IDR: A new generation of Krylov subspace methods?

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Outline

Krylov subspace methods

- Hessenberg decompositions
- Polynomial representations
- Perturbations

IDR

- IDR and IDR(s)
- IDREig
- IDR(s)Stab(ℓ) and IDRStabEig
- (Flexible and multi-shift) QMRIDR
- Perturbations

Outline

Introduction

Krylov subspace methods: approximations

$$\left.\begin{array}{l}\mathbf{x}_k, \underline{\mathbf{x}}_k, \\ \mathbf{y}_k, \underline{\mathbf{y}}_k\end{array}\right\} \in \mathcal{K}_k(\mathbf{A}, \mathbf{q}) := \operatorname{span}\{\mathbf{q}, \mathbf{A}\mathbf{q}, \ldots, \mathbf{A}^{k-1}\mathbf{q}\} = \{p(\mathbf{A})\mathbf{q} \mid p \in \mathbb{P}_{k-1}\},$$

where

$$\mathbb{P}_{k-1} := \Big\{\sum_{j=0}^{k-1} \alpha_j z^j \mid \alpha_j \in \mathbb{C},\ 0 \leqslant j < k\Big\},$$

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to solutions of linear systems

$$\mathbf{A}\mathbf{x} = \mathbf{r}_0 \ (= \mathbf{b} - \mathbf{A}\mathbf{x}_0), \qquad \mathbf{A} \in \mathbb{C}^{n\times n}, \quad \mathbf{b}, \mathbf{x}_0 \in \mathbb{C}^n,$$

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and (partial) eigenproblems

$$\mathbf{A}\mathbf{v} = \mathbf{v}\lambda, \qquad \mathbf{A} \in \mathbb{C}^{n\times n}.$$

Hessenberg decompositions

Construction of basis vectors resembled in structure of arising Hessenberg decomposition

$$\mathbf{A}\mathbf{Q}_k = \mathbf{Q}_{k+1}\underline{\mathbf{H}}_k,$$

where

- $\mathbf{Q}_{k+1} = (\mathbf{Q}_k, \mathbf{q}_{k+1}) \in \mathbb{C}^{n\times(k+1)}$ collects basis vectors,
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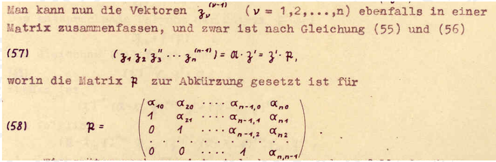
Aspects of perturbed Krylov subspace methods: captured with perturbed Hessenberg decompositions

$$\mathbf{A}\mathbf{Q}_k + \mathbf{F}_k = \mathbf{Q}_{k+1}\underline{\mathbf{H}}_k,$$

$\mathbf{F}_k \in \mathbb{C}^{n\times k}$ accounts for perturbations (finite precision & inexact methods).

Karl Hessenberg & “his” matrix + decomposition

„Behandlung linearer Eigenwertaufgaben mit Hilfe der Hamilton-Cayleyschen Gleichung“, Karl Hessenberg, 1. Bericht der Reihe „Numerische Verfahren“, July, 23rd 1940, page 23:



Man kann nun die Vektoren $\mathfrak{z}_\nu^{(\nu-1)}$ ($\nu = 1,2,\dots,n$) ebenfalls in einer Matrix zusammenfassen, und zwar ist nach Gleichung (55) und (56)

(57) $$(\mathfrak{z}_1\,\mathfrak{z}_2'\,\mathfrak{z}_3''\cdots\mathfrak{z}_n^{(n-1)}) = \mathfrak{A}\cdot\mathfrak{Z}' = \mathfrak{Z}'\cdot\mathfrak{P},$$

worin die Matrix $\mathfrak{P}$ zur Abkürzung gesetzt ist für

(58) $$\mathfrak{P} = \begin{pmatrix} \alpha_{10} & \alpha_{20} & \cdots & \alpha_{n-1,0} & \alpha_{n0} \\ 1 & \alpha_{21} & \cdots & \alpha_{n-1,1} & \alpha_{n1} \\ 0 & 1 & \cdots & \alpha_{n-1,2} & \alpha_{n2} \\ \cdot & \cdot & \cdots & \cdot & \cdot \\ 0 & 0 & \cdots & 1 & \alpha_{n,n-1} \end{pmatrix}.$$

- Hessenberg decomposition, Eqn. (57),
- Hessenberg matrix, Eqn. (58).

