Iterative linear solvers for PDE-constrained optimization involving fluid flow

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joint work with
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Let $\boldsymbol{A} \in \mathbb{R}^{\boldsymbol{n} \times \boldsymbol{n}}$ be symmetric and positive definite

$$\min_{\boldsymbol{x}} \ \frac{1}{2}\boldsymbol{x}^T \boldsymbol{A} \boldsymbol{x} - \boldsymbol{x}^T \boldsymbol{b}$$

equivalent to solving

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

Constrained Optimization and Saddle-point problems:

$$\min_x \; \frac{1}{2}x^T A x - x^T b$$

subject to $Bx = c$

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Lagrangian: $\mathcal{L}(x, \lambda) = \frac{1}{2}x^T A x - x^T b + (Bx - c)^T \lambda$

λ : Lagrange multipliers.

$$\begin{array}{lll} \min_x & \Rightarrow & Ax + B^\star \lambda = b \\ \max_\lambda & \Rightarrow & Bx = c \end{array}$$

$$\Rightarrow \begin{bmatrix} A & B^T \\ B & 0 \end{bmatrix} \begin{bmatrix} x \\ \lambda \end{bmatrix} = \begin{bmatrix} b \\ c \end{bmatrix}$$

(*Benzi, Golub & Liesen (2005)*)

Classic problem of this type: the Stokes problem

'Minimise energy subject to conserving mass' $\Rightarrow$

$$\begin{aligned} -\nabla^2 \vec{\mathbf{y}} + \nabla \mathbf{p} &= \mathbf{u} \\ \text{subject to} \qquad \nabla \cdot \vec{\mathbf{y}} &= \mathbf{0} \end{aligned}$$

$\vec{\mathbf{y}}$: velocity, $\quad \mathbf{p}$: pressure, $\quad \mathbf{u}$: body forces

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$\vec{\mathbf{y}}$: velocity, $\mathbf{p}$: pressure, $\mathbf{u}$: body forces

Mixed finite elements/MAC finite difference approximation:

$$\begin{bmatrix} \underline{\boldsymbol{K}} & \boldsymbol{B}^{\boldsymbol{T}} \\ \boldsymbol{B} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \boldsymbol{y} \\ \boldsymbol{p} \end{bmatrix} = \begin{bmatrix} \boldsymbol{u} \\ \boldsymbol{g} \end{bmatrix}, \quad \underline{\boldsymbol{K}} = \begin{bmatrix} \boldsymbol{K} & \mathbf{0} \\ \mathbf{0} & \boldsymbol{K} \end{bmatrix} \quad \text{in } \mathbb{R}^{\mathbf{2}}$$

$\boldsymbol{K}$: discrete Laplacian

$$\left[\begin{array}{cc} \underline{\boldsymbol{K}} & \boldsymbol{B}^T \\ \boldsymbol{B} & \mathbf{0} \end{array}\right]$$

is symmetric indefinite $\rightarrow$ MINRES Krylov subspace iterative solver (*Paige & Saunders (1975)*)

Preconditioning?

$$\left[\begin{array}{cc} \underline{\boldsymbol{K}} & \boldsymbol{B}^{\boldsymbol{T}} \\ \boldsymbol{B} & \mathbf{0} \end{array}\right]$$

is symmetric indefinite $\rightarrow$ MINRES Krylov subspace iterative solver (*Paige & Saunders (1975)*)

Preconditioning?

Block diagonal/triangular preconditioners

Block diagonal/triangular preconditioners:

based on observation (*Murphy, Golub & W (2000), Korzak(1999)*)

$$\begin{bmatrix} A & B^T \\ B & 0 \end{bmatrix}$$

preconditioned by

- $\begin{bmatrix} A & 0 \\ 0 & S \end{bmatrix}$ has 3 distinct eigenvalues $\quad (1, \frac{1}{2} \pm \frac{\sqrt{5}}{2})$
- $\begin{bmatrix} A & B^T \\ 0 & S \end{bmatrix}$ has 2 distinct eigenvalues

where $S = BA^{-1}B^T$ (Schur Complement)

$\Rightarrow$ MINRES /GMRES terminates in 3 / 2 iterations

$\Rightarrow$ want approximations $\widehat{A},\ \widehat{S} \Rightarrow$ 3 / 2 clusters

$\Rightarrow$ fast convergence

For Stokes problem:

$\boldsymbol{A} = \underline{\boldsymbol{K}}$ is discrete Laplacians: use $\widehat{\boldsymbol{A}} =$multigrid cycles

