Deflation acceleration for Computational Fluid Dynamics problems

Kees Vuik

Delft Institute of Applied Mathematics

c.vuik@math.tudelft.nl

http://ta.twi.tudelft.nl/users/vuik/

Model order reduction, coupled problems and optimization

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Contents

1. Introduction

Incompressible Stokes equation

$$
\begin{aligned}
-\nu \Delta \mathbf{u} + \text{grad } p &= \mathbf{f}, \\
\text{div } \mathbf{u} &= 0.
\end{aligned}
$$

Finite volumes, staggered grid

$$
\begin{pmatrix}
\mathbf{Q}_1 & \mathbf{O} & \mathbf{O} & \mathbf{G}_1 \\
\mathbf{O} & \mathbf{Q}_2 & \mathbf{O} & \mathbf{G}_2 \\
\mathbf{O} & \mathbf{O} & \mathbf{Q}_3 & \mathbf{G}_3 \\
\mathbf{G}_1^T & \mathbf{G}_2^T & \mathbf{G}_3^T & 0
\end{pmatrix}
\begin{pmatrix}
u_1 \\ u_2 \\ u_3 \\ p
\end{pmatrix}
=
\begin{pmatrix}
b_1 \\ b_2 \\ b_3 \\ b_4
\end{pmatrix}
$$

SIMPLE method (Patankar)

$\mathbf{D} = diag(\mathbf{Q})$ and $\mathbf{R} = -\mathbf{G}^T\mathbf{D}^{-1}\mathbf{G}$

SIMPLE algorithm

1. Choose an initial estimate p^*.
2. Solve $\mathbf{Q}u^* = b_1 - \mathbf{G}p^*$.
3. Solve $\mathbf{R}\delta p = b_2 - \mathbf{G}^T u^*$.
4. Compute $u = u^* - \mathbf{D}^{-1}\mathbf{G}\delta p$
   and $p := p^* + \delta p$.
5. If not converged take $p^* = p$ and go to 2.

This BIM can be used as preconditioner within GCR (Eisenstat, Elman and Schultz).

Solution methods

Efficient solution of a linear system, where A is SPD,

$$Ax = b.$$

Conjugate Gradient, Preconditioner, Projection Acceleration.

The convergence of CG depends on the effective condition number.

Projection Acceleration to eliminate the effect of small eigenvalues.

