Projected Krylov Methods for Unsymmetric Augmented Systems

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Outline

Problem Statement and Context

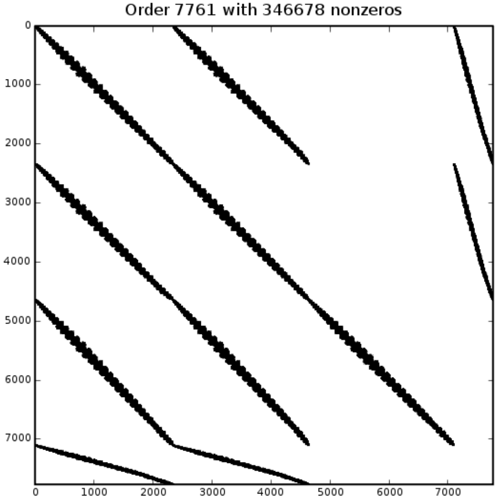
$$\begin{bmatrix} A & B^T \\ B & 0 \end{bmatrix} \begin{bmatrix} u \\ p \end{bmatrix} = \begin{bmatrix} b \\ d \end{bmatrix}$$

- Optimization and Control, incl. least squares (A symmetric),
- Multi immiscible fluid flow with free surface,
- Fictitious domains method for flow around obstacle,
- Electromagnetism, image restoration, ...

Denote the augmented matrix $K(A)$.

- Do not want to assemble A,
- B "flat" and contributes marginally to density of $K(A)$,
- Can assemble B,
- Can compute Ap but not $A^T p$.

Typical Block Structure



Density($K(A)$): 0.315%, A accounts for 0.279%, B for 0.036%

Assumptions and Basic Results

Do not assume A symmetric or positive (semi-)definite, but:

1. B full row rank,
2. $\mathcal{N}(A) \cap \mathcal{N}(B) = \{0\}$,
3. $\mathcal{R}(A \mid \mathcal{N}(B)) \cap \mathcal{R}(B^T) = \{0\}$.

where

$$\mathcal{R}(A \mid \mathcal{N}(B)) = \{v = Aw \text{ for some } w \in \mathcal{N}(B)\}$$

Theorem

$K(A)$ is nonsingular $\Longleftrightarrow$ assumptions 1–3

Theorem (Preconditioners)

$G = G^T$ positive definite over $\mathcal{N}(B) \Longrightarrow K(G)$ nonsingular

Direct Application of Iterative Methods

System size: $n + m = 7761$, itmax $= 6(n + m)$, no preconditioner

Solver	Iterations	Residual	Workspace	Time (s)
BCG	46566	0.1329880e+02	54327	21.95
DBCG	46567	0.4489614e+01	85371	23.02
CGNR	46567	0.1537764e−04	38805	21.25
BCGSTAB	46567	0.3111281e−04	62088	21.95
TFQMR	46567	0.8147863e−04	85371	23.11
GMRES	46566	0.6374488e+97	132108	28.33
FGMRES	46566	0.3499084e+96	248519	28.63
DQGMRES	46566	0.1387398e+95	256177	44.45

F77 implementations from SPARSKIT [Saad]

Nullspace Methods

$$Au + B^T p = b, \quad \text{and} \quad Bu = d.$$

Let Z = orthonormal basis for $\mathcal{N}(B)$. Any solution u^* has the form

$$u^* = Zu_{\mathrm{Z}}^* + B^T u_{\mathrm{B}}^*.$$

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and

$$Z^T AZ\; u_Z^* = Z^T(b - AB^T u_B^*) \qquad \leftarrow \text{concentrate on this system.}$$

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$$Z^T AZ \; u_\mathrm{Z}^* = Z^T(b - AB^T u_\mathrm{B}^*) \qquad \leftarrow \text{concentrate on this system.}$$

Worry about p^* later.

Problem: Computing Z is too costly. Worry about it in a minute.

Krylov Menu

- $K(A)$ is always indefinite (unless B vanishes): eliminate CG,
- $K(A)$ is not symmetric: eliminate MINRES and SYMMLQ,
- Do not want to compute $A^T p$: eliminate Bi-CG and QMR.

