hat{\mathcal{K}}_1^{(k)} - \tilde{\mathcal{K}}_1^{(k)} \qquad \rightsquigarrow \qquad \text{round off errors}$$

LDL^T-type splitting of $\mathcal{R}(X_k)$ with $X_k = L_kD_kL_k^T$

$$G_k = \left[C^T,\quad A^TL_k,\quad L_k\right] \in \mathbb{R}^{n\times(q+2\ell_k)},$$

$$S_k = \begin{bmatrix} I_q & 0 & 0 \\ 0 & 0 & D_k \\ 0 & D_k & -D_kL_k^TBB^TL_kD_k \end{bmatrix} \in \mathbb{R}^{(q+2\ell_k)\times(q+2\ell_k)}$$

Implications for Lyapunov solvers

Alternating Directions Implicit (ADI)

Solve

$$AX + XA^T = -GG^T \qquad \text{with } X = ZZ^T.$$

Classical low-rank ADI [Benner/Kürschner/S. '13]

INPUT: ADI shifts $p_1, \dots, p_\ell \in \mathbb{C}$, tolerance ε, G

1: $W_0 = G,\ Z_0 = [\ ],\ j = 1$
2: **while** $\|W_{j-1}W_{j-1}^T\|_2 \geq \varepsilon\|GG^T\|_2$ **do**
3: Solve $(A + p_j I)V_j = W_{j-1}$ for V_j.
4: $W_j = W_{j-1} - 2p_j V_j$,
5: $Z_j = [Z_{j-1},\ \sqrt{-2p_j}V_j]$
6: $j = j + 1$
7: **end while**

Implications for Lyapunov solvers

Alternating Directions Implicit (ADI)

Solve

$$AX + XA^T = -GSG^T \qquad \text{with } X = LDL^T.$$

Low-rank LDL-type ADI [Lang/Mena/S. '14]

INPUT: ADI shifts $p_1, \ldots, p_\ell \in \mathbb{C}$, tolerance ε, G, S

1: $W_0 = G,\ Z_0 = [\,],\ j = 1$
2: **while** $\|W_{j-1} S W_{j-1}^T\|_2 \geq \varepsilon \|GSG^T\|_2$ **do**
3: Solve $(A + p_j I)V_j = W_{j-1}$ for V_j.
4: $W_j = W_{j-1} - 2p_j V_j$,
5: $L_j = [L_{j-1},\ V_j]$
6: $j = j + 1$
7: **end while**
8: $D_j = -2\,\mathrm{diag}\left(\mathrm{Re}\,(p_1), \ldots, \mathrm{Re}\,(p_j)\right) \otimes S$

$\otimes \ldots$ Kronecker product

Implications for Lyapunov solvers

Krylov subspace methods

Solve

$$AX + XA^T = -GG^T \qquad \text{with } X = ZZ^T.$$

Classical low-rank Krylov subspace methods

INPUT: Set of shifts $\mu = (\mu_1, \ldots, \mu_s) \in \mathbb{C}^s$.

1: Compute orthonormal basis V of, e.g.,

$$\mathcal{RK}_s(A, G, \mu) \subset \mathbb{R}^{n\times(s+1)k} \text{ or } \mathcal{K}_{2s}(A, A^{-s}G) = \subset \mathbb{R}^{n\times(2s+1)k}.$$

2: Compute solution Y of the small-scale Lyapunov equation

$$V^TAVY + YV^TAV = -V^TGG^TV, \text{ with } \quad X = VYV^T.$$

3: Compute decomposition $Y = \hat{Z}\hat{Z}^T$ and set $Z := V\hat{Z}, X := ZZ^T$.

Implications for Lyapunov solvers

Krylov subspace methods

Solve

$$AX + XA^T = -GSG^T \qquad \text{with } X = LDL^T.$$

Low-rank LDL-type Krylov subspace method

INPUT: Set of shifts $\mu = (\mu_1, \ldots, \mu_s) \in \mathbb{C}^s$.

1: Compute orthonormal basis L of, e.g.,

$$\mathcal{RK}_s(A, G, \mu) \subset \mathbb{R}^{n\times(s+1)k} \text{ or } \mathcal{K}_{2s}(A, A^{-s}G) =\subset \mathbb{R}^{n\times(2s+1)k}.$$

2: Compute solution D of the small-scale Lyapunov equation

$$L^TALD + DL^TAL = -L^TGSG^TL, \text{ with } \quad X = LDL^T.$$

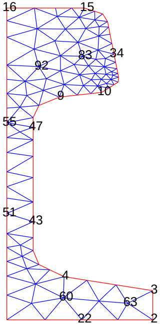
3: FREE TIME

Numerical experiments

ADI based implementation

- Finite time LQR problem for 2D heat equation.