- geometric mutigrid: relaxed Jacobi smoothing, standard grid transfers
- algebraic multigrid: `HSL` routine `HSL_MI20` *(Boyle, Mihajlovic & Scott (2007))*

$\widehat{S}$ for Stokes problem:

Babuska-Brezzi stability $\Rightarrow$ Schur Complement spectrally equivalent to the finite element identity matrix, the mass matrix, M ie. the Gram matrix of the finite element basis functions $\{\phi_j, j = 1, \ldots, n\}$ in $L_2(\Omega), \Omega \subset \mathbb{R}^d$:

$$BA^{-1}B^T \approx \nabla \cdot (\nabla^2)^{-1} \nabla \approx Id \rightarrow M$$

Specifically $\exists \gamma > 0, \Gamma \leq \sqrt{d}$ such that

$$\gamma \leq \frac{x^T BA^{-1}B^T x}{x^T M x} \leq \Gamma$$

$$\text{where} \qquad M = \{m_{i,j}\}, \quad m_{i,j} = \int_\Omega \phi_i \phi_j$$

(*Bank, Welfert & Yserentant ('90), Silvester & W ('94), Griffiths ('95)*)

Mass matrix is effectively preconditioned by its diagonal D=diag(M) *(W (1987))*

eg. for Q1 (bilinear) elements in 2-dimensions (rectangles)

eigenvalues of $D^{-1}M$ all in $[\mathbf{1/4, 9/4}]$

eg. for Q1 (trilinear) finite elements in 3-dimensions (bricks)

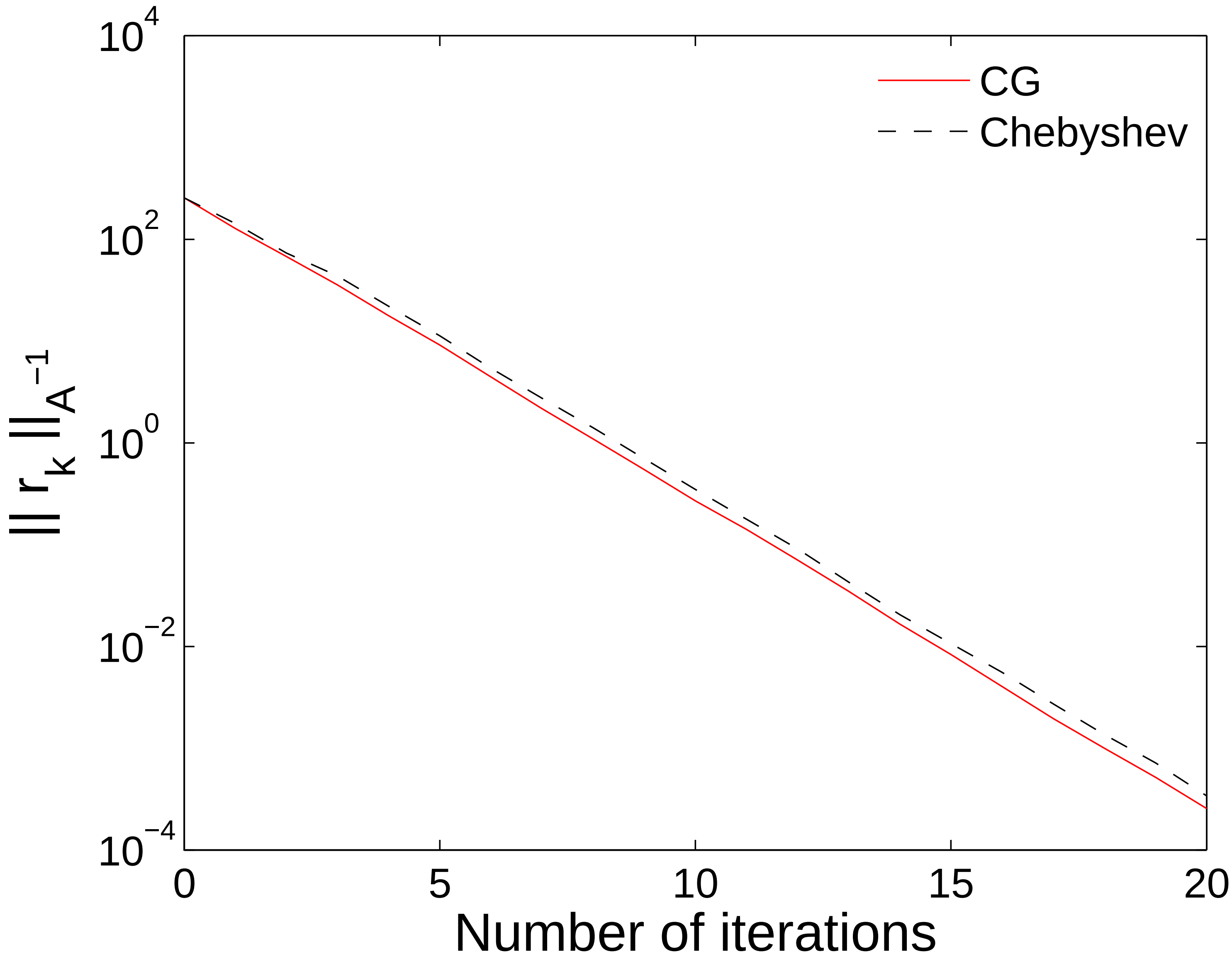
eigenvalues of $D^{-1}M$ all in $[\mathbf{1/8, 27/8}]$