Leaves CGNE, CGNR, CGS, TFQMR, Bi-CGSTAB, GMRES(m).

- CGNE and CGNR "square the conditioning",
- CGS exhibits erratic convergence,
- GMRES is quite memory hungry.

At this point, concentrate efforts on Bi-CGSTAB and TFQMR.

Preconditioned Bi-CGSTAB for $R_1^{-T} M R_2^{-1} x = R_1^{-T} y$

1. $x_0 \in \mathbb{R}^n, \;\; r_0 = b - Mx_0, \;\; \bar{r}_0^T r_0 \neq 0, \;\; d_0 = r_0, \;\; k = 0.$
2. Solve $C\bar{d}_k = d_k$, set $\alpha_k = \dfrac{\bar{r}_0^T r_k}{\bar{r}_0^T M \bar{d}_k}$,
3. $s_k = r_k - \alpha_k M \bar{d}_k$, solve $C\bar{s}_k = s_k$,
4. $\omega_k = \dfrac{(R_1^{-T} s_k)^T (R_1^{-T} M \bar{s}_k)}{\|R_1^{-T} M \bar{s}_k\|_2^2}$,
5. $x_{k+1} = x_k + \alpha_k \bar{d}_k + \omega_k \bar{s}_k$,
6. $r_{k+1} = s_k - \omega_k M \bar{s}_k$,
7. $\beta_k = \dfrac{\alpha_k}{\omega_k} \dfrac{\bar{r}_0^T r_{k+1}}{\bar{r}_0^T r_k}$,
8. $d_{k+1} = r_{k+1} + \beta_k (d_k - \omega_k M \bar{d}_k)$.

$C = R_1^T R_2$ is the preconditioner.

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4. $\omega_k = \dfrac{(R_1^{-T} s_k)^T (R_1^{-T} M\bar{s}_k)}{\|R_1^{-T} M\bar{s}_k\|_2^2} \approx \dfrac{s_k^T M\bar{s}_k}{\|M\bar{s}_k\|_2^2}$,
5. $x_{k+1} = x_k + \alpha_k \bar{d}_k + \omega_k \bar{s}_k$,
6. $r_{k+1} = s_k - \omega_k M\bar{s}_k$,
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Apply Bi-CGSTAB to Nullspace System

$Z^T AZ \; u = Z^T(b - AB^T u^*_{\mathrm{B}})$ $\qquad C = Z^T GZ$

Choose an initial u_0^Z.

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$$\begin{aligned} r_0^Z &= Z^T(b - AB^T u_B^*) - Z^T AZ\ u_0^Z \\ &= Z^T \left(b - A(Zu_0^Z + B^T u_B^*)\right) \\ &= Z^T(b - Au_0) \\ &= Z^T r_0. \end{aligned}$$

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Similarly, $r_k^{\mathrm{Z}} = Z^T r_k,\ \ d_k^{\mathrm{Z}} = Z^T d_k,\ \ Z\bar{d}_k^{\mathrm{Z}} = \bar{d}_k$, so

$$Z^T GZ \quad \bar{d}_k^{\mathrm{Z}} = \qquad\qquad d_k^{\mathrm{Z}}$$

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Similarly, $r^Z_k = Z^T r_k$, $d^Z_k = Z^T d_k$, $Z\bar{d}^Z_k = \bar{d}_k$, so

$$\bar{d}^Z_k = \quad (Z^T GZ)^{-1} \quad d^Z_k$$

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i.e.

$$\bar{d}_k = P_G(d_k) \quad \text{oblique projection onto } \mathcal{N}(B)$$

Projected Preconditioned Bi-CGSTAB

1. $u_0 \in \mathbb{R}^n$, $r_0 = b - Au_0$, $(Z\bar{r}_0)^T r_0 \neq 0$, $d_0 = r_0$, $k = 0$.
2. Compute $\bar{d}_k = P_G(d_k)$, set $\alpha_k = \dfrac{(Z\bar{r}_0)^T r_k}{(Z\bar{r}_0)^T A\bar{d}_k}$,
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Choice of Fixed Vector

- $\bar{r}_0 = Z^T \tilde{r}_0$ for some $\tilde{r}_0 \in \mathbb{R}^n$. Then

$$(Z\bar{r}_0)^T v = (ZZ^T \tilde{r}_0)^T v = P_I(\tilde{r}_0)^T v.$$

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Upon picking $\tilde{r}_0 = r_0$, we ask that $r_0 \not\perp \mathcal{N}(B)$.