$$
\begin{aligned}
c \cdot \rho \frac{\partial}{\partial t} x &= \lambda \Delta x, && \xi \in \Omega \\
\lambda \frac{\partial}{\partial n} x &= \kappa(u_k - x), && \xi \in \Gamma_k,\ 1 \leq k \leq 7, \\
\frac{\partial}{\partial n} x &= 0, && \xi \in \Gamma_7.
\end{aligned}
$$

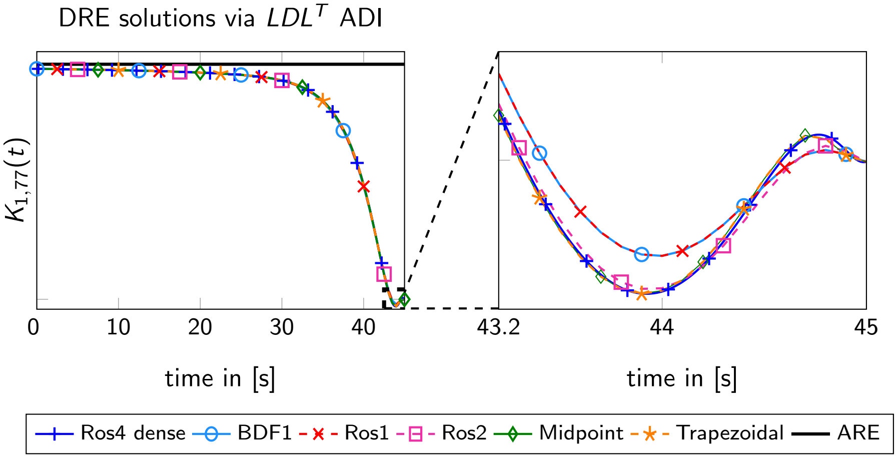


- FEM discretization with $n = 371$ states, $m = 7$ inputs, and $q = 6$ outputs
- computations with $\tau = 0.1$ on $[0, 45]s$
- evaluations for one component of the feedback $K = -B^T XE$

http://simulation.uni-freiburg.de/downloads/benchmark/Steel%20Profiles%20(38881)/

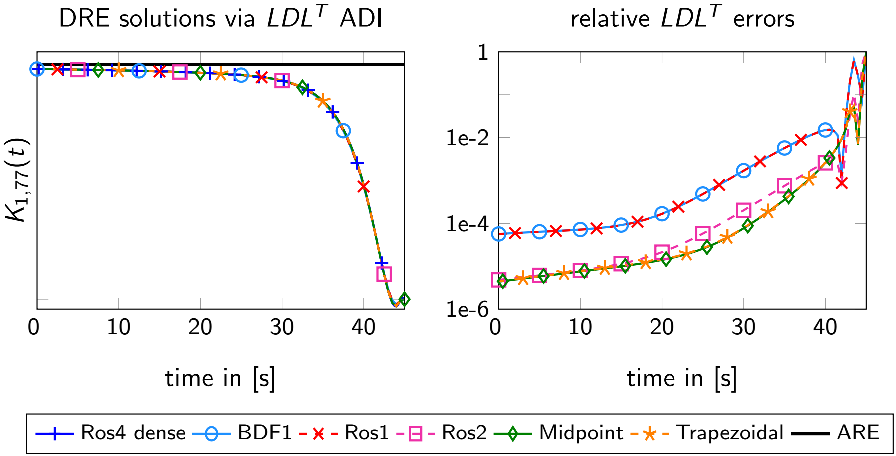
Numerical experiments

ADI based implementation



Numerical experiments

ADI based implementation



Numerical experiments

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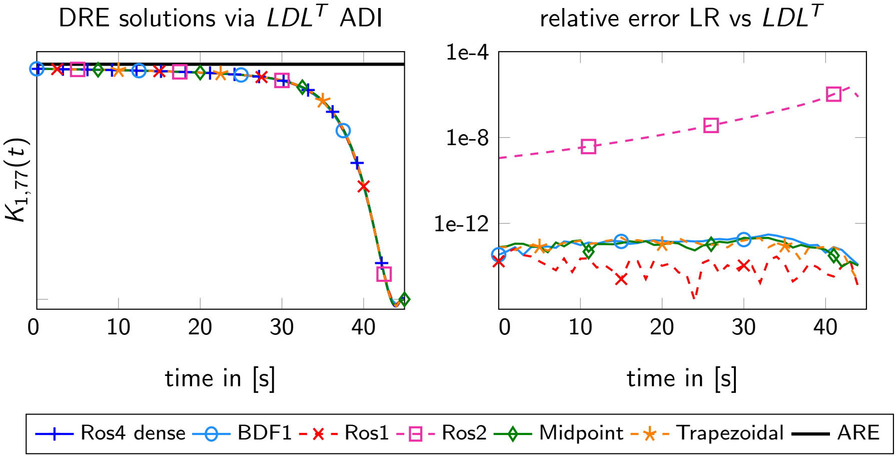