independently of mesh size h (ie. independently of discrete problem dimension)

Could use $\widehat{S} = D$ but better a few iterations of a diagonally preconditioned iteration for M:

- diagonally scaled Conjugate Gradients: leads to a nonlinear preconditioner
- diagonally scaled Chebyshev (semi-)iteration: is linear and we have precise eigenvalue inclusion intervals

(*W & Rees (2008))*



10^4
10^2
10^0
10^{-2}
10^{-4}
$\| r_k \|_{A^{-1}}$
0
5
10
15
20
Number of iterations
CG
Chebyshev

For Stokes problem:

$$P = \begin{bmatrix} \widehat{A} & 0 \\ 0 & \widehat{S} \end{bmatrix} = \begin{bmatrix} A_{AMG} & 0 \\ 0 & T_{20}(D^{-1}M) \end{bmatrix}$$

Here: Q2-Q1 mixed finite element (Taylor-Hood),
$\widehat{A} = A_{AMG}$: 1 AMG V-cycle

h	Iterations	CPU time (s)
2^{-2} (187)	19	0.015
2^{-3} (659)	24	0.073
2^{-4} (2,467)	26	0.082
2^{-5} (9,539)	28	0.21
2^{-6} (37,507)	29	3.80
2^{-7} (148,739)	29	15.5

PDE-constrained Optimization

General problem:

Given $\Omega \subset \mathbb{R}^2$ or $\mathbb{R}^3$, $\widehat{y} \in L_2(\Omega)$ as some desired state then for some (regularisation) parameter β

$$\min_{y,u} \; \frac{1}{2}\|y - \widehat{y}\|^2_{L_2(\Omega)} + \frac{\beta}{2}\|u\|^2_{L_2(\Omega)}$$

subject to

$$\mathcal{L}y = u \quad \text{in } \; \Omega, \qquad y = \widehat{y} \quad \text{on } \; \partial\Omega$$

where $\mathcal{L}$ represents a partial differential operator can also include simple bounds on the control:

$$\underline{\mathbf{u}} \leq \mathbf{u} \leq \overline{\mathbf{u}}$$

and even bounds on the state (via Moreau-Yoshida regulrization)

$$\underline{\mathbf{y}} \leq \mathbf{y} \leq \overline{\mathbf{y}}$$

also boundary control...

Simple sample problem:

desirable $\widehat{\mathbf{y}}$, controlable body force $\mathbf{u}$

$$\min_{\mathbf{y},\mathbf{u}} \frac{1}{2}\|\mathbf{y}-\widehat{\mathbf{y}}\|^2_{L_2(\Omega)} + \frac{\beta}{2}\|\mathbf{u}\|^2_{L_2(\Omega)}$$

subject to

$$-\nabla^2 \mathbf{y} = \mathbf{u} \quad \text{in } \Omega, \qquad \mathbf{y} = \widehat{\mathbf{y}} \quad \text{on } \partial\Omega$$

$$\min_{\mathrm{y},\mathrm{u}} \frac{1}{2}\|\mathrm{y}-\widehat{\mathrm{y}}\|^2 + \frac{\beta}{2}\|\mathrm{u}\|^2$$

$$\text{subject to} \qquad -\nabla^2 \mathrm{y} = \mathrm{u} \quad \text{in } \Omega, \qquad \mathrm{y} = \widehat{\mathrm{y}} \quad \text{on } \partial\Omega$$

