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An iterative algorithm for the partial QZ reduction of very large generalized eigenproblems

Gerard Sleijpen
Henk van der Vorst
Diederik Fokkema

Universiteit Utrecht
Department of Mathematics

http://www.math.ruu.nl/people/sleijpen

Example: MHD

- Interaction plasma and magnetic field
- Fluid eqns + Maxwell
- **Applications**:
  stability tokamak plasmas,
  coronal loops, solar flares

Linear MHD

$$
\begin{aligned}
\frac{\partial \rho}{\partial t} &= -\nabla \cdot (\rho \mathbf{V}) \\
\rho \frac{\partial \mathbf{V}}{\partial t} &= -\rho(\mathbf{V}\cdot\nabla)\mathbf{V} - \nabla p \\
&\quad +(\nabla \times \mathbf{B}) \times \mathbf{B} \\
\frac{\partial p}{\partial t} &= -(\mathbf{V}\cdot\nabla)p - \gamma p \nabla\cdot\mathbf{V} \\
&\quad +(\gamma-1)\eta(\nabla\times\mathbf{B})^2 \\
\frac{\partial \mathbf{B}}{\partial t} &= \nabla\times(\mathbf{V}\times\mathbf{B}) - \nabla\times(\eta\nabla\times\mathbf{B}) \\
\text{with} \quad & \nabla\cdot\mathbf{B} = 0
\end{aligned}
$$

- Linearise around an equilibrium
- Assume solutions of the form $e^{\lambda t}$: generalized eigenproblem

Linear MHD (2)

- Block tridiagonal matrices:
  $100 - 2\,000$ blocks of size $80 - 320$
  $\Rightarrow$ matrices of order $8\,000 - 640\,000$

For smallest systems:

- Shift-and-Invert IRA
  (Sorensen)
- Shift-and-Invert Lanczos
  (Cullum et al)
- Jacobi-Davidson, no inversion
  (Booten, Fokkema, Sleijpen, van der Vorst)

Problem and Approach

Problem: find one or more eigenvalues of $\mathbf{A}\mathbf{x} = \lambda\,\mathbf{B}\mathbf{x}$

$\mathbf{A}$ and $\mathbf{B}$ unsymmetric, large

CONVENTIONAL APPROACH:
Shift-and-Invert

$$(\mathbf{A} - \sigma\mathbf{B})^{-1}\mathbf{B}\mathbf{x} = \tilde{\lambda}\,\mathbf{x}$$

$$\tilde{\lambda} = \frac{1}{\lambda - \sigma}, \qquad \lambda = \sigma + \frac{1}{\tilde{\lambda}}$$

Apply Arnoldi, convergence to eigenvalues closest to σ

Problem: $(\mathbf{A} - \sigma\mathbf{B})^{-1}$

QZ Method

Compute orthogonal $\mathbf{Q}$ and $\mathbf{Z}$:

$$\mathbf{A}\mathbf{Q} = \mathbf{Z}\mathbf{S}, \qquad \mathbf{B}\mathbf{Q} = \mathbf{Z}\mathbf{T}$$

such that $\mathbf{S}$ and $\mathbf{T}$ are upper triangular.

Columns $\mathbf{q}_i$:
Generalized Schur vectors

Eigenvalue: $\mathbf{S}_{i,i}/\mathbf{T}_{i,i}$

Iterative approach based upon
Jacobi-Davidson method

Projection

$$(\mathbf{A} - \lambda\mathbf{B})\mathbf{x} = 0$$

Petrov-Galerkin conditions:
Find $\mathbf{x}_m \in \{\mathbf{v}_1, \ldots, \mathbf{v}_m\}$ such that

$$(\mathbf{A} - \theta\mathbf{B})\mathbf{x}_m \perp \{\mathbf{w}_1, \ldots, \mathbf{w}_m\}$$

With $\mathbf{V}_m \equiv [\,\mathbf{v}_1\,|\,\mathbf{v}_2\,|\,\ldots\,|\,\mathbf{v}_m\,]$,
$\mathbf{W}_m \equiv [\,\mathbf{w}_1\,|\,\mathbf{w}_2\,|\,\ldots\,|\,\mathbf{w}_m\,]$,
and $\mathbf{x}_m = \mathbf{V}_m\,y$:

$$(\mathbf{W}_m^*\,\mathbf{A}\mathbf{V}_m - \theta\mathbf{W}_m^*\,\mathbf{B}\mathbf{V}_m)\,y = 0$$