Karl Hessenberg (* September 8th, 1904, † February 22nd, 1959)

Important Polynomials

Residuals of OR and MR approximation

$$\mathbf{x}_k := \mathbf{Q}_k \mathbf{z}_k \qquad \text{and} \qquad \underline{\mathbf{x}}_k := \mathbf{Q}_k \underline{\mathbf{z}}_k$$

with coefficient vectors

$$\mathbf{z}_k := \mathbf{H}_k^{-1} \mathbf{e}_1 \|\mathbf{r}_0\| \qquad \text{and} \qquad \underline{\mathbf{z}}_k := \underline{\mathbf{H}}_k^{\dagger} \underline{\mathbf{e}}_1 \|\mathbf{r}_0\|$$

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Convergence of OR and MR depends on (harmonic) Ritz values.

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polynomial representation

$$\mathbf{r}_k = \mathcal{R}_k(\mathbf{A})\mathbf{r}_0 - \sum_{\ell=1}^{k} z_{\ell k}\mathcal{R}_{\ell+1:k}(\mathbf{A})\mathbf{f}_\ell + \mathbf{F}_k\mathbf{z}_k$$

(all trailing square Hessenberg matrices are assumed to be regular).

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Convergence: $\mathbf{F}_k\mathbf{z}_k$ bounded (inexact methods) & $\mathcal{R}_{\ell+1:k}(\mathbf{A})$ “small”.

Outline

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1979	First talk on IDR
1980	Proceedings
1989	CGS
1992	IDR $\rightsquigarrow$ BiCGStab
1993	BiCGStab2, BiCGStab(ℓ)
later	“acronym explosion” . . .

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IDR(s) is a Krylov subspace method $\rightsquigarrow$ all techniques from 90's applicable!

IDR(s)

IDR spaces:

$$\mathcal{G}_0 := \mathcal{K}(\mathbf{A}, \mathbf{q}), \qquad \text{(full Krylov subspace)}$$
$$\mathcal{G}_j := (\alpha_j \mathbf{A} + \beta_j \mathbf{I})(\mathcal{G}_{j-1} \cap \mathcal{S}), \quad j \geqslant 1, \quad \alpha_j, \beta_j \in \mathbb{C}, \quad \alpha_j \neq 0,$$

where

$$\text{codim}(\mathcal{S}) = s, \quad \text{e.g.,} \quad \mathcal{S} = \text{span}\,\{\widetilde{\mathbf{R}}_0\}^{\perp}, \quad \widetilde{\mathbf{R}}_0 \in \mathbb{C}^{n \times s}.$$

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Interpreted as Sonneveld spaces (Sleijpen, Sonneveld, van Gijzen 2010):

$$\mathcal{G}_j = \mathcal{S}_j(P_j, \mathbf{A}, \widetilde{\mathbf{R}}_0) := \left\{ P_j(\mathbf{A})v \mid v \perp \mathcal{K}_j(\mathbf{A}^\mathsf{H}, \widetilde{\mathbf{R}}_0) \right\},$$
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Image of shrinking space: Induced Dimension Reduction.

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IDR spaces nested:

$$\{\mathbf{o}\} = \mathcal{G}_{\mathrm{jmax}} \subsetneq \cdots \subsetneq \mathcal{G}_{j+1} \subsetneq \mathcal{G}_{j} \subsetneq \mathcal{G}_{j-1} \subsetneq \cdots \subsetneq \mathcal{G}_{2} \subsetneq \mathcal{G}_{1} \subsetneq \mathcal{G}_{0}.$$

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IDR(s)

Generalized Hessenberg decomposition:

$$\mathbf{A}\mathbf{V}_k = \mathbf{A}\mathbf{G}_k\mathbf{U}_k = \mathbf{G}_{k+1}\underline{\mathbf{H}}_k,$$

where $\mathbf{U}_k \in \mathbb{C}^{k\times k}$ upper triangular.

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Structure of Sonneveld pencils:

