NAG/Oxford U. Comp. Lab, Workshop Precond., Sept., 2000

Some preconditioning techniques for eigenvalue problems

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Problem and Approach

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

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

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

Program

- Jacobi-Davidson
- Preconditioning
- Multi-level ILU
  - Updating the preconditioner
  - Initial guesses
  - Numerical examples
- Domain Decomposition

Petrov-Galerkin approach

Find $\mathbf{u} \in \mathcal{V}_k = \{\mathbf{v}_1, \ldots, \mathbf{v}_k\}$ such that

$$\mathbf{r} = (\mathbf{A} - \theta\mathbf{B})\mathbf{u} \perp \mathcal{W}_k = \{\mathbf{w}_1, \ldots, \mathbf{w}_k\}.$$

$(\theta, \mathbf{u})$ **Petrov pair** w.r.t.
search subspace $\mathcal{V}_k$ & **test** subspace $\mathcal{W}_k$.

In practice. $k \ll n$

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

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

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

JACOBI-DAVIDSON

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

Compute *residual vector*

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

Also compute auxiliary vector:

$$\gamma\,\mathbf{z} \equiv (\beta\mathbf{A} + \alpha\mathbf{B})\mathbf{u}$$

Find correction $\mathbf{t}$ for $\mathbf{u}$ with $\mathbf{u}^*\mathbf{t} = 0$ and

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

Correction equation approximately solved with e.g. a few steps of precond. GMRES

$\mathbf{t}$ expansion vector $\mathbf{V}_k$: $\quad \mathbf{v}_{k+1} \equiv \mathrm{GS}_{\mathbf{V}_k}(\mathbf{t})$
$\mathbf{s} \equiv (\beta\mathbf{A} + \alpha\mathbf{B})\mathbf{t}$ exp. v. $\mathbf{W}_k$: $\quad \mathbf{w}_{k+1} \equiv \mathrm{GS}_{\mathbf{W}_k}(\mathbf{s})$

Solve approximately

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

<u>**Any** preconditioned it. method</u> can be used.

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

Preconditioning equation:

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

Solution:

$\mathbf{K}\,\mathbf{c} = \mathbf{s} - \mathbf{z}\,\alpha, \quad \alpha$ such that $\quad \mathbf{c} \perp \mathbf{u},$

or

$\mathbf{c} = \mathbf{K}^{-1}\mathbf{s} - \mathbf{K}^{-1}\mathbf{z}\,\alpha \qquad$ where, with

$\mathbf{y} \equiv \mathbf{K}^{-1}\mathbf{z}$ & $\mu \equiv \mathbf{u}^*\mathbf{y}, \quad \alpha = \mu^{-1}(\mathbf{u}^*\mathbf{K}^{-1}\mathbf{s}).$

or

$$\mathbf{c} = \mathbf{K}^\dagger\mathbf{s} \equiv (\mathbf{I} - \mathbf{y}\mu^{-1}\mathbf{u}^*)\mathbf{K}^{-1}\mathbf{s}$$

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

$\mathbf{K} \approx \mathbf{A} - \theta\,\mathbf{B}, \qquad (\mathbf{I} - \mathbf{z}\,\mathbf{z}^*)\,\mathbf{K}\,(\mathbf{I} - \mathbf{u}\,\mathbf{u}^*)\,\mathbf{c} = \mathbf{s}.$

$\mathbf{K}^\dagger \equiv (\mathbf{I} - \mathbf{y}\mu^{-1}\mathbf{u}^*)\mathbf{K}^{-1}$ with $\mathbf{y} \equiv \mathbf{K}^{-1}\mathbf{z}$, $\mu \equiv \mathbf{u}^*\mathbf{y}$

Explicit left preconditioning

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

Note that $\mathbf{K}^\dagger\mathbf{s} \perp \mathbf{z}$. $\qquad$ In part., $\mathbf{K}^\dagger\mathbf{r} \perp \mathbf{z}$.