Apply standard QZ (LAPACK) for projected matrices
$\mathbf{W}_m^*\,\mathbf{A}\mathbf{V}_m$ and $\mathbf{W}_m^*\,\mathbf{B}\mathbf{V}_m$

Standard QZ

Find orthogonal U_L and U_R:

$$U_L^*(\mathbf{W}_m^*\,\mathbf{A}\mathbf{V}_m)U_R = S_A$$

$$U_L^*(\mathbf{W}_m^*\,\mathbf{B}\mathbf{V}_m)U_R = S_B$$

S_A and S_B are upper-triangular ordered such that leading elements define eigenvalue closest to σ

Eigenpair approximation $(\mathbf{x}_m, \theta)$;

$$\mathbf{x}_m = \mathbf{V}_m\,U_R(:,1), \qquad \theta = S_B(1,1)/S_A(1,1)$$

At convergence we have
$\mathbf{x}$: the first column of $\mathbf{Q}$

$\mathbf{z}_1 \in \mathrm{span}(\mathbf{A}\mathbf{q}_1, \mathbf{B}\mathbf{q}_1)$ $\quad (\mathbf{A}\mathbf{Q} = \mathbf{Z}\mathbf{S},\ \mathbf{B}\mathbf{Q} = \mathbf{Z}\mathbf{T})$
Therefore, $\mathbf{W}_m$ taken as $\alpha\,\mathbf{A}\mathbf{V}_m - \beta\,\mathbf{B}\mathbf{V}_m$
(we selected: $\alpha = 1$, $\beta = \sigma$)

JACOBI-DAVIDSON

How to expand $\mathbf{V}_m$ (and $\mathbf{W}_m$)?

Compute *residual vector*

$$\mathbf{r} \equiv (\mathbf{A} - \theta\mathbf{B})\mathbf{x}_m$$

Also compute auxiliary vector:

$$\gamma\,\mathbf{z} \equiv (\mathbf{A} - \sigma\mathbf{B})\mathbf{x}_m$$

Find correction $\mathbf{v}$ for $\mathbf{x}_m$ with

$$\mathbf{x}_m^*\mathbf{v} = 0$$

and

$$(\mathbf{I} - \mathbf{z}\,\mathbf{z}^*)(\mathbf{A} - \theta\mathbf{B})(\mathbf{I} - \mathbf{x}_m\,\mathbf{x}_m^*)\mathbf{v} = -\mathbf{r}$$

Correction equation approximately solved with few steps of GMRES

$\mathbf{v}_{m+1} \equiv \mathbf{v} \;\Rightarrow\; \mathbf{V}_{m+1}$
$\mathbf{w}_{m+1} \equiv (\mathbf{A} - \sigma\mathbf{B})\mathbf{v} \;\Rightarrow\; \mathbf{W}_{m+1}$

How to continu?

Expansion of Schur Form:

$$\mathbf{A}\,[\mathbf{Q}_k, \mathbf{q}] = [\mathbf{Z}_k, \mathbf{z}] \begin{bmatrix} S_k & s \\ & \alpha \end{bmatrix}$$

and

$$\mathbf{B}\,[\mathbf{Q}_k, \mathbf{q}] = [\mathbf{Z}_k, \mathbf{z}] \begin{bmatrix} T_k & t \\ & \beta \end{bmatrix}$$

with $\mathbf{Q}_k^*\mathbf{q} = 0, \quad \mathbf{Z}_k^*\mathbf{z} = 0.$

This leads to

$$(\mathbf{I} - \mathbf{Z}_k\mathbf{Z}_k^*)(\beta\mathbf{A} - \alpha\mathbf{B})(\mathbf{I} - \mathbf{Q}_k\mathbf{Q}_k^*)\mathbf{q} = \mathbf{0}$$

$(\mathbf{q}, \lambda \equiv \alpha/\beta)$ eigenpair of:

$$(\mathbf{I} - \mathbf{Z}_k\mathbf{Z}_k^*)(\mathbf{A} - \lambda\mathbf{B})(\mathbf{I} - \mathbf{Q}_k\mathbf{Q}_k^*)$$

Apply "JD - algorithm with Schur form" for this matrix pair $\Rightarrow$ $\mathbf{q}$ and $\mathbf{z}$.