$$\mathbf{H}_k = \begin{pmatrix}
\times & \times & \times & \times & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ \\
+ & \times & \times & \times & \times & \circ & \circ & \circ & \circ & \circ & \circ & \circ \\
\circ & + & \times & \times & \times & \times & \circ & \circ & \circ & \circ & \circ & \circ \\
\circ & \circ & + & \times & \times & \times & \times & \circ & \circ & \circ & \circ & \circ \\
\circ & \circ & \circ & + & \times & \times & \times & \times & \circ & \circ & \circ & \circ \\
\circ & \circ & \circ & \circ & + & \times & \times & \times & \times & \circ & \circ & \circ \\
\circ & \circ & \circ & \circ & \circ & + & \times & \times & \times & \times & \circ & \circ \\
\circ & \circ & \circ & \circ & \circ & \circ & + & \times & \times & \times & \times & \circ \\
\circ & \circ & \circ & \circ & \circ & \circ & \circ & + & \times & \times & \times & \times \\
\circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & + & \times & \times & \times \\
\circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & + & \times & \times \\
\circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & + & \times
\end{pmatrix}, \quad
\begin{pmatrix}
\times & \times & \times & \times & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ \\
\circ & \times & \times & \times & \times & \circ & \circ & \circ & \circ & \circ & \circ & \circ \\
\circ & \circ & \times & \times & \times & \times & \circ & \circ & \circ & \circ & \circ & \circ \\
\circ & \circ & \circ & \times & \times & \times & \times & \circ & \circ & \circ & \circ & \circ \\
\circ & \circ & \circ & \circ & \times & \times & \times & \times & \circ & \circ & \circ & \circ \\
\circ & \circ & \circ & \circ & \circ & \times & \times & \times & \times & \circ & \circ & \circ \\
\circ & \circ & \circ & \circ & \circ & \circ & \times & \times & \times & \times & \circ & \circ \\
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\circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \times & \times \\
\circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \times
\end{pmatrix} = \mathbf{U}_k$$

IDREig

Eigenvalues of Sonneveld pencil $(\mathbf{H}_k, \mathbf{U}_k)$ are roots of residual polynomials. Those distinct from roots of

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Use deflated pencil for Lanczos Ritz values (Gutknecht, Z. (2010): IDREIG). First: IDR(s)ORES, Olaf Rendel: IDR(s)BIO, Anisa Rizvanolli: IDR(s)STAB(ℓ).

IDRSTAB

IDR(s)STAB(ℓ) (Tanio & Sugihara; Sleijpen & van Gijzen): combine ideas of IDR(s) and BICGSTAB(ℓ).

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IDRSTAB (Sleijpen's implementation) recursively computes "(extended) Hessenberg matrices of basis matrices and residuals" ($k \geqslant 1$):

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\begin{array}{llll}
\mathbf{G}_{11}^{(k)}, \mathbf{r}_{11}^{(k)} & \mathbf{G}_{12}^{(k)}, \mathbf{r}_{12}^{(k)} & \cdots & \mathbf{G}_{1,\ell+1}^{(k)}, \quad \mathbf{r}_{1,\ell+1}^{(k)} \\
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\mathbf{G}_{i,j}^{(k)} &\in \mathbb{C}^{n\times s}, & \mathbf{r}_{i,j}^{(k)} &\in \mathbb{C}^{n}, \\
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Initialization using Arnoldi's method:

$$\mathbf{G}_{21}^{(1)} = \mathbf{A}\mathbf{G}_{11}^{(1)} = (\mathbf{G}_{11}^{(1)}, \mathbf{g}_{\mathsf{tmp}})\underline{\mathbf{H}}_s^{(0)},$$

$$\mathbf{r}_{11}^{(1)} = \mathbf{r}_0 - \mathbf{G}_{21}^{(1)}\boldsymbol{\alpha}^{(1)} = (\mathbf{I} - \mathbf{G}_{21}^{(1)}(\widetilde{\mathbf{R}}_0^{\mathsf{H}}\mathbf{G}_{21}^{(1)})^{-1}\widetilde{\mathbf{R}}_0^{\mathsf{H}})\mathbf{r}_0, \quad \mathbf{r}_{21}^{(1)} = \mathbf{A}\mathbf{r}_{11}^{(1)}.$$

IDRSTAB

Columnwise update (IDR part) such that diagonal blocks

- form basis of $\mathcal{G}_j \setminus \mathcal{G}_{j+1}$ with expansion $\mathcal{G}_j = \mathbf{A}(\mathcal{G}_{j-1} \cap \mathcal{S}) \rightsquigarrow \beta^{(j)} \in \mathbb{C}^{s \times s}$,
- are orthonormalized $\rightsquigarrow \underline{\mathbf{H}}_{s-1}^{(j)} \in \mathbb{C}^{s \times s-1}$

All other blocks in column treated in same manner.