Motivation

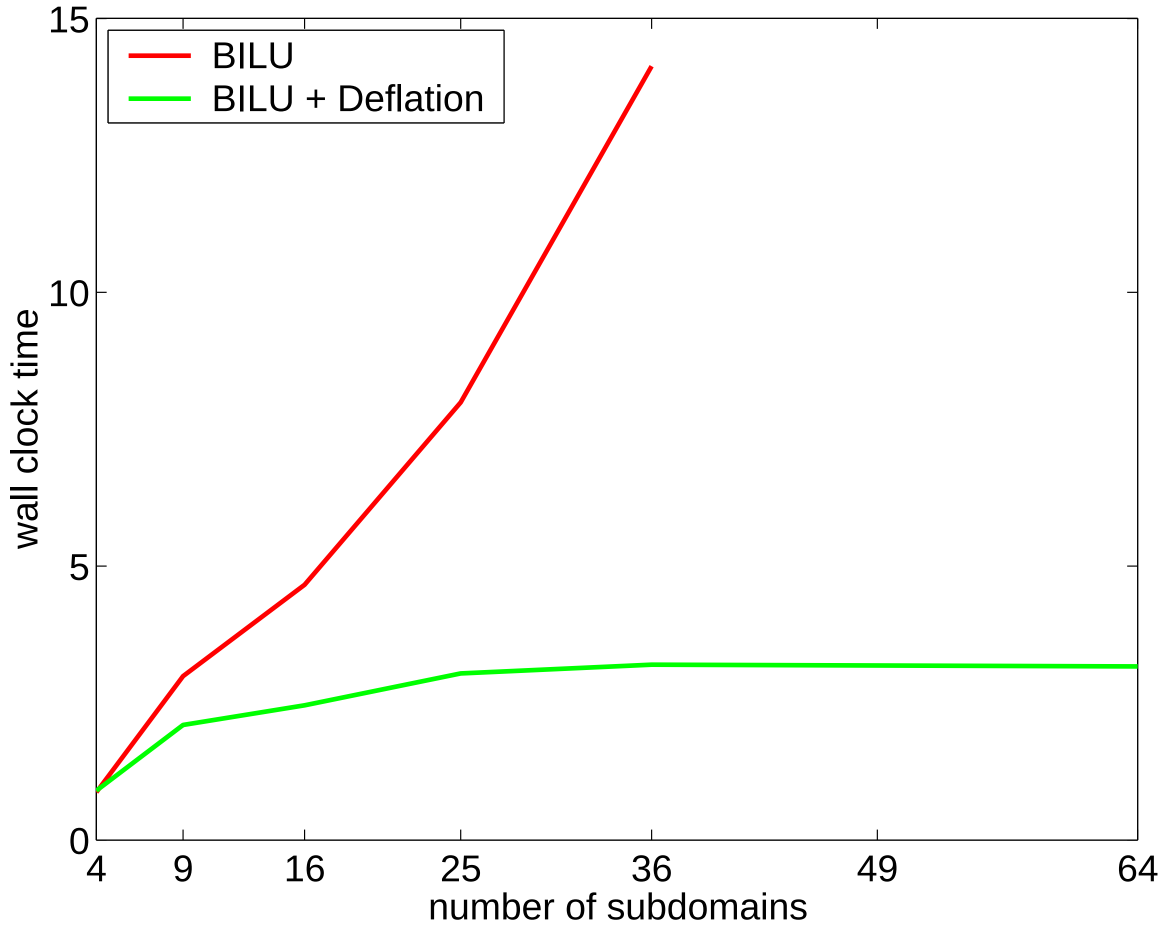
- large jumps in the coefficients
- block preconditioners (parallel)
- IC preconditioners (serial)

Projection type methods

Krylov	Ar
Preconditioned Krylov	$M^{-1}Ar$
Block Preconditioned Krylov	$\sum_{i=1}^{m}(M_i^{-1})Ar$
Block Preconditioned Deflated Krylov	$\sum_{i=1}^{m}(M_i^{-1})PAr$

Parallel scalability

subdomain grid size 50×50, wall clock time, Cray T3E



2. Projection type methods

Deflated CG and coarse grid projection vectors

Nicolaides 1987, Mansfield 1990, Kolotilina 1998, Vuik, Segal and Meijerink 1999, Saad, Yeung, Erhel and Guyomarc'h 2000, Frank and Vuik 2001, Nabben and Vuik 2004

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Additive Coarse Grid Correction

Bramble, Pasciak and Schatz 1986, Dryja and Widlund 1991, Smith, Bjorstad and Gropp 1996, Benzi, Frommer, Nabben and Szyld 2001

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Balancing (Neumann-Neumann) preconditioner
Mandel 1993, Dryja and Widlund 1995, Mandel and Brezina 1996, Pavarino and Widlund 2002

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Augmented Krylov methods, FETI

Deflation

$$Z \in \mathbb{R}^{n \times r}$$

$$Ax = b, \qquad P_D = I - AZ(Z^T AZ)^{-1} Z^T$$

Note that $P_D A$ is a symmetric, positive semi definite singular matrix.

Deflation

$$Z \in \mathbb{R}^{n \times r}$$

$$Ax = b, \qquad P_D = I - AZ(Z^TAZ)^{-1}Z^T$$

Note that P_DA is a symmetric, positive semi definite singular matrix.

We use $x = (I - P_D^T)x + P_D^Tx$

Compute both terms:

1. $(I - P_D^T)x = Z(Z^TAZ)^{-1}Z^TAx = Z(Z^TAZ)^{-1}Z^Tb$,
2. Solve $P_DA\tilde{x} = P_Db$,
3. Form $P_D^T\tilde{x}$ (Theorem: $P_D^Tx = P_D^T\tilde{x}$).