Projected matrices

The projected matrices in JD satisfy:

$$\mathbf{W}_m^*\,(\mathbf{I} - \mathbf{Z}_k\mathbf{Z}_k^*)\mathbf{A}(\mathbf{I} - \mathbf{Q}_k\mathbf{Q}_k^*)\mathbf{V}_m = \mathbf{W}_m^*\,\mathbf{A}\mathbf{V}_m$$

and

$$\mathbf{W}_m^*\,(\mathbf{I} - \mathbf{Z}_k\mathbf{Z}_k^*)\mathbf{B}(\mathbf{I} - \mathbf{Q}_k\mathbf{Q}_k^*)\mathbf{V}_m = \mathbf{W}_m^*\,\mathbf{B}\mathbf{V}_m$$

Implicit Restart

For projected matrices we compute the generalized Schur form

$$\mathbf{W}_m^*\,\mathbf{A}\mathbf{V}_m\;U_R = U_L\,S_A$$

and

$$\mathbf{W}_m^*\,\mathbf{B}\mathbf{V}_m\;U_R = U_L\,S_B$$

S_A and S_B are ordered so that

$$|S_B(i,i)/S_A(i,i) - \sigma|$$

form a nondecreasing row

The first few columns of reordered $\mathbf{V}_m$ represent best eigenvector approx's
$\Rightarrow$ can be used for restart

Some practical notes

1. After convergence of some eigenvectors: solution of correction eq. easier

2. Corr. eq. with precond. solver: preconditioning can be used more often: pays to make better preconditioning

3. For standard eigenproblems JD + QR-reduction

4. Numerical examples: maximum dimension of $\mathbf{V}_m$: 15 after restart: $m = 10$

Parallelism

Computational elements:

1. Given $\mathbf{V}_m = [\,\mathbf{v}_1 \,|\, \mathbf{v}_2 \,|\, \ldots \,|\, \mathbf{v}_m\,]$
and $\mathbf{W}_m = [\,\mathbf{w}_1 \,|\, \mathbf{w}_2 \,|\, \ldots \,|\, \mathbf{w}_m\,]$
compute $M_A \equiv \mathbf{W}_m^* \mathbf{A} \mathbf{V}_m$, $M_B \equiv \mathbf{W}_m^* \mathbf{B} \mathbf{V}_m$

   requires:
   $\mathbf{A}\mathbf{v}_m$, $\mathbf{B}\mathbf{v}_m$,
   $2m$ inner products for
   last row and column of M_A and M_B

2. QZ-algorithm for M_A and M_B
negligible if $m \ll n$

3. Form $\mathbf{x}_m = \mathbf{V}_m\, y$:
multiple update

Parallelism(2)

4. Compute $\mathbf{r} = (\mathbf{A} - \theta\mathbf{B})\mathbf{x}_m$, $\|\mathbf{r}\|_2$
and $\mathbf{z} = (\mathbf{A} - \sigma\mathbf{B})\mathbf{x}_m$, $\mathbf{z} := \mathbf{z}/\|\mathbf{z}\|_2$

   Requires: 2 updates, 2 norms

5. Solve approximately
$$(\mathbf{I} - \mathbf{z}\mathbf{z}^*)(\mathbf{I} - \mathbf{Z}_k\mathbf{Z}_k^*)\times$$
$$(\mathbf{A} - \theta\mathbf{B})(\mathbf{I} - \mathbf{Q}_k\mathbf{Q}_k^*)(\mathbf{I} - \mathbf{x}_m\mathbf{x}_m^*)\mathbf{v} = -\mathbf{r}$$
with few steps of prec. GMRES.

   Most expensive part:
   requires inner products, updates
   matrix vector products for $\mathbf{A}$ and $\mathbf{B}$

6. Orthogonalize $\mathbf{v}$ wrt $\mathbf{V}_m$, and
$$\mathbf{w} \equiv (\mathbf{A} - \sigma\mathbf{B})\mathbf{v} \text{ wrt } \mathbf{W}_m$$

Parallel Performance

For problem coming from acoustics:
$\mathbf{A}$ and $\mathbf{B}$ 19-diagonal, $n = 136\,161$

Results for interior isolated eigenvalue, on the CRAY T3D:

Processors	Elapsed time (sec)
16	206.4
32	101.3
64	52.1

For $n = 274\,625$, 64 processors:
93.3 seconds, 1.0 Gflops
(1 shift-invert step 600 sec. at peak-perf.)