<u>*The action of a precond. operator on an* $\mathbf{s}$</u>

If $\mathbf{s} \perp \mathbf{z}$

- $\mathbf{s} \leftarrow (\mathbf{A} - \theta\,\mathbf{B})\mathbf{s}$
- Solve $\mathbf{K}\mathbf{s}' = \mathbf{s}$
- $\mathbf{s} \leftarrow \mathbf{s}' - \mathbf{y}(\mu^{-1}(\mathbf{u}^*\mathbf{s}'))$

then $\mathbf{s} \perp \mathbf{z}$

Only one (skew) projection!

Preconditioning

In general is $\mathbf{A} - \theta\mathbf{B}$ indefinite:

1. ILU with fill-in
2. MILU with fill-in
3. ILQ
4. Multigrid
5. Multilevel:
   Schur complement & incomlete fact.
6. Homotopy approaches
7. Domain decomposition
8. $(\mathbf{A} - \tau\mathbf{B})^{-1}$ for fixed tau

Solutions are often non-smooth:
no basis for usage of MILU

For interior eigenvalues:
quite some fill-in needed
(or many steps with solver)

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

Excellent preconditioners

Suppose $\quad \mathbf{K}\widetilde{\mathbf{x}} \approx \mathbf{0} \quad \& \quad \widetilde{\mathbf{x}} \approx \mathbf{x}.$

and suppose $\quad \mathbf{K} : \widetilde{\mathbf{x}}^\perp \to \widetilde{\mathbf{y}}^\perp \quad$ well-conditioned,
with $\widetilde{\mathbf{y}}$ such that $\widetilde{\mathbf{y}}^*\mathbf{K} \approx \mathbf{0}$.

Expand $\mathbf{V}_k$ by the solution $\mathbf{t} \perp \mathbf{u}$ of

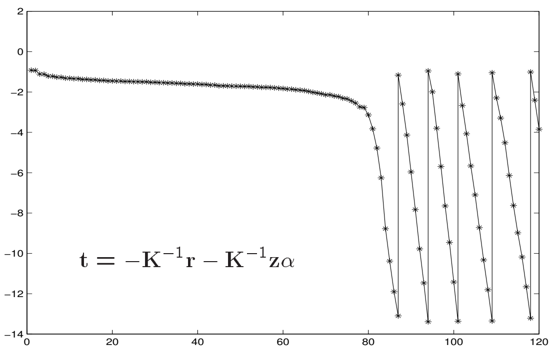
$$(\mathbf{I} - \mathbf{z}\,\mathbf{z}^*)\,\mathbf{K}\,(\mathbf{I} - \mathbf{u}\,\mathbf{u}^*)\,\mathbf{t} = -\mathbf{r}.$$

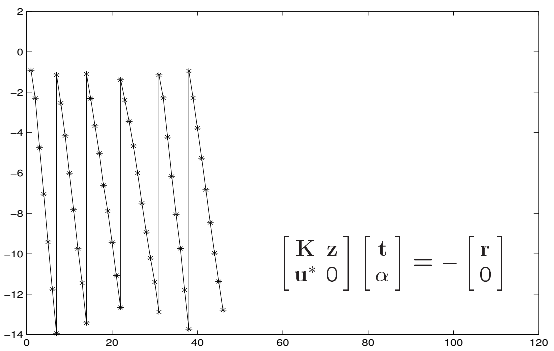
- $\mathbf{t} = -\mathbf{K}^{-1}\mathbf{r}$ [Davidson '75]
- $\mathbf{t} = -\mathbf{K}^{-1}\mathbf{r} - \mathbf{K}^{-1}\mathbf{z}\,\alpha$ [Olsen, et al '90]

If $\widetilde{\mathbf{y}}^*\mathbf{r} \not\approx 0$ then $\mathbf{K}^{-1}\mathbf{r}$, $\mathbf{K}^{-1}\mathbf{z}$ have huge (error) components in $\widetilde{\mathbf{x}}$-direction and $\mathbf{t}$ may be extremely inaccurate.