Comparison of Deflation and Additive Coarse Grid Correction

$$P_D = I - AZE^{-1}Z^T \qquad P_C = I + \sigma ZE^{-1}Z^T$$

$$M^{-1}P_D = M^{-1} - M^{-1}AZE^{-1}Z^T \qquad P_{CM^{-1}} = M^{-1} + \sigma ZE^{-1}Z^T$$

where $E = Z^T AZ$.

Work per iteration:

- 1 matrix vector product
- 1 preconditioner vector product
- 1 coarse grid operator

Comparison of Deflation and Additive Coarse Grid Correction

Definition

Eigenpair $\{\lambda_i, v_i\}$, so $Av_i = \lambda_i v_i$ with $0 < \lambda_1 \leq \ldots \leq \lambda_n$.
Take $Z = [v_1 \ldots v_r]$.

Theorem

- the spectrum of $P_D A$ is $\{0, \ldots, 0, \lambda_{r+1}, \ldots, \lambda_n\}$

- the spectrum of $P_C A$ is $\{\sigma + \lambda_1, \ldots, \sigma + \lambda_r, \lambda_{r+1}, \ldots, \lambda_n\}$

Comparison of Deflation and Additive Coarse Grid Correction

Corollary

$$cond_{eff}(P_D A) = \frac{\lambda_n}{\lambda_{r+1}} \leq \frac{\max\{\lambda_n, \sigma + \lambda_r\}}{\min\{\lambda_{r+1}, \sigma + \lambda_1\}} = cond(P_C A)$$

- The eigenvalues of $P_C A$ has a worse distribution than the eigenvalues of $P_D A$

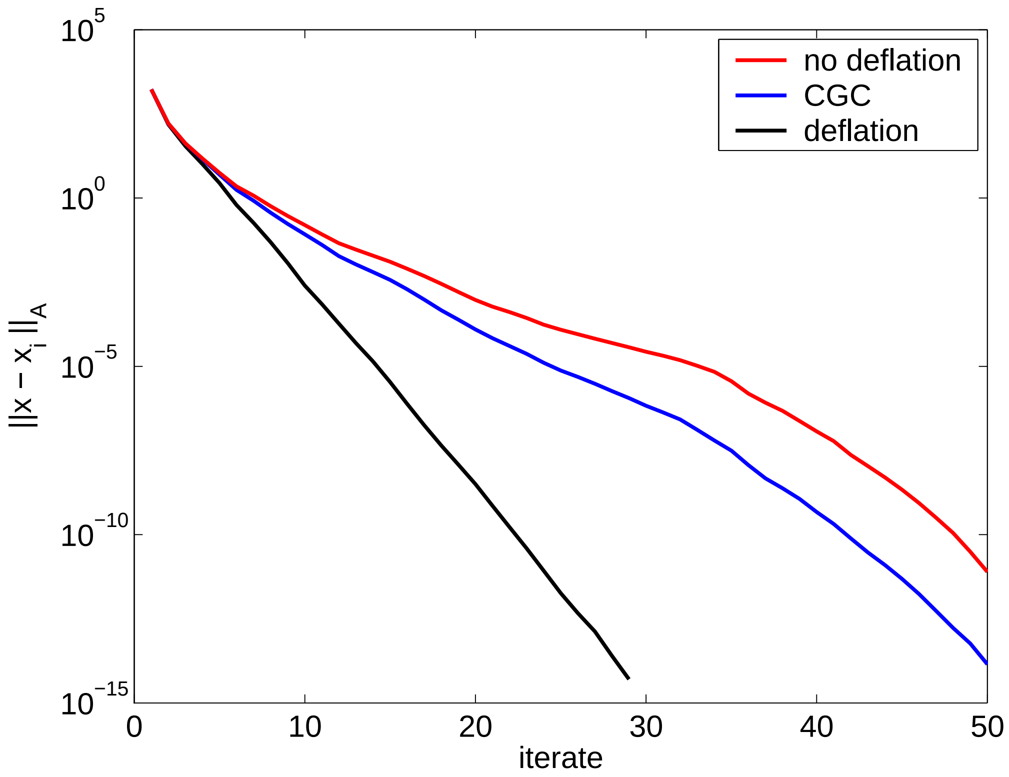
Conclusion

Deflation is asymptotically better than additive coarse grid correction!