More Details

JD-algorithm:

Sleijpen and van der Vorst

SIMAX, 17 (2), March 1996

JD: general problems

Sleijpen et al

Preprint 923, UU, 1995 (BIT 1996)

JDQR and JDQZ

Fokkema et al, Preprint 941

UU, January 1996

Parallel performance

Sleijpen et al, SIAM News, Aug. 96

these papers and others:

http://www.math.ruu.nl/people/sleijpen

http://www.math.ruu.nl/people/vorst

With $\mathbf{u} = \mathbf{x}_m$, solve approximately

$$(\mathbf{I} - \mathbf{z}\,\mathbf{z}^*)\,(\mathbf{A} - \theta\,\mathbf{B})\,(\mathbf{I} - \mathbf{u}\,\mathbf{u}^*)\,\mathbf{z} = -\mathbf{r}.$$

Any preconditioned it. method can be used.

Preconditioning: $\mathbf{M} \approx \mathbf{A} - \theta\,\mathbf{B}$

Preconditioning equation:

$$(\mathbf{I} - \mathbf{z}\,\mathbf{z}^*)\,\mathbf{M}\,(\mathbf{I} - \mathbf{u}\,\mathbf{u}^*)\,\mathbf{t} = \mathbf{s}$$

Solution:

$$\mathbf{M}\,\mathbf{t} = \mathbf{s} + \mathbf{z}\,\alpha \quad \text{such that} \quad \mathbf{t} \perp \mathbf{u},$$

or

$$\mathbf{t} = \mathbf{M}^{-1}\mathbf{s} + \mathbf{M}^{-1}\mathbf{z}\,\alpha \qquad \&$$

$$\alpha = (\mathbf{u}^*\mathbf{M}^{-1}\mathbf{z})^{-1}(\mathbf{u}^*\mathbf{M}^{-1}\mathbf{s}).$$

$\mathbf{M} \approx \mathbf{A} - \theta\,\mathbf{B}$, $\quad (\mathbf{I} - \mathbf{z}\,\mathbf{z}^*)\,\mathbf{M}\,(\mathbf{I} - \mathbf{u}\,\mathbf{u}^*)\,\mathbf{t} = \mathbf{s}$

What if $\mathbf{M}\tilde{\mathbf{x}} = 0$ **&** $\tilde{\mathbf{x}} \approx \mathbf{x}$**?**

[joint work with F. Wubs, Groningen U]

Suppose

$\mathbf{M} : \tilde{\mathbf{x}}^\perp \to \tilde{\mathbf{y}}^\perp$ well-cond., Cond. nmb $\mathcal{C}$

with $\tilde{\mathbf{y}}$ such that $\mathbf{y}^*\mathbf{M} = \mathbf{0}$.

Use equivalent aumented system:

$$\begin{bmatrix} \mathbf{M} & \mathbf{z} \\ \mathbf{u}^* & 0 \end{bmatrix} \begin{bmatrix} \mathbf{t} \\ \alpha \end{bmatrix} = \begin{bmatrix} \mathbf{s} \\ 0 \end{bmatrix}$$

Condition augmented system:

$$\sim \quad \mathcal{C} \cdot \mathrm{Cond}_M(0) \cdot 1/\cos(\mathbf{x}_m, \tilde{\mathbf{x}}) \cdot \underbrace{1/\cos(\mathbf{z}, \tilde{\mathbf{y}})}_{\approx\ \mathrm{Cond}_{\mathbf{B}^{-1}\mathbf{A}}(\lambda)}$$

$\mathbf{A}\mathbf{x} = \mathbf{b}$

[Saad 94, Botta & Wubs 97]

MRILU

Reorder & partition

$$\mathbf{A}^{(0)} = \mathbf{A} - \tau\mathbf{B} = \begin{bmatrix} \mathbf{A}_1 & \mathbf{E} \\ \mathbf{F} & \mathbf{A}_2 \end{bmatrix}$$

such that $\mathbf{A}_1 \approx \mathbf{D} := \mathrm{diag}(\mathbf{A}_1)$

Take $\mathbf{M}^{(0)} = \mathbf{M} = \begin{bmatrix} \mathbf{D} & \mathbf{E} \\ \mathbf{F} & \mathbf{A}_2 \end{bmatrix}$

Use Schur complement $\widetilde{\mathbf{A}}_2 = \mathbf{A}_2 - \mathbf{F}\mathbf{D}^{-1}\mathbf{E}$

for solving $\mathbf{M}\begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} b \\ c \end{bmatrix}$:

- solve (approximately) $\widetilde{\mathbf{A}}_2\,y = c - \mathbf{G}\mathbf{D}^{-1}b$
- solve exactly $\mathbf{D}\,x = b - \mathbf{E}\,y$

Can be repeated with

$\mathbf{A}$ replaced by $\mathbf{A}^{(1)} = \widetilde{\mathbf{A}}_2$, etc.