If $\widetilde{\mathbf{y}}^*\mathbf{r} \approx 0$ then $\mathbf{t}$ may be sufficiently accurate.
Note that: $\widetilde{\mathbf{y}}^*\mathbf{r} \approx 0$ if $\widetilde{\mathbf{y}} \approx\in \mathbf{W}_k$.

$\widetilde{\mathbf{y}} \approx\in \mathbf{W}_k$ if $\widetilde{\mathbf{y}} \approx\in \mathbf{W}_0$ or (Davidson & $\mathbf{K}^* = \mathbf{K}$ & $\mathbf{W}_k = \mathbf{V}_k$)





Excellent preconditioners

Suppose $\quad \mathbf{K}\widetilde{\mathbf{x}} \approx \mathbf{0} \quad \& \quad \widetilde{\mathbf{x}} \approx \mathbf{x}.$

and suppose $\mathbf{K} : \widetilde{\mathbf{x}}^\perp \to \widetilde{\mathbf{y}}^\perp$ well-cond., Cond. nmb $\mathcal{C}$
with $\widetilde{\mathbf{y}}$ such that $\widetilde{\mathbf{y}}^*\mathbf{K} \approx \mathbf{0}$.

Expand $\mathbf{V}_k$ by the solution $\mathbf{t} \perp \mathbf{u}$ of

$$(\mathbf{I} - \mathbf{z}\,\mathbf{z}^*)\,\mathbf{K}\,(\mathbf{I} - \mathbf{u}\,\mathbf{u}^*)\,\mathbf{t} = -\mathbf{r}.$$

Use equivalent augmented system:

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

Cond(projected system)

$$\sim \quad \text{Cond(augmented system)}$$

$$\sim \quad \mathcal{C} \cdot \text{Cond}_K(\widetilde{\lambda}) \cdot \frac{1}{\cos(\mathbf{u}, \widetilde{\mathbf{x}})} \cdot \underbrace{\frac{1}{\cos(\mathbf{z}, \widetilde{\mathbf{y}})}}_{\approx\, \text{Cond}_{\mathbf{B}^{-1}\mathbf{A}}(\lambda)}$$

[Botta & Wubs '99, vd Ploeg & Botta & Wubs '96]

[Saad '96, Reusken '96, Bank & Wagner '00]

MRILU, NGILU, ILUM, MLILU

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 conditioned Schur complement)

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

with

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

$\widetilde{\mathbf{A}}_2$ Schur complement of $\mathbf{K}_1$ in $\mathbf{K}$:

$$\widetilde{\mathbf{A}}_2 = \mathbf{A}_2 - \mathbf{E}_\ell\mathbf{K}_1^{-1}\mathbf{E}_u$$

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

$\mathbf{K}_1$ well-conditioned, $\mathbf{A}_2$ low dimensional

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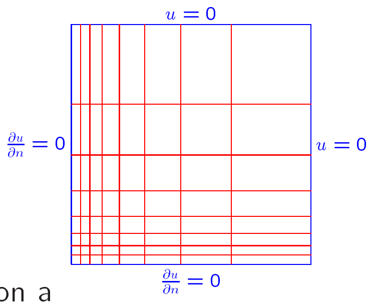
$$\begin{bmatrix} \mathbf{K} & \mathbf{z} \\ \mathbf{u}^* & 0 \end{bmatrix} = \begin{bmatrix} \mathbf{K}_1 & \mathbf{E}_u & \mathbf{z}_1 \\ \mathbf{E}_\ell & \mathbf{A}_2 & \mathbf{z}_2 \\ \mathbf{u}_1^* & \mathbf{u}_2^* & 0 \end{bmatrix} =$$

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

$\begin{bmatrix} \widetilde{\mathbf{A}}_2 & \widetilde{\mathbf{z}}_2 \\ \widetilde{\mathbf{u}}_2^* & \beta \end{bmatrix}$ well conditioned & low dimensional
allows "exact" direct methods

$$\widetilde{\mathbf{u}}_2^* \equiv \mathbf{u}_2^* - \mathbf{u}_1^*\mathbf{K}_1^{-1}\mathbf{E}_u, \quad \widetilde{\mathbf{z}}_2 \equiv \mathbf{z}_2 - \mathbf{E}_\ell\mathbf{K}_1^{-1}\mathbf{z}_1, \quad \beta \equiv -\mathbf{u}_1^*\mathbf{K}_1^{-1}\mathbf{z}_1$$