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New cycle (STAB part, $\mathbf{r}_{21}^{(k+1)} = \mathbf{A}\mathbf{r}_{11}^{(k+1)}$, $\gamma^{(\ell)} \in \mathbb{C}^s$ such that $\|\mathbf{r}_{11}^{(k+1)}\| = \min$):

$$\mathbf{r}_{11}^{(k+1)} = \mathbf{r}_{1,\ell+1}^{(k)} - \sum_{i=1}^{\ell} \mathbf{r}_{i+1,\ell+1}^{(k)} \gamma_i^{(\ell)}, \quad \begin{cases} \mathbf{G}_{11}^{(k+1)} = \mathbf{G}_{1,\ell+1}^{(k)} - \sum_{i=1}^{\ell} \mathbf{G}_{i+1,\ell+1}^{(k)} \gamma_i^{(\ell)}, \\ \mathbf{G}_{21}^{(k+1)} = \mathbf{G}_{2,\ell+1}^{(k)} - \sum_{i=1}^{\ell} \mathbf{G}_{i+2,\ell+1}^{(k)} \gamma_i^{(\ell)}. \end{cases}$$

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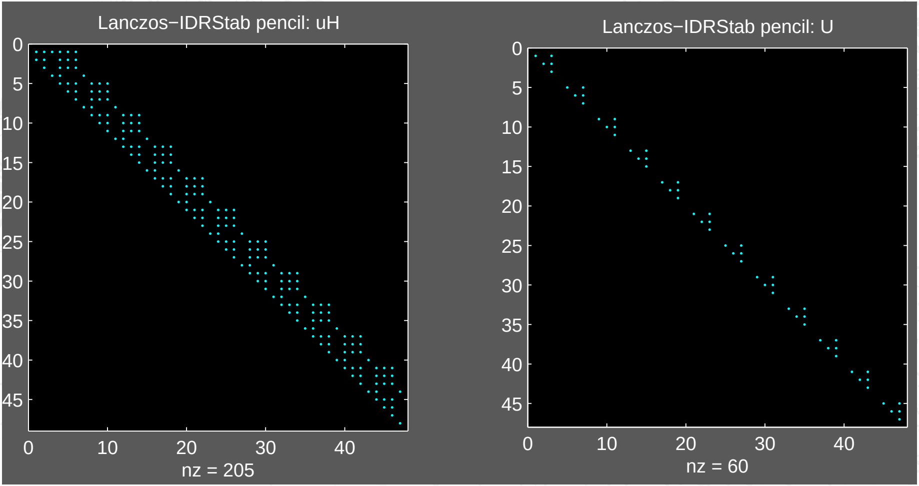
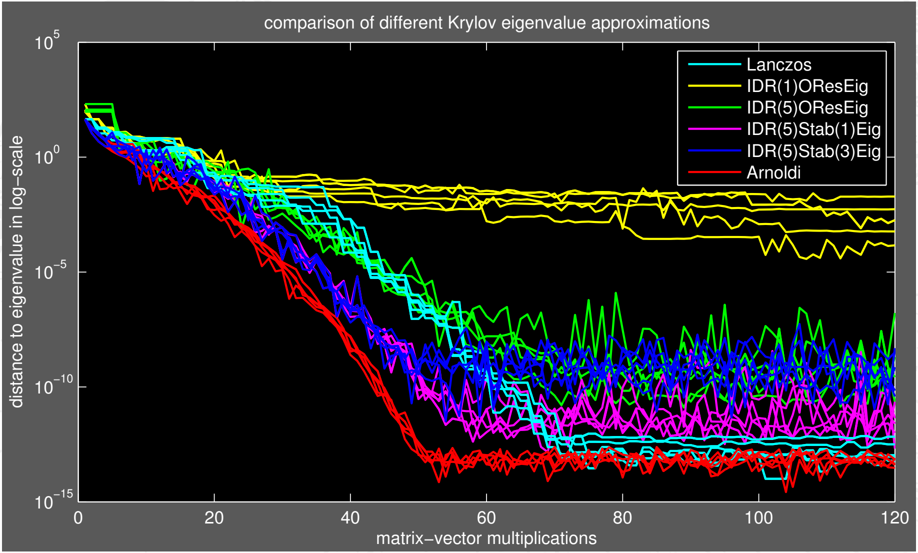
Anisa Rizvanolli: $\rightsquigarrow$ Lanczos-IDRSTAB pencil for eigenvalues, IDRSTABEIG.