Discretisation: finite elements

$\mathrm{y}_h = \sum y_j \phi_j, \;\; y = (y_1, y_2, \ldots, y_n)^T$
$\mathrm{u}_h = \sum u_j \phi_j, \;\; u = (u_1, u_2, \ldots, u_n)^T$

$$\min_{y,u} \;\; \frac{1}{2} y^T M y + y^T b + \frac{\beta}{2} u^T M u$$

$$\text{subject to} \qquad K y = M u + d$$

$M = \{m_{i,j}\}, m_{i,j} = \int_\Omega \phi_i \phi_j$ — mass matrix

$K = \{k_{i,j}\}, k_{i,j} = \int_\Omega \nabla\phi_i \cdot \nabla\phi_j$ — stiffness matrix
as before

so, Lagrangian:

$$\frac{1}{2}\boldsymbol{y}^T M \boldsymbol{y} + \boldsymbol{y}^T \boldsymbol{b} + \frac{\beta}{2}\boldsymbol{u}^T M \boldsymbol{u} + \boldsymbol{\lambda}^T (K\boldsymbol{y} - M\boldsymbol{u} - \boldsymbol{d})$$

stationarity $\Rightarrow$ Saddle point system

$$\begin{bmatrix} M & 0 & K^T \\ 0 & \beta M & -M \\ K & -M & 0 \end{bmatrix} \begin{bmatrix} \boldsymbol{y} \\ \boldsymbol{u} \\ \boldsymbol{\lambda} \end{bmatrix} = \begin{bmatrix} -\boldsymbol{b} \\ 0 \\ \boldsymbol{d} \end{bmatrix}$$

$$\text{Note} \quad B = \begin{bmatrix} K & -M \end{bmatrix} \quad \text{and} \quad A = \begin{bmatrix} M & 0 \\ 0 & \beta M \end{bmatrix}$$

in usual saddle point form

$$\begin{bmatrix} A & B^T \\ B & 0 \end{bmatrix}$$

$$\textbf{Recall} \quad \boldsymbol{B} = \begin{bmatrix} \boldsymbol{K} & -\boldsymbol{M} \end{bmatrix} \quad \textbf{and} \quad \boldsymbol{A} = \begin{bmatrix} \boldsymbol{M} & \mathbf{0} \\ \mathbf{0} & \boldsymbol{\beta M} \end{bmatrix}$$

so $\widehat{\boldsymbol{S}}$? $\quad \boldsymbol{S = BA^{-1}B^T}$ (Schur Complement)

$$\begin{aligned} &= \begin{bmatrix} \boldsymbol{K} & -\boldsymbol{M} \end{bmatrix} \begin{bmatrix} \boldsymbol{M}^{-1} & \mathbf{0} \\ \mathbf{0} & \frac{1}{\boldsymbol{\beta}}\boldsymbol{M}^{-1} \end{bmatrix} \begin{bmatrix} \boldsymbol{K}^T \\ -\boldsymbol{M} \end{bmatrix} \\ &= \frac{1}{\boldsymbol{\beta}}\boldsymbol{M} + \boldsymbol{K M^{-1} K^T} \end{aligned}$$

Unless approx $\boldsymbol{\beta} < 10^{-6}$ dominant part is $\widehat{\boldsymbol{S}} = \boldsymbol{K M^{-1} K^T}$