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

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

MRILU

Reorder & partition

$$\mathbf{A}^{(0)} = \mathbf{A} = \begin{bmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} \\ \mathbf{A}_{21} & \mathbf{A}_{22} \end{bmatrix}$$

such that (i) $\mathbf{A}_{11}$ is well-conditioned
(ii) $\mathbf{A}_{11}$ is κn by κn with $0 < \kappa \leq 1$
(iii) $\mathbf{A}_{11} \approx \mathbf{D} :=$ diag($\mathbf{A}_{11}$)

Take $\mathbf{K}^{(0)} = \begin{bmatrix} \mathbf{D} & \mathbf{A}_{12} \\ \mathbf{A}_{21} & \mathbf{A}_{22} \end{bmatrix} = \begin{bmatrix} \mathbf{D} & \mathbf{0} \\ \mathbf{A}_{21} & \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{I} & \mathbf{D}^{-1}\mathbf{A}_{12} \\ \mathbf{0} & \widetilde{\mathbf{A}}_{22} \end{bmatrix}$

For sparseness in the Schur complement:
lump small off-diagonal elem. to the diagonal.
'Small' with respect to diagonal elements.

To be repeated with
$\mathbf{A}$ replaced by $\mathbf{A}^{(1)} \equiv \widetilde{\mathbf{A}}_{22}$, etc.

$\mathbf{K} \approx \mathbf{A} - \tau\mathbf{B}$

Can the preconditioner be updated efficiently if better approximations θ for λ become available?

$$\begin{aligned} \mathbf{A} - \theta\mathbf{B} &= (\mathbf{A} - \tau\mathbf{B}) - (\theta - \tau)\mathbf{B} \\ &\approx \mathbf{K} - (\theta - \tau)\mathbf{B} \\ &= \mathbf{K}(\mathbf{I} - (\theta - \tau)\mathbf{K}^{-1}\mathbf{B}) \end{aligned}$$

For ease of explanation, we assume $\tau = 0$
(else replace $\mathbf{A}$ by $\mathbf{A} - \tau\mathbf{B}$, etc.)

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

$\mathbf{K}_1$ well-conditioned, $\mathbf{A}_2$ low dimensional

Improving the preconditioner

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

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

Neumann series:

$$(\mathbf{K}_1-\theta\mathbf{B}_1)^{-1} \approx \mathbf{C}_1 \equiv (\mathbf{I}+\theta[\mathbf{K}_1^{-1}\mathbf{B}_1])\mathbf{K}_1^{-1}$$

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

Computational aspects

$$\mathbf{M}_\theta \begin{bmatrix} \mathbf{t}_1 \\ \mathbf{t}_2 \end{bmatrix} = \begin{bmatrix} \mathbf{s}_1 \\ \mathbf{s}_2 \end{bmatrix}$$ to be solved as:

(1) Solve $\mathbf{K}_1\mathbf{t}_1 = \mathbf{s}_1$

(1′) $\mathbf{t}_1 \leftarrow \mathbf{t}_1 + \theta[\mathbf{K}_1^{-1}\mathbf{B}_1]\mathbf{t}_1$

(2) $\widetilde{\mathbf{t}}_2 = \mathbf{s}_2 - \mathbf{E}_\ell\mathbf{t}_1 - \theta\mathbf{F}_\ell\mathbf{t}_1$

(3) Solve $(\widetilde{\mathbf{A}}_2-\theta\widetilde{\mathbf{B}}_2)\mathbf{t}_2 = \widetilde{\mathbf{t}}_2$

(4) $\widetilde{\mathbf{t}}_1 \leftarrow [\mathbf{K}_1^{-1}\mathbf{E}_u]\mathbf{t}_2 - \theta[\mathbf{K}_1^{-1}\mathbf{F}_u]\mathbf{t}_2$

