Structure preserving GMRES methods for solving large Lyapunov equations

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Outline

1. Motivation
2. GMRES in low rank arithmetics
   - GMRES
   - LRCF-ADI
3. Numerical results

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Basic Idea of Model reduction

Linear circuit equations are modelled by a linear descriptor system:

$$\begin{aligned} \mathcal{E}\dot{x} &= \mathcal{A}x + \mathcal{B}u \qquad && \mathcal{E}, \mathcal{A} \in \mathbb{R}^{n,n}, \quad \mathcal{B} \in \mathbb{R}^{n,m} \\ y &= \mathcal{C}x && \mathcal{C} \in \mathbb{R}^{p,n} \qquad . \end{aligned}$$

Approximate it by a reduced order system:

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Balanced truncation

- Compute a system equivalence transformation and truncate the system.
- E singular:
  Requires the solution of 2 dual continuous-time algebraic Lyapunov equations (Proper Gramians) and 2 dual discrete-time algebraic Lyapunov equations (Improper Gramians).

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Proper Gramians X, Y

Generalized projected Lyapunov equations

$$EXA^T + AXE^T = -P_l BB^T P_l^T, \quad X_p = P_r^T X P_r$$
$$E^T YA + A^T YE = -P_r^T C^T CP_r, \quad Y_p = P_l Y P_l^T$$

$E, A \in R^{n \times n} \quad B, C^T \in R^{n \times n_s}$

- r.h.s. is symmetric and low rank i.e. $n_s \ll n$
- E singular
- P_r, P_l are projectors on right and left deflating subspaces of $\lambda E - A$ corresponding to finite eigenvalues
- $\lambda E - A$ asymptotically stable: the solution exists and is unique

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$$EX_pA^T + AX_pE^T = -B_pB_p^T$$
$$E^TY_pA + A^TY_pE = -C_p^TC_p$$

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Structure

$\mathcal{L} := A \otimes E + E \otimes A \ldots$ Lyapunov operator
$\mathcal{X}_p = \text{vec}(X_p) \qquad \mathcal{B}_p = \text{vec}(B_p B_p^T)$

Lyapunov equation

$$EX_pA^T + AX_pE^T = -B_pB_p^T$$

$E, A \in R^{n \times n}$ $B_p \in R^{n \times n_s}$

Linear equation

$$\mathcal{L}\mathcal{X}_p = -\mathcal{B}_p$$

$\mathcal{L} \in R^{n^2 \times n^2}$ $\mathcal{B}_p \in R^{n^2 \times 1}$

Structure preservation principle

- Properties of X_p: low rank, symmetric, positive semidefinite
- Linear combination and matrix-vector multiplication preserve low rank and symmetry
- Objective: Structure preserving Krylov-subspace methods, e.g. GMRES
- Use factorization $\mathcal{X} = VZV^T =$ 

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GMRES

Properties

- Iterative method for solving $\mathcal{L}\mathcal{X}_p = -\mathcal{B}_p$
- Calculates an orthonormal basis of m-dimensional Krylov space $\mathcal{K}_m(\mathcal{R}_0, \mathcal{L}) = \text{span}(\mathcal{R}_0, \mathcal{L}\mathcal{R}_0, \ldots, \mathcal{L}^{m-1}\mathcal{R}_0)$
- Solution $\mathcal{X}_m$ minimizes residual.

GMRES [Saad & Schultz'86,Saad '92]

Algorithm

- Initialize: choose $\mathcal{X}_0$ and dimension m
- Arnoldi process:
  1. compute $\mathcal{R}_0 = \mathcal{B}_p - \mathcal{L}\mathcal{X}_0,\ h_{1,0} = \|\mathcal{R}_0\|,\ \mathcal{V}_1 = \frac{\mathcal{R}_0}{h_{1,0}}$
  2. for $j = 1 \dots m$
     a) solve $\mathcal{W}_j = M^{-1}\mathcal{V}_j$
     b) compute $\mathcal{V}_{j+1} = \mathcal{L}\mathcal{W}_j$
     c) orthogonalize $\mathcal{V}_{j+1}$ on all previous $\mathcal{V}_i$ via MGS
  3. Let $W_m := [\mathcal{W}_1 \dots \mathcal{W}_m]$
- Compute solution $\mathcal{X}_m = \mathcal{X}_0 + W_m\mathcal{Y}_m$ with $\mathcal{Y}_m$ minimizes $\|h_{1,0}e_1 - H_m\mathcal{Y}\|$
- Restart : If *not converged* $\mathcal{X}_0 = \mathcal{X}_m$

Low rank arithmetics

We only need 4 types of operations to formulate Krylov-subspace methods in low rank arithmetics.