Structure of (undeflated) Lanczos-IDRSTAB pencil



A comparison: IDR based eigenvalue solvers



QMRIDR

MR methods: use extended Hessenberg matrix

$$\mathbf{x}_k := \mathbf{Q}_k \underline{\mathbf{z}}_k, \quad \underline{\mathbf{z}}_k := \underline{\mathbf{H}}_k^{\dagger} \underline{\mathbf{e}}_1 \|\mathbf{r}_0\|.$$

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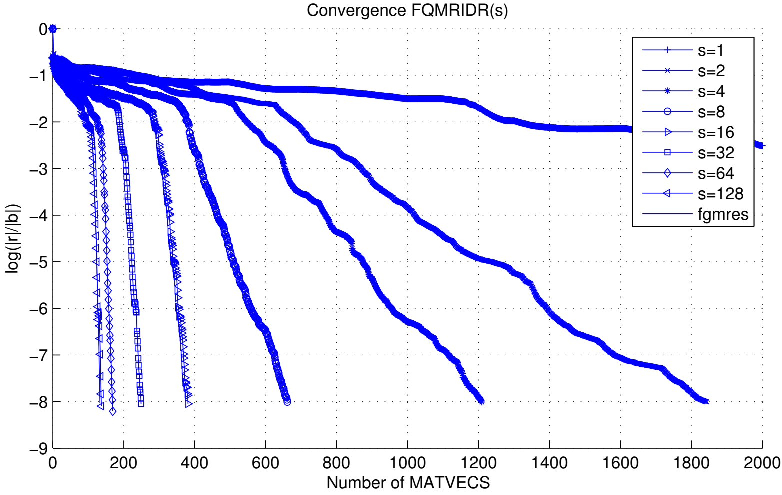
Olaf Rendel, Gerard Sleijpen, Martin van Gijzen: $\rightsquigarrow$ QMRIDRStab.

Flexible QMRIDR(s)



Perturbations

IDR based on short recurrences, i.e., Lanczos based.

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Lanczos	IDR
deviation	deviation
multiple Ritz values	ghost polynomial roots
delay of convergence	delay of convergence
attainable accuracy: condition	attainable accuracy: worse than Lanczos
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Lanczos	IDR
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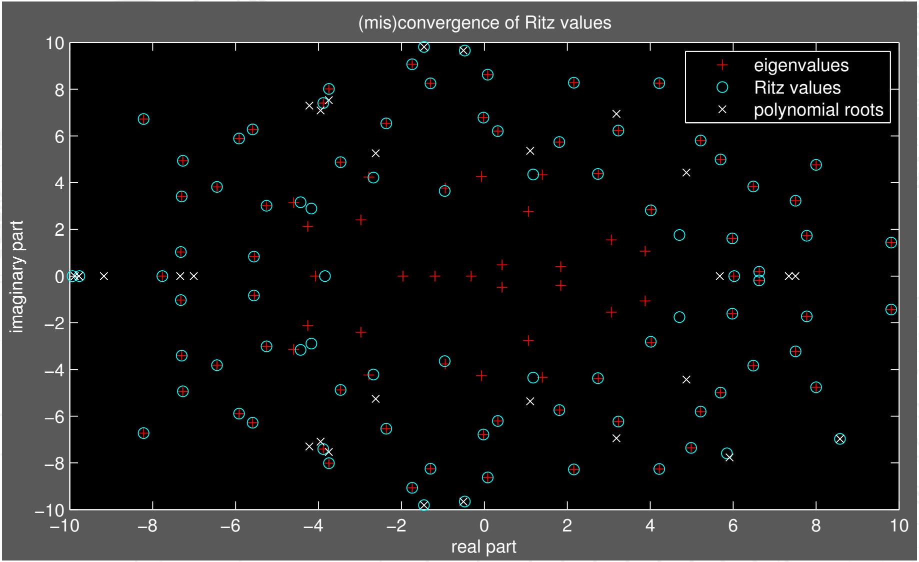
But:

- IDR transpose-free,
- easy to implement,
- more stable (for large values of s),
- often close to “optimal” methods (for large values of s).

IDR(3)STAB(3): "Ghost polynomial roots"



Conclusion and Outview

- IDR is both old (original IDR, CGS, BiCGStab, BiCGStab2, BiCGStab(ℓ), ...) and new (IDR(s), IDRStab, QMRIDR, ...).

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- The analysis & development of IDR based methods is a new branch of Krylov subspace methods.
- The pencils of IDR based methods are specially structured pencils (adapted backward stable algorithms; perturbation theory, ...).

Thank you for your attention!

In case of questions feel free to ask Anisa, Olaf & myself at any time.

This talk is partially based on the following technical reports:

Eigenvalue computations based on IDR, Martin H. Gutknecht and Z., Bericht 145, Institut für Numerische Simulation, TUHH, 2010,

Flexible and multi-shift induced dimension reduction algorithms for solving large sparse linear systems, Martin B. van Gijzen, Gerard L.G. Sleijpen, and Z., Bericht 156, Institut für Numerische Simulation, TUHH, 2011.