(4′) $\mathbf{t}_1 \leftarrow \mathbf{t}_1 - \widetilde{\mathbf{t}}_1 - \theta[\mathbf{K}_1^{-1}\mathbf{B}_1]\widetilde{\mathbf{t}}_1$

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

$$= \begin{bmatrix} \mathbf{K}_1^{-1}\mathbf{B}_1 & \mathbf{K}_1^{-1}\mathbf{F}_u \\ \mathbf{F}_\ell - \mathbf{E}_\ell\mathbf{K}_1^{-1}\mathbf{B}_1 & \mathbf{B}_2 - \mathbf{E}_\ell\mathbf{K}_1^{-1}\mathbf{F}_u \end{bmatrix}$$

$$\widetilde{\mathbf{B}}_2 = [\mathbf{B}_2 - \mathbf{E}_\ell\mathbf{K}_1^{-1}\mathbf{F}_u] - [\mathbf{F}_\ell - \mathbf{E}_\ell\mathbf{K}_1^{-1}\mathbf{B}_1][\mathbf{K}_1^{-1}\mathbf{E}_u]$$

Improving the preconditioner

Construction of the update of the precond.:

– Use ordering and partioning for $\mathbf{K}$ also for $\mathbf{B}$
– Apply elimination for $\mathbf{A}$ also to $\mathbf{B}$
  to compute $\mathbf{K}_1^{-1}\mathbf{B}_1$, $\mathbf{K}_1^{-1}\mathbf{F}_u$, and $\widetilde{\mathbf{B}}_2$
– Store these matrices.

Application of the updated preconditioner:
– For each θ update the low dim. $\widetilde{\mathbf{A}}_2 - \theta\widetilde{\mathbf{B}}_2$.

Computational costs for the construction and for the application of the update are (virtually) independent of θ and are low as compared to the costs for $\mathbf{K}$.

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

Accurate initial guesses

Since $\mathbf{M}_\theta \approx \mathbf{K} - \theta\mathbf{B} \approx \mathbf{A} - \theta\mathbf{B}$ for θ small,

we will have that (Bauer-Fike)

$(\theta, \mathbf{u}) \approx (\lambda, \mathbf{x})$ if $\mathbf{M}_\theta\mathbf{u} = \mathbf{0}$ and θ small.

$(\theta, \mathbf{u})$ is called pre-eigenpair if $\mathbf{M}_\theta\mathbf{u} = \mathbf{0}$.

Solving $\mathbf{M}_\theta\mathbf{u} = \mathbf{0}$

(3) Compute $(\theta, \mathbf{u}_2)$ s.t. $(\widetilde{\mathbf{A}}_2 - \theta\widetilde{\mathbf{B}}_2)\mathbf{u}_2 = \mathbf{0}$

(4) $\mathbf{u}_1 = [\mathbf{K}_1^{-1}\mathbf{E}_u]\mathbf{u}_2 - \theta[\mathbf{K}_1^{-1}\mathbf{F}_u]\mathbf{u}_2$

(4′) $\mathbf{u}_1 \leftarrow -\mathbf{u}_1 - \theta[\mathbf{K}_1^{-1}\mathbf{B}_1]\mathbf{u}_1$

Experiments

– Wanted eigenvalues: 6 absolute smallest.
– $6 \leq \dim(\text{search subspace}) \leq 11$.
– Test subspace: $\mathbf{z} = (\mathbf{A} - \tau\mathbf{B})\mathbf{u}$
(harmonic Petrov v.)
– Appr. eigenpair accepted if $\|\mathbf{r}\| \leq 10^{-12}$