Results for eigenvectors

The eigenvalues of A are $1, 2, 3, \ldots, 99, 100$.

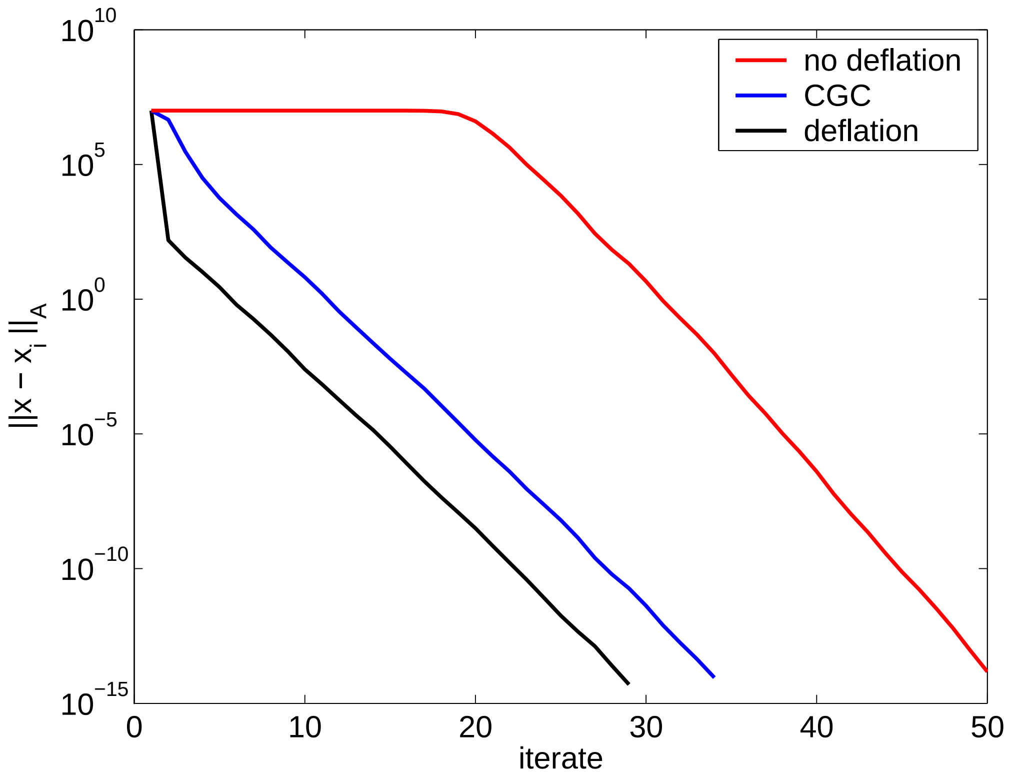
The eigenvectors $v_1, \ldots, v_{10}$ are used as projection vectors.



Results for eigenvectors

The eigenvalues of A are $10^{-6}, \ldots 10^{-6}, 11, 12, 13, \ldots, 99, 100$.

The eigenvectors $v_1, \ldots, v_{10}$ are used as projection vectors.



Comparison of Deflation and the Balancing preconditioner

$$M^{-1}P_D = M^{-1} - M^{-1}AZE^{-1}Z^T$$

$$P_B = (I - ZE^{-1}Z^TA)M^{-1}(I - AZE^{-1}Z^T) + ZE^{-1}Z^T$$

$$P_B = P_D^TM^{-1}P_D + ZE^{-1}Z^T$$

Work per iteration:

	Deflation	Balancing (depends on implementation)
matrix vector product	1	3
preconditioner vector product	1	1
coarse grid operator	1	2

Comparison of Deflation and the Balancing preconditioner

Take $Z = [v_1 \ldots v_r]$ and $M = I$.