Hence preconditioner for

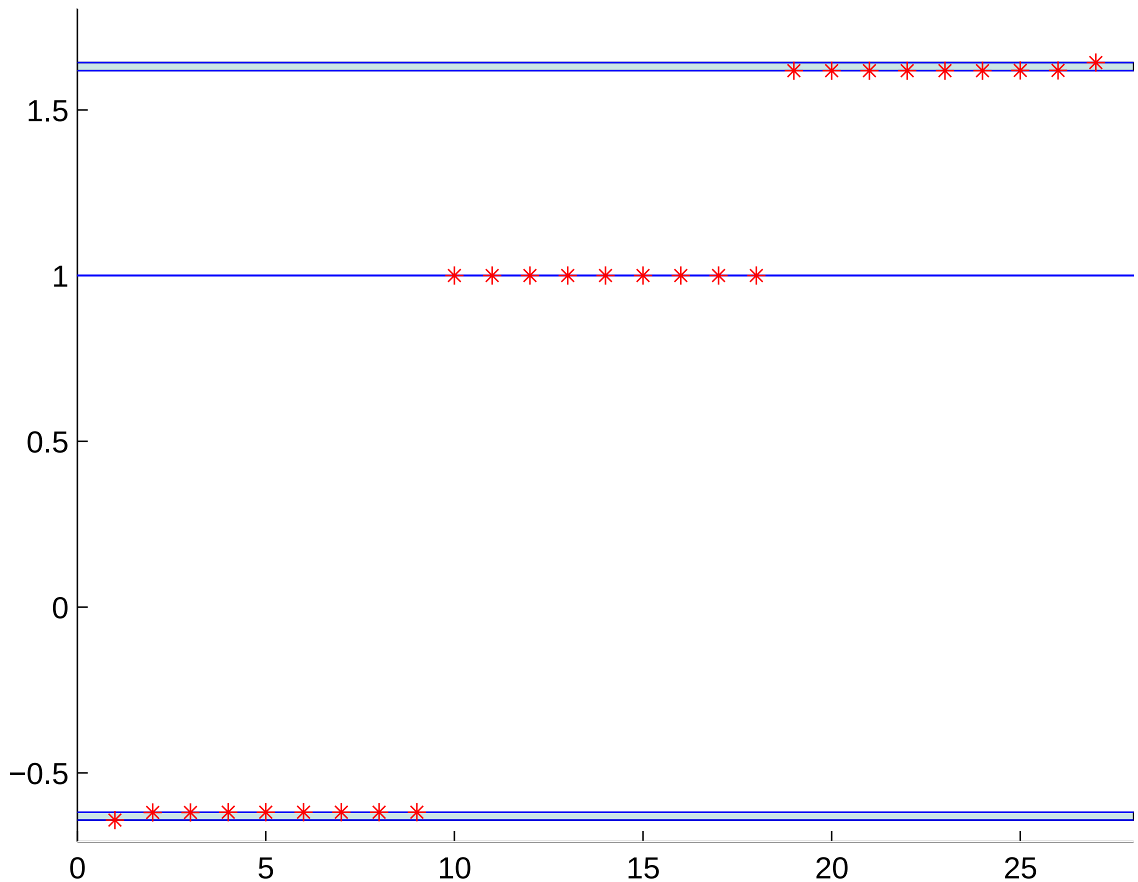
$$\mathcal{A} = \begin{bmatrix} M & 0 & K^T \\ 0 & \beta M & -M \\ K & -M & 0 \end{bmatrix} \text{ is } \mathcal{P} = \begin{bmatrix} M & 0 & 0 \\ 0 & \beta M & 0 \\ 0 & 0 & KM^{-1}K^T \end{bmatrix}$$

Eigenvalues ν of $\mathcal{P}^{-1}\mathcal{A}$

$$\begin{aligned} \nu &= 1, \\ \frac{1}{2}\left(1+\sqrt{5+\frac{2\alpha_1 h^4}{\beta}}\right) \leq \ \nu \ &\leq \frac{1}{2}\left(1+\sqrt{5+\frac{2\alpha_2}{\beta}}\right) \\ \text{or } \ \frac{1}{2}\left(1-\sqrt{5+\frac{2\alpha_2}{\beta}}\right) \leq \ \nu \ &\leq \frac{1}{2}\left(1-\sqrt{5+\frac{2\alpha_1 h^4}{\beta}}\right), \end{aligned}$$

where $\alpha_1, \ \alpha_2$ are positive constants independent of h.

$$\mathcal{P} = \begin{bmatrix} M & 0 & 0 \\ 0 & \beta M & 0 \\ 0 & 0 & KM^{-1}K^T \end{bmatrix}, \quad \beta = 10^{-2}$$



But

$$\mathcal{P} = \begin{bmatrix} M & 0 & 0 \\ 0 & \beta M & 0 \\ 0 & 0 & KM^{-1}K^T \end{bmatrix}$$

still expensive to use in practice so employ approximations

$$\widehat{M} \simeq M \quad \text{and} \quad \widehat{K} \simeq K$$

giving

$$\mathcal{P} = \begin{bmatrix} \widehat{M} & 0 & 0 \\ 0 & \beta\widehat{M} & 0 \\ 0 & 0 & \widehat{K}M^{-1}\widehat{K^T} \end{bmatrix} = \begin{bmatrix} \widehat{A} & 0 \\ 0 & \widehat{S} \end{bmatrix}$$

Important subtlety:

$$\widehat{\boldsymbol{K}} \simeq \boldsymbol{K}$$

does *not* imply that

$$\widehat{\boldsymbol{K}} M^{-1} \widehat{\boldsymbol{K}^{\boldsymbol{T}}} \simeq \boldsymbol{K} M^{-1} \boldsymbol{K}^{\boldsymbol{T}}$$

or indeed that

$$\widehat{\boldsymbol{K}} \widehat{\boldsymbol{K}^{\boldsymbol{T}}} \simeq \boldsymbol{K} \boldsymbol{K}^{\boldsymbol{T}}$$

without further conditions which are satisfied in this case
(Braess & Peisker (1986))

$$\mathcal{P} = \begin{bmatrix} \widehat{M} & 0 & 0 \\ 0 & \beta\widehat{M} & 0 \\ 0 & 0 & \widehat{K}M^{-1}\widehat{K^T} \end{bmatrix} = \begin{bmatrix} \widehat{A} & 0 \\ 0 & \widehat{S} \end{bmatrix}$$

so $\widehat{M}$?: $T_{20}(D^{-1}M)$ as before

For $\mathcal{L} = -\nabla^2$, K is a discrete Laplacian: use multigrid cycles as before