Target τ is reset after each detection of an eigenpair: τ smallest eigenvalue

$$\mathbf{V}^*\mathbf{A}\mathbf{V}y = \theta\mathbf{V}^*\mathbf{B}\mathbf{V}y$$

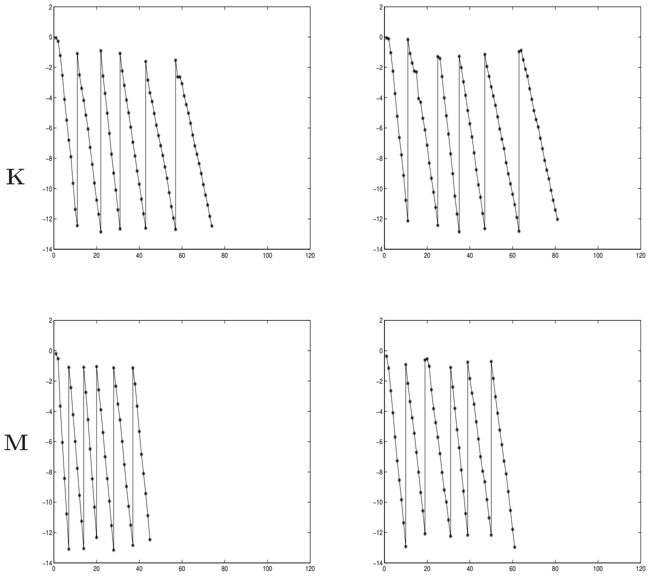
with $\mathbf{V}$ orth. matrix current search subspace

Initial search subspace
for $\mathbf{K}$: $\mathbf{V} = [\mathbf{v}_1]$ random
for $\mathbf{M}$: $\mathbf{V} = [\mathbf{u}_1, \ldots, \mathbf{u}_6]$ smallest pre-eigenvectors.

$$\begin{cases} \Delta u + c(u_x + u_y) = \lambda u & \text{on} \quad [0,1]^2 \\ u(0,y) = u(x,0) = 0, & u_x(1,y) = u_y(x,1) = 0 \end{cases}$$

uniform mesh, central differences

$\mathbf{M}$ versus $\mathbf{K}$



'high' fill (30+8) 'moderate' fill (19+5)

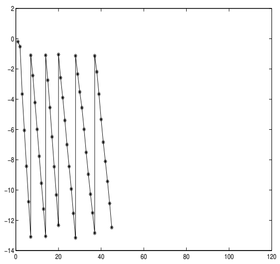
On a grid of 32×32 unknowns.

Pre-eigenvalues, targets and computed eigenvalues for the convection-diffusion problem

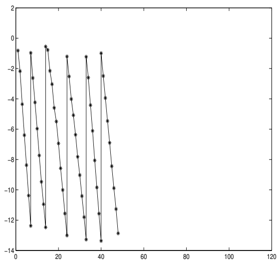
	K-variant					
target	0	25.0	25.1	44.9	64.1	83.8
computed eigenvalue	5.14	24.8	24.8	44.5	64.1	83.8
	M-variant					
pre-eigenvalue	5.13	25.3	25.6	46.6	67.9	69.0
target	5.13	25.2	25.0	44.9	65.0	64.5
computed eigenvalue	5.14	24.8	24.8	44.5	64.1	64.1

Grid independence

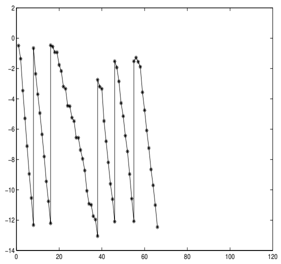
Use the M-variant



32×32
(fill 30+8)



64×64 (fill 34+9)

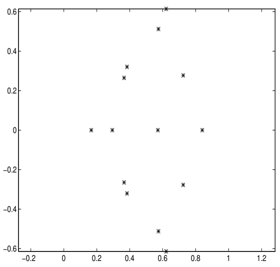


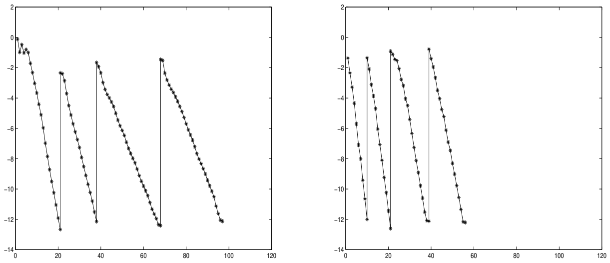
128×128 (fill 37+10)