Theorem

- the spectrum of $P_D A$ is $\{0, \ldots, 0, \lambda_{r+1}, \ldots, \lambda_n\}$

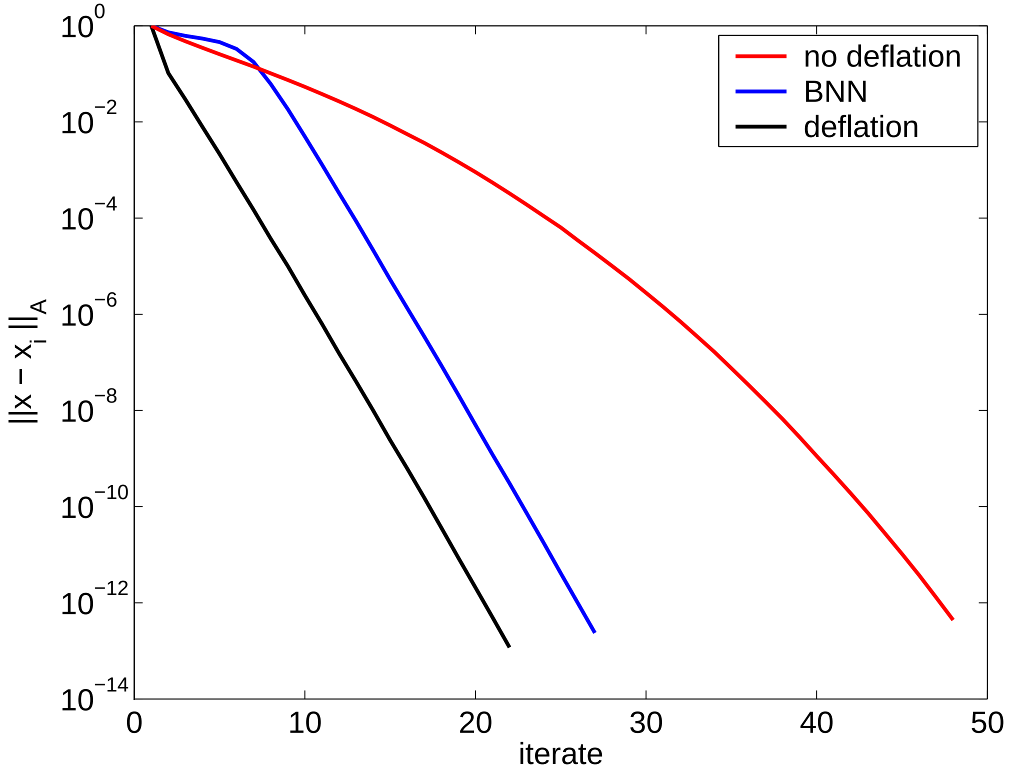
- the spectrum of $P_B A$ is $\{1, \ldots, 1, \lambda_{r+1}, \ldots, \lambda_n\}$

$$cond_{eff}(P_D A) = \frac{\lambda_n}{\lambda_{r+1}} \leq \frac{\max\{\lambda_n, 1\}}{\min\{\lambda_{r+1}, 1\}} = cond(P_B A)$$

Deflation is asymptotically better than Balancing!