Computing Projections

$$\bar{v} = P_I(v) \iff \begin{bmatrix} I & B^T \\ B & 0 \end{bmatrix} \begin{bmatrix} \bar{v} \\ w \end{bmatrix} = \begin{bmatrix} v \\ 0 \end{bmatrix} \qquad K(I)$$

$$\bar{v} = P_G(v) \iff \begin{bmatrix} G & B^T \\ B & 0 \end{bmatrix} \begin{bmatrix} \bar{v} \\ w \end{bmatrix} = \begin{bmatrix} v \\ 0 \end{bmatrix} \qquad K(G)$$

Rely on symmetric indefinite factorization of $K(I)$ and/or $K(G)$.

Stabilizing the Projected Krylov Method

As in [Gould, Hribar & Nocedal, 2001], note that

$$\begin{bmatrix} I & B^T \\ B & 0 \end{bmatrix} \begin{bmatrix} \bar{s}_k \\ h_k \end{bmatrix} = \begin{bmatrix} s_k \\ 0 \end{bmatrix}.$$

and $\bar{s}_k \to 0$ while $s_k \not\to 0$. Cancellation follows:

$$\bar{s}_k = s_k - B^T h_k \quad \text{and} \quad \|s_k\| \approx \|B^T h_k\|.$$

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Solution: solve equivalently

$$\begin{bmatrix} I & B^T \\ B & 0 \end{bmatrix} \begin{bmatrix} \bar{s}_k \\ \tilde{h}_k \end{bmatrix} = \begin{bmatrix} s_k - B^T \lambda \\ 0 \end{bmatrix}.$$

with λ chosen such that $\|s_k - B^T \lambda\| \approx \|\bar{s}_k\|$.

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Ideal value $\lambda = \tilde{h}_k \approx \tilde{h}_{k-1}$.

Recovering the Pressure

p solves

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Equivalently,

$$\begin{bmatrix} I & B^T \\ B & 0 \end{bmatrix} \begin{bmatrix} w \\ p \end{bmatrix} = \begin{bmatrix} b - Au \\ 0 \end{bmatrix}$$

Finding an Initial Point

$$u^* = Zu_{\mathrm{Z}}^* + B^T u_{\mathrm{B}}^*, \qquad \text{with} \qquad BB^T u_{\mathrm{B}}^* = d.$$

$$\begin{bmatrix} I & B^T \\ B & 0 \end{bmatrix} \begin{bmatrix} w \\ -u_{\mathrm{B}}^* \end{bmatrix} = \begin{bmatrix} 0 \\ d \end{bmatrix}$$

$$w = B^T u_{\mathrm{B}}^* \qquad \text{with} \qquad Bw = d.$$

Test Problems

Implementation

- Flexible Fortran 90/95 modules,
- Projections computed with MA57 from HSL, METIS ordering,
- Could also use MA27 or MA47 from HSL Archive.

Flow of an incompressible viscous Newtonian fluid in a domain Ω which contains a (potentially moving) subdomain Ω^*:

$$\begin{aligned}
\left(\frac{\partial \vec{v}}{\partial t} + \vec{v} \cdot \mathrm{grad}\ \vec{v} \right) + \mu \nabla^2 \vec{v} + \mathrm{grad}\ p = \vec{f} \qquad & \text{in } \Omega, \\
\mathrm{div}\ \vec{v} = 0 \qquad & \text{in } \Omega, \\
\vec{v} = \vec{v^*} \qquad & \text{on } \Gamma^*,
\end{aligned}$$

Numerical Results ($G = I$)

Problem I: Two immiscible fluids in a cavity

$n_A = 7,092, \quad m_B = 669, \quad LBL^T \approx 0.12s, \quad \text{nnz}(L) \approx 27,658$

Instance	nnz(A)	nnz(B)	Matvecs	Rel. Res.	Time (s)
iter-5	168,103	40,198	5,864	9.7e−09	19.50
iter-7	168,030	40,174	5,282	4.5e−09	17.70
iter-8	168,054	40,160	4,842	3.2e−09	16.22