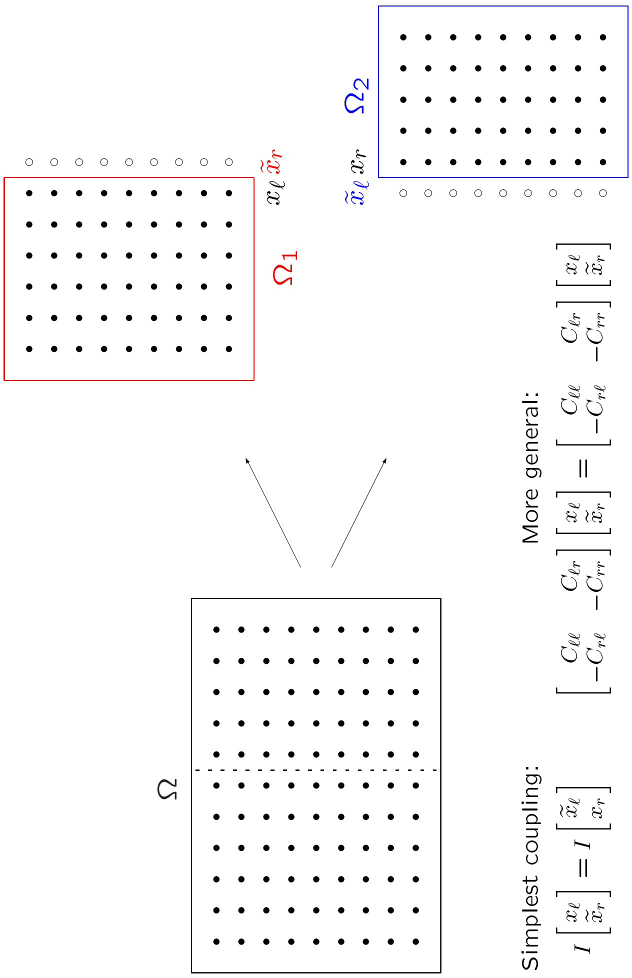
Incompressible Navier-Stokes

relevant eigenvalues

Stability stationary sol.
Fin. diff. on a stagg. grid of 675 unknowns.
$\mathrm{B} = \mathrm{diag}(1, 1, 0, 1, 1, 0, \ldots)$



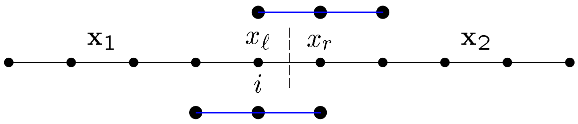




[Tan & Borsboom '95, Tan '95]

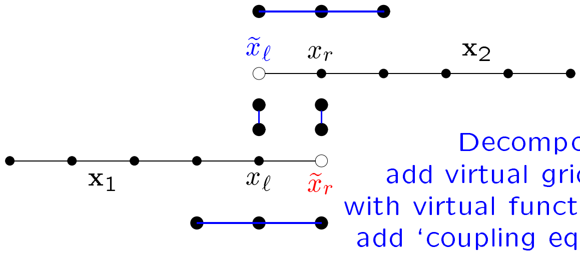
Domain decomposition with enhanced systems

1-dimensional



Represents stencil for coupling the function val. x_{i-1}, $x_\ell \equiv x_i$, $x_r \equiv x_{i+1}$ at the grid pints $i-1$, i, $i+1$

Decompose and enhance:



Decompose grid, add virtual grid-points with virtual function val., add 'coupling equations' to identify x_ℓ with $\tilde{x}_\ell, \ldots$

Simplest coupling: $\quad I \begin{bmatrix} x_\ell \\ \tilde{x}_r \end{bmatrix} = I \begin{bmatrix} \tilde{x}_\ell \\ x_r \end{bmatrix}$