Tools LR-BLAS

1. $\mathcal{Y} = \mathcal{Y} + \alpha\mathcal{X}$ — Addition
2. $\mathcal{Y} = \alpha\mathcal{L}\mathcal{X} + \beta\mathcal{Y}$ — Generalized matrix-vector multiplication
3. $\alpha = \|\mathcal{Y}\|$ — Norm
4. $\alpha = (\mathcal{Y}, \mathcal{X})$ — Scalar product

After 1) and 2) the rank of the result may increase. Strategy?

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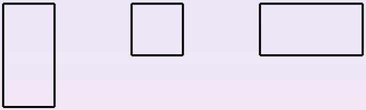
Rank truncation strategy

Rank of $\mathcal{X} = VZV^T$ need to be reduced w.r.t. given tolerance.

1. Perform $QR\Pi$ decomposition of $V = QR\Pi$
   take first r_1 rows of R
   $\hat{Q} = Q(:, 1 : r_1), \hat{R} = R(1 : r_1, :)$
2. Compute EVD of $\hat{R}Z\hat{R}^T = U\Sigma U^T$
   take first r_2 eigenvalues in Σ
   $\hat{U} = U(:, 1 : r_2), \hat{\Sigma} = \Sigma(1 : r_2, 1 : r_2)$



$$\mathcal{X} = V \; Z \; V^T$$

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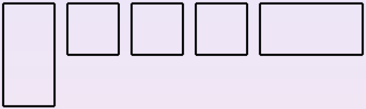

$\mathcal{X} = QR\,Z\,R^T Q^T$

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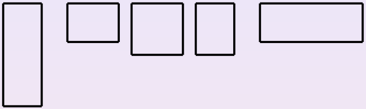

$\mathcal{X} = \hat{Q}\hat{R}\, Z\, \hat{R}^T \hat{Q}^T$

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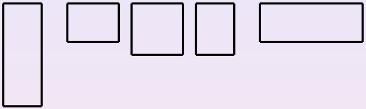

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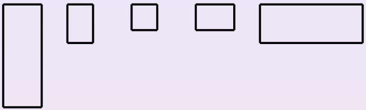

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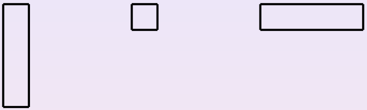

$\mathcal{X} = \hat{V}\,\hat{\Sigma}\,\hat{V}^T$

Result

- $\mathcal{X} = \hat{V}\hat{\Sigma}\hat{V}^T$ with $\hat{V} = \hat{Q}\hat{U}$
- $\hat{V}$ unitary matrix
- $\hat{\Sigma}$ diagonal matrix

Preconditioning

Properties

- Must preserve structure (important fact)
- Should increase convergence rate
- Natural candidate: LRCF-ADI

  Apply 1 cycle of LRCF-ADI to

$$E\mathcal{W}_jA^T + A\mathcal{W}_jE^T = -P_l\mathcal{V}_jP_l^T \qquad P_r^T\mathcal{W}_jP_r.$$

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ADI-methods

Alternating **D**irect **I**mplicit

Overview of Development

- Decompose linear equation into 2 (Finite Differences for elliptic PDE's) [Peacemen, Rachford '55]
- ADI-iteration for L. equations [Wachspress '88]

$$(E + \tau_j A)X_{j-\frac{1}{2}} = -B_p B_p^T - X_{j-1}(E - \tau_j A)^T$$
$$(E + \tau_j A)X_j = -B_p B_p^T - X_{j-\frac{1}{2}}^T(E - \tau_j A)^T$$

- Rewrite as one step iteration and work with low rank factors $X_j = Z_j Z_j^T$ [Penzl' 99]
- Reversing the order of the shifts [Li, White '02]
- Apply to generalized L. equations [Benner '04, Stykel '08]

LRCF-ADI [Stykel '08]

Low **R**ank **C**holesky **F**actor-**A**lternating **D**irect **I**mplicit computes the Cholesky-Factor Z of the solution $X = ZZ^T$.