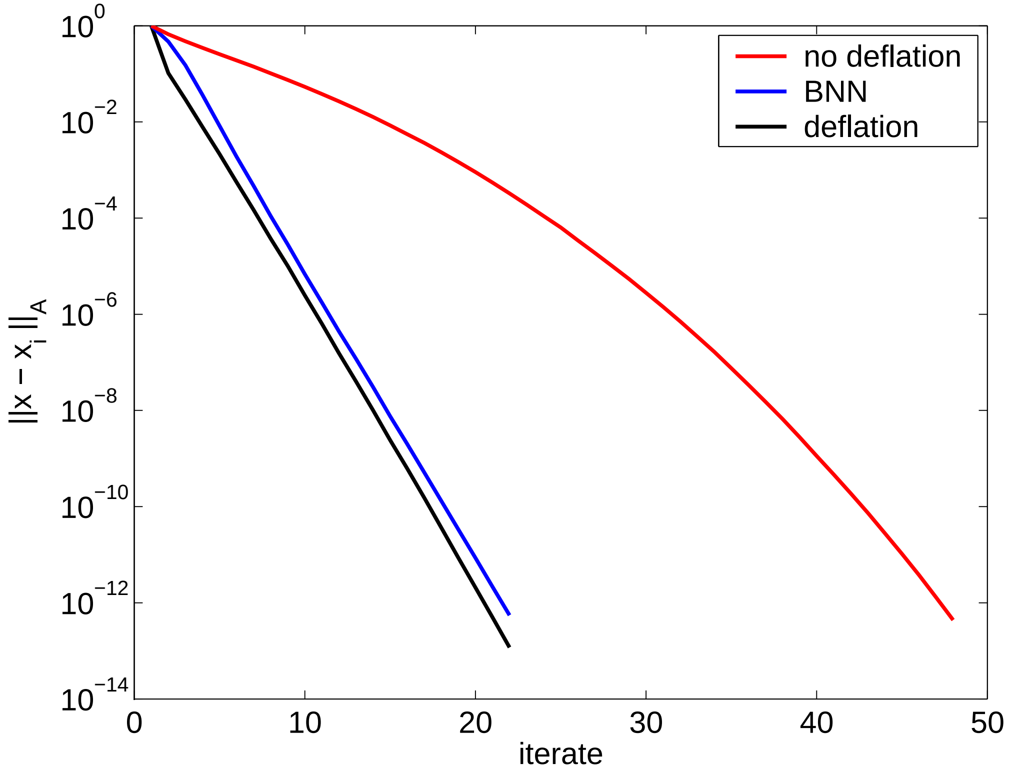
Results for eigenvectors $v_1, \ldots, v_{10}$

The eigenvalues of A are $1, 2, 3, \ldots, 99, 100$.



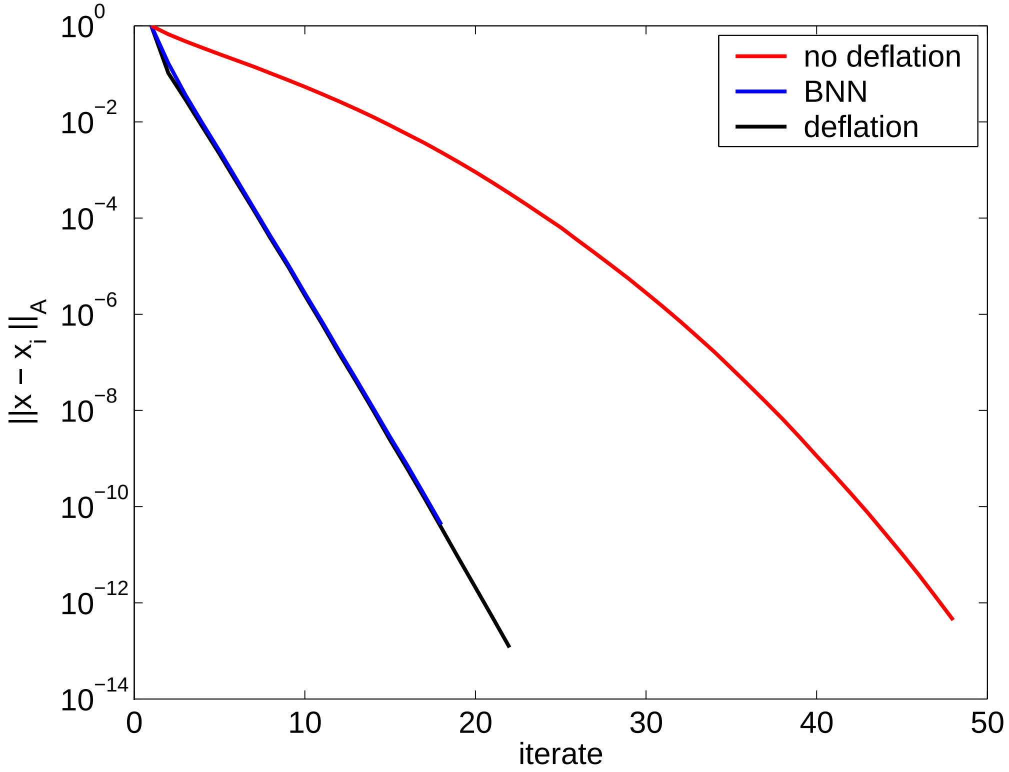
Results for eigenvectors $v_1, \ldots, v_{10}$