Numerical experiments

ADI based implementation

	time in s			avg. rel. err.*
	LR	LDL	speedup	LRvsLDL
BDF1	1 909.53	1 299.17	1.4698	1.87e-14
Ros1	845.74	658.11	1.2851	1.85e-15
Ros2	4 514.19	1 242.30	3.6337	2.97e-08
Midpoint	2 598.54	1 494.33	1.7389	1.50e-14
Trapezoidal	2 602.14	1 180.55	2.2042	1.53e-14

Table: Timings, average relative errors between standard low-rank and the LDL^T based methods of the steel profile example with $n = 371$ on the time interval $[0, 45]$ s, τ=1e-1.

*one component of the feedback

Numerical experiments

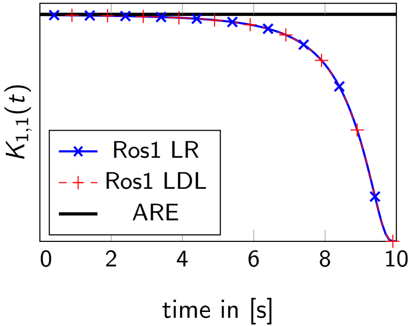
Extended Krylov subspace based implementation

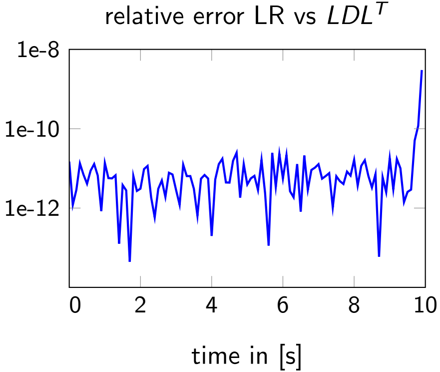
- CAREX benchmark[1] Example 4.2 [Abels/Benner '99]
- variable system size, here:
  - $n = 1\,000$ states,
  - $m = 1$ inputs,
  - $q = 1$ outputs
- computations on $[0, 10]s$ with $\tau = 0.01$
- evaluations for $(1, 1)$-component of the feedback $K = -B^T XE$

[1] available from www.slicot.org

Numerical experiments

Extended Krylov subspace based implementation





	time in s			avg. rel. err.
	LR	LDL	speedup	LRvsLDL
Ros1	421.98	254.57	1.6576	2.05e-08

Constant coefficient matrices

Idea: global projection (w.r.t. time)

Find a constant matrix L and move the time dependence solely to D, e.g., using model reduction on $\Sigma(A, B, C)$.

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Idea: global projection (w.r.t. time)

Find a constant matrix L and move the time dependence solely to D, e.g., using model reduction on $\Sigma(A, B, C)$.

Then:

- storage requirements are drastically reduced,
- only a small dense DRE needs to be solved,
- Schur form reuse in step equations
  $\rightsquigarrow$ acceleration by BLAS-3-/multicore-enabled solvers
  [Jonsson/Kågström '02, Köhler/S. '14]
- Parallel in time integration via PARAREAL is relatively straight forward [Köhler/Lang/S. '15]

Constant coefficient matrices

Idea: global projection (w.r.t. time)

Find a constant matrix L and move the time dependence solely to D, e.g., using model reduction on $\Sigma(A, B, C)$.

Then:

- storage requirements are drastically reduced,
- only a small dense DRE needs to be solved,
- Schur form reuse in step equations
  $\rightsquigarrow$ acceleration by BLAS-3-/multicore-enabled solvers
  [Jonsson/Kågström '02, Köhler/S. '14]
- Parallel in time integration via PARAREAL is relatively straight forward [Köhler/Lang/S. '15]

Problem [Mehrmann/Voigt '15]

What is good for $\Sigma(A, B, C)$ is not necessarily good for the DRE.

Conclusions, Outlook & References

Conclusion

- Need to solve ALEs with indefinite right hand sides ($s > 1$)
- LDL^T factorization improves both ADI and Krylov methods
  - avoids complex arithmetic, cancellation
  - reduces number of system solves
  - natural decomposition for Krylov methods
- Memory management: double buffering, global projection, property of interest

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Outlook

- adaptive time stepping,
- validity conditions and subspace selection for the global projection approach,
- comparison to operator splitting approach [Hansen/Stillfjord '14]

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Thank you!