Continuity – or couplings equations::

$$\begin{bmatrix} C_{\ell\ell} & C_{\ell r} \\ -C_{r\ell} & -C_{rr} \end{bmatrix} \begin{bmatrix} x_\ell \\ \tilde{x}_r \end{bmatrix} = \begin{bmatrix} C_{\ell\ell} & C_{\ell r} \\ -C_{r\ell} & -C_{rr} \end{bmatrix} \begin{bmatrix} x_\ell \\ \tilde{x}_r \end{bmatrix}$$

Two domains

Left domain:

a. interior unknowns $\mathbf{x}_1$

b. boundary unknowns x_ℓ

c. unknowns on virtual points: $\tilde{x}_r$

Right domain:

a. interior unknowns $\mathbf{x}_2$

b. boundary unknowns x_r

c. unknowns on virtual points: $\tilde{x}_\ell$

W-P Tang [92]: add one set of virtual points, split stencils that couple across the interface.

Tan [95]: add two sets of virtual points (s.t. no stencils across interface), add cont. eq.

Enhanced matrix

Enhanced system

$$
\left[\begin{array}{ccc|ccc}
\mathbf{A}_{11} & \mathbf{A}_{1\ell} & \mathbf{A}_{1r} & 0 & 0 & 0 \\
\mathbf{A}_{\ell 1} & A_{\ell\ell} & A_{\ell r} & 0 & 0 & 0 \\
\mathbf{0} & C_{\ell\ell} & C_{\ell r} & -C_{\ell\ell} & -C_{\ell r} & 0 \\
\hline
0 & -C_{r\ell} & -C_{rr} & C_{r\ell} & C_{rr} & \mathbf{0} \\
0 & 0 & 0 & A_{r\ell} & A_{rr} & \mathbf{A}_{r2} \\
0 & 0 & 0 & \mathbf{A}_{2\ell} & \mathbf{A}_{2r} & \mathbf{A}_{22}
\end{array}\right]
\begin{bmatrix} \mathbf{x}_1 \\ x_\ell \\ \tilde{x}_r \\ \tilde{x}_\ell \\ x_r \\ \mathbf{x}_2 \end{bmatrix}
=
\begin{bmatrix} \mathbf{b}_1 \\ b_\ell \\ 0 \\ 0 \\ b_r \\ \mathbf{b}_2 \end{bmatrix}
$$

$$\mathbf{A}_C \underset{\sim}{\mathbf{x}} = \underline{\mathbf{b}}, \quad \mathbf{K}_C \text{ block diagonal part}$$

'Schwart' iteration = block Jacobi:
submatrices outside boxes $\rightarrow$ right-hand side
(with x-values of previous it.)

With $C \equiv \begin{bmatrix} C_{\ell\ell} & C_{\ell r} \\ -C_{r\ell} & -C_{rr} \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix}$
Dirichlet-Neumann coupling

Tan ['95]: general couplings for 6 point stencils along the interface.

More Details

JD-algorithm:

Sleijpen and van der Vorst
SIMAX, 17 (1996), pp. 401–425.

JD: general problems

Sleijpen, Booten, Fokkema, and van der Vorst
BIT, 36:3 (1996), pp. 595–633.

JDQR and JDQZ

Fokkema, Sleijpen, and van der Vorst,
SISC, 20 (1999), pp. 94–125.

Preconditioning

Sleijpen, van der Vorst, Meijerink,
ETNA, 7 (1998), pp. 75–89.
Sleijpen and Wubs,
Preprint 1117, Aug. 1999.

these papers and others:
http://www.math.uu.nl/people/sleijpen
http://www.math.uu.nl/people/vorst

JD-correction equation

Solve approximately $\mathbf{t} \perp \mathbf{u}$

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

Practical procedure

a. Enhance $\mathbf{A} - \theta\mathbf{I}$ and $\mathbf{r}$

b. Take for $\mathbf{K}_C$ the block Jacobi-part

c. Do m steps of GMRES

d. Undo enhancement: take average

$$t_\ell \leftarrow (t_\ell + \tilde{t}_\ell)/2, \quad t_r \leftarrow (t_r + \tilde{t}_r)/2$$