The eigenvalues of A are $0.1, 0.2, 0.3, \ldots, 9.9, 10$.



Results for eigenvectors $v_1, \ldots, v_{10}$

The eigenvalues of A are $0.01, 0.02, 0.03, \ldots, 0.99, 1$.



3. Projection vectors

Two classes

- eigenvector based
- domain decomposition based

Exact eigenvectors

Properties

- expensive to obtain
- all components of the vectors are nonzero
- projection is easy
- much theory available

Approximate eigenvectors

Krylov subspace approximation

Properties

- cheap/expensive to obtain
- all components of the vectors are nonzero
- more suitable for non symmetric Krylov solvers

References

Morgan, Saad, Yeung, Ehrel, Guyomarch, Burrage, Pohl, Baglama, Calvetti, Reichel, Golub

Approximate eigenvectors

Physical approximation

Properties

- problem dependent
- the vectors are sparse
- suitable for parallel computing

References

Lynn, Timlake, Meijerink, Segal, Vuik, Wijma

Approximate eigenvectors

Previous solution approximation

Properties

- cheap/expensive to obtain
- all components of the vectors are nonzero
- not sure that bad eigenvalues are removed

References

Clemens, Wilke, Schuhman, Weiland

Domain decomposition

All vectors, except on the interfaces

Properties

- cheap to obtain
- many sparse vectors
- (large) subproblems should be solved accurately

References

Dostal

Domain decomposition

Some vectors per subdomain (constant 1, constant + linear 4)

Properties

- cheap to obtain
- black box
- sparse vectors (total memory 1 to 4 vectors)
- suitable for parallel computing
- bad eigenvectors are removed

References

Nicolaides, Mansfield, Fischer, De Gersem, Vandewalle, Hameyer, Frank, Padiy, Axelsson, Polman, Vuik, Nabben, Verkaik, Vermolen, Segal, Waisman, Fish, Tuminaro, Widlund

4. Conclusions

- Projection is a usefull technique to accelerate preconditioned Krylov subspace methods
- Deflation needs less iterations than additive coarse grid correction, and uses the same amount of work per iteration
- Deflation uses less (approximately the same) iterations as Balancing, but uses less work per iteration.
- Balancing needs less iterations than additive coarse grid correction.
- The choice of the projection vectors is important for the success of a projection method.

Further information

- http://ta.twi.tudelft.nl/nw/users/vuik/pub_it_def.html

- C. Vuik, A. Segal and J.A. Meijerink
  An efficient preconditioned CG method for the solution of a class of layered problems with extreme contrasts in the coefficients
  J. Comp. Phys., 152, pp. 385-403, 1999.
- J. Frank and C. Vuik
  On the construction of deflation-based preconditioners
  SIAM Journal on Scientific Computing, 23, pp. 442–462, 2001
- R. Nabben and C. Vuik
  A comparison of Deflation and Coarse Grid Correction applied to porous media flow
  SIAM J. on Numerical Analysis, 42, pp. 1631-1647, 2004
- R. Nabben and C. Vuik
  A comparison of Deflation and the Balancing preconditioner
  SIAM Journal on Scientific Computing, to appear