In our examples:

$\widehat{K}$ is the action of 2 V-cycles

$\widehat{M}$ is the action of 20 Chebyshev semi-iterative steps

Example problem: $\Omega = [0,1]^d, d = 2,3$

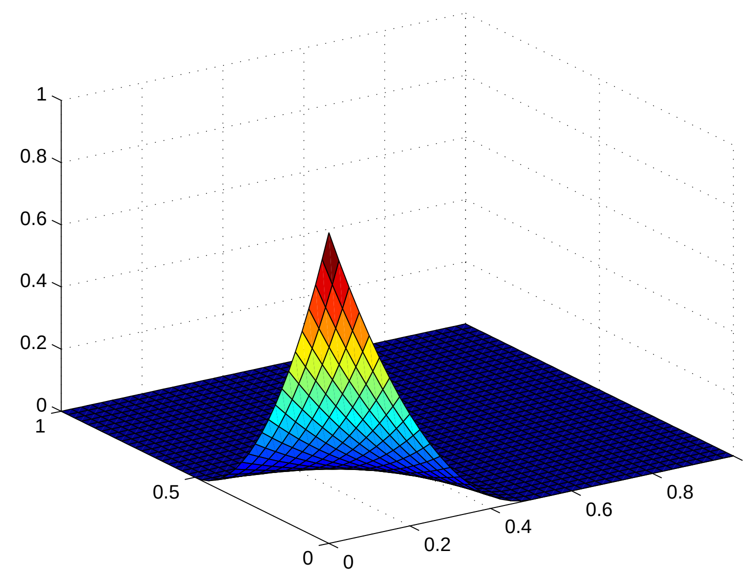
$$\min_{\mathbf{y},\mathbf{u}} \frac{1}{2}\|\mathbf{y} - \widehat{\mathbf{y}}\|^2_{L_2(\Omega)} + \frac{\beta}{2}\|\mathbf{u}\|^2_{L_2(\Omega)}$$

subject to

$$-\nabla^2 \mathbf{y} = \mathbf{u} \quad \text{in } \Omega, \qquad \mathbf{y} = \widehat{\mathbf{y}} \quad \text{on } \partial\Omega$$