MRILU

Reorder & Partition

$$\mathbf{A} - \tau\mathbf{B} = \begin{bmatrix} \mathbf{A}_1 & \mathbf{E}_u \\ \mathbf{E}_\ell & \mathbf{A}_2 \end{bmatrix}$$

with • $\mathbf{A}_1$ well conditioned

• $\mathbf{A}_2$ of low dimension
(with ill. cond. Schur complement)

$$\mathbf{K} = \begin{bmatrix} \mathbf{K}_1 & \mathbf{E}_u \\ \mathbf{E}_\ell & \mathbf{A}_2 \end{bmatrix} = \begin{bmatrix} \mathbf{K}_1 & 0 \\ \mathbf{E}_\ell & \widetilde{\mathbf{A}}_2 \end{bmatrix} \begin{bmatrix} \mathbf{I} & \mathbf{K}_1^{-1}\mathbf{E}_u \\ 0 & \mathbf{I} \end{bmatrix}$$

with $\mathbf{K}_1$ block ILU $\mathbf{A}_1$

$\widetilde{\mathbf{A}}_2$ Schur complement wrt $\mathbf{K}_1$

$$\mathbf{K} = \begin{bmatrix} \mathbf{K}_1 & \mathbf{E}_u \\ \mathbf{E}_\ell & \mathbf{A}_2 \end{bmatrix} = \begin{bmatrix} \mathbf{K}_1 & 0 \\ \mathbf{E}_\ell & \widetilde{\mathbf{A}}_2 \end{bmatrix} \begin{bmatrix} \mathbf{I} & \mathbf{K}_1^{-1}\mathbf{E}_u \\ 0 & \mathbf{I} \end{bmatrix}$$

$$\begin{bmatrix} \mathbf{K} & \mathbf{z} \\ \mathbf{u}^* & 0 \end{bmatrix} = \begin{bmatrix} \mathbf{K}_1 & \mathbf{E}_u & \mathbf{z}_1 \\ \mathbf{E}_\ell & \mathbf{A}_2 & \mathbf{z}_2 \\ \mathbf{u}_1^* & \mathbf{u}_{2*} & 0 \end{bmatrix} =$$

$$\begin{bmatrix} \mathbf{K}_1 & 0 & 0 \\ \mathbf{E}_\ell & \widetilde{\mathbf{A}}_2 & \tilde{\mathbf{z}}_2 \\ \tilde{\mathbf{u}}_1 & \tilde{\mathbf{u}}_2 & \beta \end{bmatrix} \begin{bmatrix} \mathbf{I} & \mathbf{K}_1^{-1}\mathbf{E}_u & \mathbf{K}_1^{-1}\mathbf{z}_1 \\ \mathbf{0} & \mathbf{I} & \mathbf{0} \\ \mathbf{0}^* & \mathbf{0}^* & 1 \end{bmatrix}$$

$\begin{bmatrix} \widetilde{\mathbf{A}}_2 & \tilde{\mathbf{z}}_2 \\ \tilde{\mathbf{u}}_2 & \beta \end{bmatrix}$ well conditioned & low dimensional

allows "exact" direct methods

$$\mathbf{K} = \begin{bmatrix} \mathbf{K}_1 & \mathbf{E}_u \\ \mathbf{E}_\ell & \mathbf{A}_2 \end{bmatrix} = \begin{bmatrix} \mathbf{K}_1 & 0 \\ \mathbf{E}_\ell & \widetilde{\mathbf{A}}_2 \end{bmatrix} \begin{bmatrix} \mathbf{I} & \mathbf{K}_1^{-1}\mathbf{E}_u \\ 0 & \mathbf{I} \end{bmatrix}$$