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$n_A = 30,320, \quad m_B = 2,645, \quad LBL^T \approx 0.64s, \quad \text{nnz}(L) \approx 145,651$

Instance	nnz(A)	nnz(B)	Matvecs	Rel. Res.	Time (s)
iter-2	541,545	86,083	2,696	3.0e−07	37.75
iter-6	795,404	86,063	1,540	9.8e−09	23.61

Numerical Results ($G = I$)

Problem II: Rectangular cavity, fixed circular obstacle (single fluid)

1. Mesh around obstacle
   $n_{\mathrm{A}} = 49,995,\ m_{\mathrm{B}} = 6,530,\ LBL^T \approx 1.45s,\ \mathrm{nnz}(L) \approx 383,272$
2. Fictitious domains
   $n_{\mathrm{A}} = 53,597,\ m_{\mathrm{B}} = 7,330,\ LBL^T \approx 1.86s,\ \mathrm{nnz}(L) \approx 444,637$

Instance	nnz(A)	nnz(B)	Matvecs	Rel. Res.	Time (s)
1	$1,009,071$	$383,094$	366	4.1e−07	9.76
2	$1,139,724$	$413,640$	382	3.9e−05	11.40

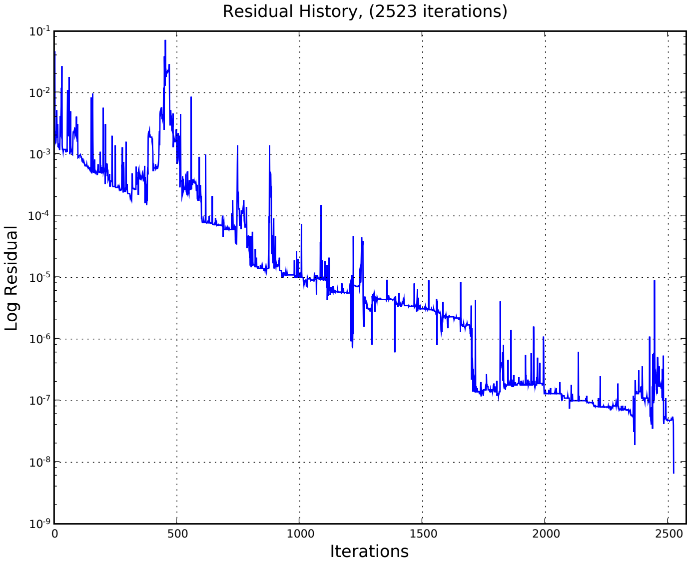
Numerical Results ($G = I$)

Problem III: Von Karmann "vortices"
Rectangular cavity, fixed circular obstacle

1. Mesh around obstacle, single fluid
   $n_A = 49,690$, $m_B = 6,336$, $LBL^T \approx 1.46s$, $\text{nnz}(L) \approx 424,618$
2. Mesh around obstacle, two immiscible fluids
   $n_A = 86,685$, $m_B = 7,345$, $LBL^T \approx 2.78s$, $\text{nnz}(L) \approx 523,249$
3. Fictitious domains, two immiscible fluids
   $n_A = 87,196$, $m_B = 7,579$, $LBL^T \approx 3.97s$, $\text{nnz}(L) \approx 587,336$

Instance	nnz(A)	nnz(B)	Matvecs	Rel. Res.	Time (s)
1	1,094,691	408,039	416	1.6e−07	11.73
2	2,069,305	507,380	131	1.9e−07	6.28
3	2,084,752	512,015	119	3.8e−08	5.78

Typical Evolution of Residual



Next Steps

- Populate Projected Krylov Library,
- Evaluate various preconditioners,
- When $G \neq I$,

$$\omega_k = \frac{P_I(s_k)^T A\bar{s}_k}{\|P_I(A\bar{s}_k)\|_2^2} \approx \frac{P_G(s_k)^T A\bar{s}_k}{\|P_G(A\bar{s}_k)\|_2^2},$$

- Inexact projections (iteratively, inexact / incomplete B).

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That's all Folks!

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