Q1 (bilinear) finite elements, $\beta = 10^{-2}$

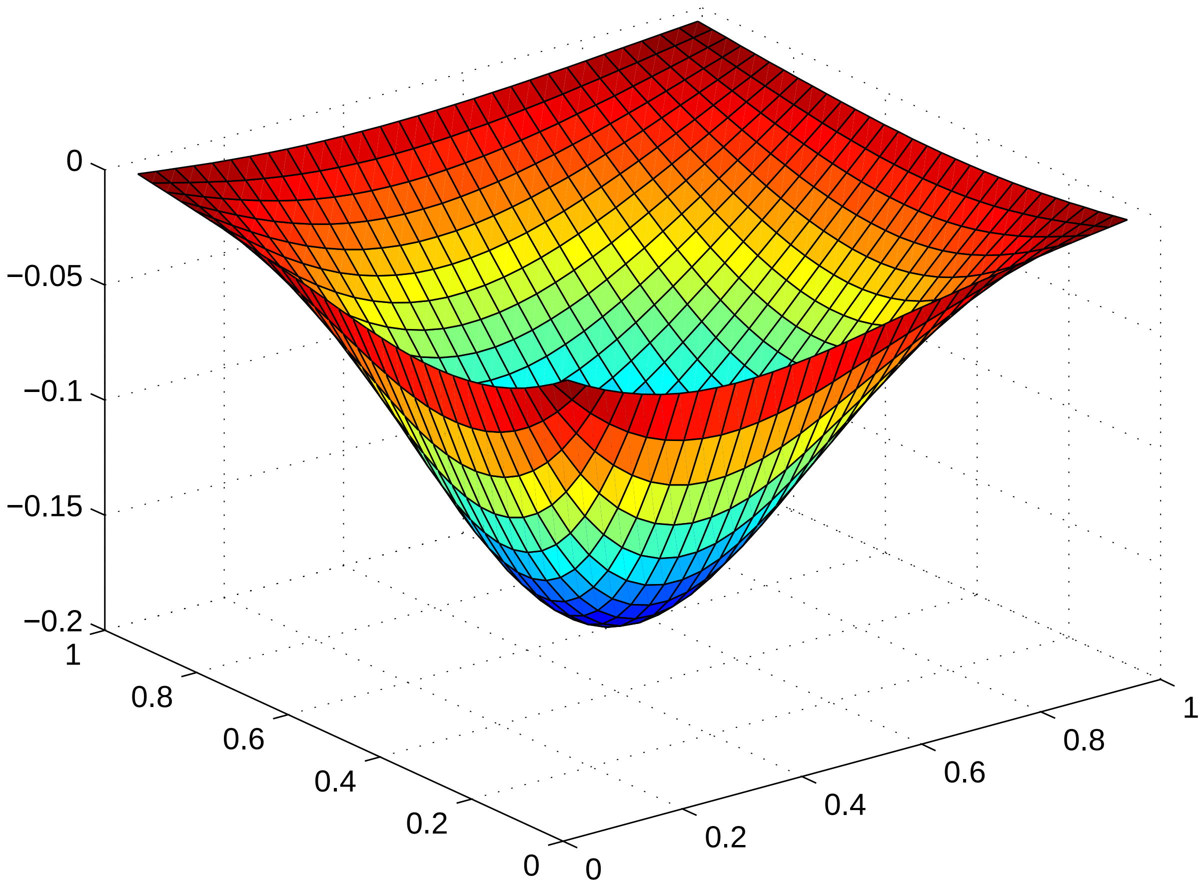
$\widehat{\mathbf{y}}$:



CPU times (MINRES iterations) in 2D, tol 10^{-6}

h	3n	backslash	MINRES ($\mathcal{P}_{AMG}$)	MINRES ($\mathcal{P}_{MG}$)
2^{-2}	27	0.0003	0.02 (7)	0.13 (7)
2^{-3}	147	0.002	0.03 (9)	0.16 (9)
2^{-4}	675	0.01	0.05 (9)	0.21 (9)
2^{-5}	2883	0.08	0.14 (9)	0.41 (9)
2^{-6}	11907	0.46	0.61 (9)	1.29 (9)
2^{-7}	48387	3.10	2.61 (9)	5.09 (9)
2^{-8}	195075	15.5	15.0 (11)	23.6 (9)
2^{-9}	783363	—	75.6 (11)	136 (9)

Control:



CPU times (MINRES iterations) in 3D, tol 10^{-6}

h	3n	backslash	MINRES ($\mathcal{P}_{AMG}$)	MINRES ($\mathcal{P}_{MG}$)
2^{-2}	81	0.001	0.02 (7)	0.14 (8)
2^{-3}	1029	0.013	0.13 (9)	0.26 (8)
2^{-4}	10125	25.1	1.89 (8)	1.69 (8)
2^{-5}	89373	—	22.1 (8)	15.9 (8)
2^{-6}	750141	—	—	230 (10)

Stokes Control

$$\min_{\mathbf{y},\mathbf{p},\mathbf{u}} \frac{1}{2}\|\vec{\mathbf{y}} - \hat{\mathbf{y}}\|^2_{L^2(\Omega)} + \frac{1}{2}\|\mathbf{p} - \hat{\mathbf{p}}\|^2_{L^2(\Omega)} + \frac{\beta}{2}\|\mathbf{u}\|^2_{L^2(\Omega)}$$

$$\text{subject to} \qquad \begin{aligned} -\nabla^2\vec{\mathbf{y}} + \nabla\mathbf{p} &= \mathbf{u} \\ \nabla\cdot\vec{\mathbf{y}} &= 0 \end{aligned}$$

$\vec{\mathbf{y}}$: velocity, $\mathbf{p}$: pressure.