Improved preconditioner

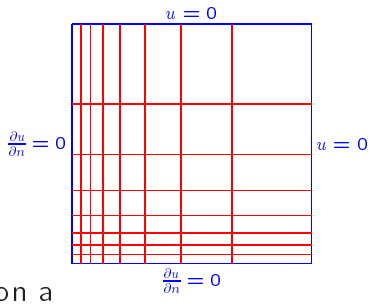
$$\mathbf{A} - \theta\mathbf{B} = (\mathbf{A} - \tau\mathbf{B}) - (\theta - \tau)\mathbf{B}$$

$$\approx \mathbf{K} - \delta\mathbf{B} = \begin{bmatrix} \mathbf{K}_1 - \delta\mathbf{B}_1 & \mathbf{E}_u - \delta\mathbf{F}_u \\ \mathbf{E}_\ell - \delta\mathbf{F}_\ell & \mathbf{A}_2 - \delta\mathbf{B}_2 \end{bmatrix}$$

Neumann series:
$(\mathbf{K}_1 - \delta\mathbf{B}_1)^{-1} \approx \mathbf{C}_1 \equiv \mathbf{K}_1^{-1} + \delta\,\mathbf{K}_1^{-1}\mathbf{B}_1\mathbf{K}_1^{-1}$

$$\mathbf{M}_\theta = \begin{bmatrix} \mathbf{C}_1^{-1} & 0 \\ \mathbf{E}_\ell - \delta\mathbf{F}_\ell & \widetilde{\mathbf{A}}_2 - \delta\tilde{\mathbf{B}}_2 \end{bmatrix} \begin{bmatrix} \mathbf{I} & \mathbf{C}(\mathbf{E}_u - \delta\mathbf{F}_u) \\ 0 & \mathbf{I} \end{bmatrix}$$

Note that $\mathbf{M}_\theta\tilde{\mathbf{x}} = 0 \quad \Rightarrow \quad \theta \approx \lambda$



Numerical Example

2d Laplace operator on a
streched $N \times N$ regular grid.

Dirichlet on east & north boundary
Neumann on west and south boundary

Preconditioned for 3 smallest eigenvalues
$\epsilon = 10^{-8}$
(3 eigenvalues detected at machine precision)

N	Cond($\mathbf{A}$)	fill in	levels	# JD steps
7	$2.4\,10^5$	5.6	3	7
15	$7.4\,10^6$	7.3	8	10
31	$7.3\,10^7$	7.9	12	12
63	$6.1\,10^8$	8.4	17	13

Numerical Example

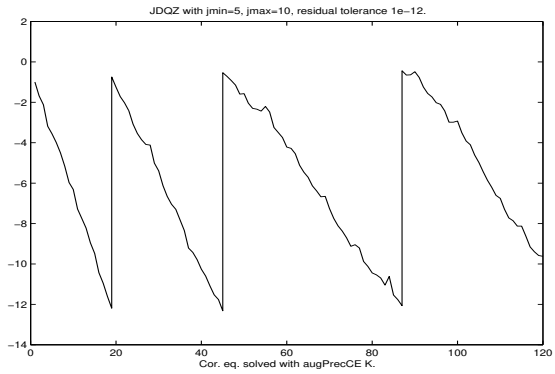
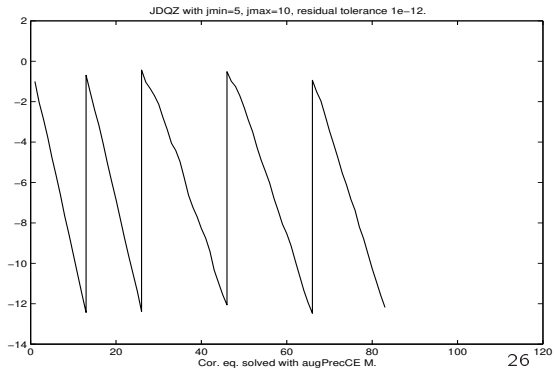
Linearized incompressible Navier Stokes (Re=100).
Discretized on 17×17 stag. grid, upwind

Generalized eigenproblem of dim. $3 \times 15 \times 15$

$$\mathbf{A}\mathbf{x} = \lambda\,\mathbf{B}$$

Find 5 eigenvalues with smallest real part

Corr. eq. solved with 1 step precond. GMRES

[Olsen's method]

Maximum dimension $\mathbf{V}_m$: 10
after restart: $m = 5$.