Algorithm

1. compute shift parameters $\tau_1, ...\tau_j$
2. $z_1 = \sqrt{-2\tau_1}(E + \tau_1 A)^{-1} B_p$
   $Z = [z_1]$
3. For $i = 2 \ldots j \ldots$
   $z_i = P_{i-1} z_{i-1}$, with
   $P_i = \frac{\sqrt{-2\tau_{i+1}}}{\sqrt{-2\tau_i}}[I - (\tau_{i+1} + \tau_i)(E + \tau_{i+1} A)^{-1} A]$
   $Z = [Z \; z_i]$
   end for

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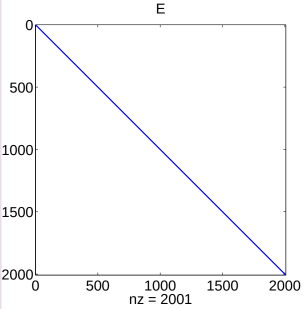
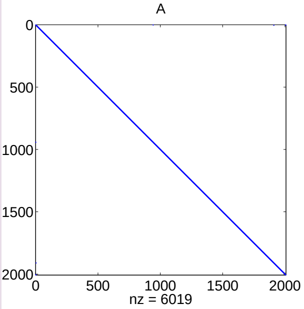
All computations were done on a workstation with Intel(R) Xeon(TM) MP CPU 3.66GHz and 16GB RAM using Matlab©Version 7.7.0.471 (R2008b).

Example Circuit n=2007 RC-chain

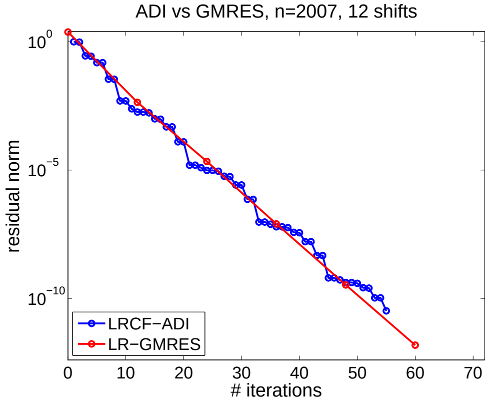
2002 capacitors, 2003 resistors, 3 voltage sources





Example circuits were provided by NEC.

Exact solve $E + \tau_i A$ (LU)



method	rank X_p	cpu-time [s]
LRCF-ADI	98	4,0
LR-GMRES	95	5,8

- same number of iterations
- comparable runtime
- convergence criterion cheaper

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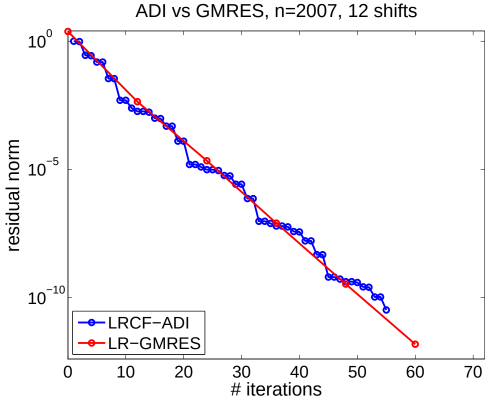

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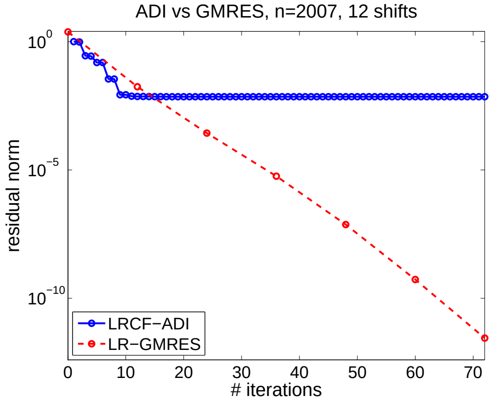

[* M. Bollhöfer et.al. ILUPACK - preconditioning software package. Available online at http://ilupack.tu-bs.de/. Release V2.2, November 2008.]

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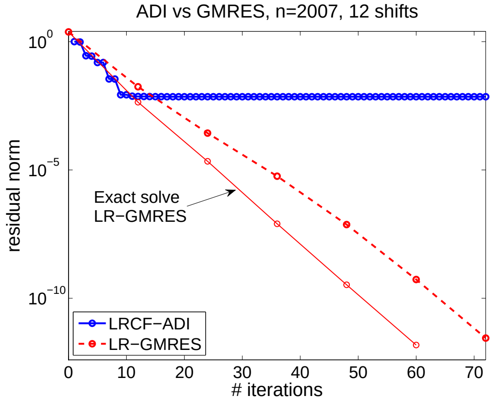

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Benefits

- Structure preservation (low rank, symmetry) is fulfilled
- More robust against perturbations
- Same number of iterations as LR-CFADI together with a comparable runtime

Future work

- Use QMR as Krylov subspace method
- Integration in PABTEC
- C implementation
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