Mixed finite elements for (forward) Stokes problem:

$$\begin{bmatrix} \underline{K} & B^T \\ B & 0 \end{bmatrix} \begin{bmatrix} y \\ p \end{bmatrix} = \begin{bmatrix} u \\ g \end{bmatrix}, \ \underline{K} = \begin{bmatrix} K & 0 \\ 0 & K \end{bmatrix} \quad \text{in } \mathbb{R}^2$$

Cost functional

$$\frac{1}{2}\boldsymbol{y}^T\boldsymbol{M_y}\boldsymbol{y} - \boldsymbol{y}^T\boldsymbol{b} + \frac{1}{2}\boldsymbol{p}^T\boldsymbol{M_p}\boldsymbol{p} - \boldsymbol{p}^T\boldsymbol{d} + \frac{\boldsymbol{\beta}}{2}\boldsymbol{u}^T\boldsymbol{M_u}\boldsymbol{u}$$

combined with constraint via the Lagrangian $\Rightarrow$

$$\begin{bmatrix} \boldsymbol{M_y} & \mathbf{0} & \mathbf{0} & \underline{\boldsymbol{K}} & \boldsymbol{B}^T \\ \mathbf{0} & \boldsymbol{M_p} & \mathbf{0} & \boldsymbol{B} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \boldsymbol{\beta M_u} & -\boldsymbol{M_u} & \mathbf{0} \\ \underline{\boldsymbol{K}} & \boldsymbol{B}^T & -\boldsymbol{M_u} & \mathbf{0} & \mathbf{0} \\ \boldsymbol{B} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \boldsymbol{y} \\ \boldsymbol{p} \\ \boldsymbol{u} \\ \boldsymbol{\lambda} \\ \boldsymbol{\mu} \end{bmatrix} = \begin{bmatrix} \boldsymbol{b} \\ \boldsymbol{d} \\ \mathbf{0} \\ \boldsymbol{h} \\ \boldsymbol{k} \end{bmatrix}.$$

Schur Complement:

$$\left[\begin{array}{cc} \frac{\boldsymbol{K}}{\boldsymbol{B}} & \boldsymbol{B}^{\boldsymbol{T}} \\ & \boldsymbol{0} \end{array} \right] \left[\begin{array}{cc} \boldsymbol{M}_{\boldsymbol{y}}^{-1} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{M}_{\boldsymbol{p}}^{-1} \end{array} \right] \left[\begin{array}{cc} \frac{\boldsymbol{K}}{\boldsymbol{B}} & \boldsymbol{B}^{\boldsymbol{T}} \\ & \boldsymbol{0} \end{array} \right] + \frac{\boldsymbol{1}}{\boldsymbol{\beta}} \boldsymbol{M}_{\boldsymbol{u}}$$

and again ignore 2nd term for moderate $\boldsymbol{\beta}$

So overall block diagonal preconditioner requires:

$\widehat{\boldsymbol{M}_{\boldsymbol{y}}}, \widehat{\boldsymbol{M}_{\boldsymbol{p}}}, \widehat{\boldsymbol{M}_{\boldsymbol{u}}} \rightarrow$ Chebyshev

and 2 Stokes approximations

Stokes preconditioners:

$$\widehat{\begin{bmatrix} \underline{\boldsymbol{K}} & \boldsymbol{B}^T \\ \boldsymbol{B} & \boldsymbol{0} \end{bmatrix}} = \begin{bmatrix} \widehat{\underline{\boldsymbol{K}}} & \boldsymbol{0} \\ \boldsymbol{B} & \widehat{\boldsymbol{M}_p} \end{bmatrix}$$

and

$$\widehat{\begin{bmatrix} \underline{\boldsymbol{K}} & \boldsymbol{B}^T \\ \boldsymbol{B} & \boldsymbol{0} \end{bmatrix}} = \begin{bmatrix} \widehat{\underline{\boldsymbol{K}}} & \boldsymbol{B}^T \\ \boldsymbol{0} & \widehat{\boldsymbol{M}_p} \end{bmatrix}$$

on left and right respectively where $\widehat{\underline{\boldsymbol{K}}}$ is multigrid cycles for each discrete scalar Laplacian as before (*Silvester & W (1993), Klawonn (1998)*)

Gives symmetric Schur complement approximation

Here: Q2-Q1 mixed finite elements for cavity flow

4 AMG V-cycles to approx each $\boldsymbol{K}$

20 Chebyshev semi-iterations for each $\boldsymbol{M}$

$\boldsymbol{h}$	Iterations	CPU time (s)
$\mathbf{2^{-2}}$ (344)	26	0.48
$\mathbf{2^{-3}}$ (1,512)	31	1.05
$\mathbf{2^{-4}}$ (6,344)	33	3.69
$\mathbf{2^{-5}}$ (25,992)	33	18.0
$\mathbf{2^{-6}}$ (105,224)	34	84.2
$\mathbf{2^{-7}}$ (423,432)	34	342

recall: 29 MINRES iterations for forward Stokes solve (but only 1 AMG V-cycle) $\Rightarrow$ approx 10 times more work to solve the control problem than a single PDE solve.

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