Introduction to Saddle Point Problems

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Motivation and goals

Let A be a real, symmetric, $n \times n$ matrix and let $f \in \mathbf{R}^n$ be given.

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Let $\langle \cdot, \cdot \rangle$ denote the standard inner product in \mathbf{R}^n .

Consider the following two problems:

Obve Au = f
Minimize the function J(u) = ¹/₂ ⟨Au, u⟩ − ⟨f, u⟩

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Consider the following two problems:

Note that $\nabla J(u) = Au - f$. Hence, if A is positive definite (SPD), the two problems are equivalent, and there exists a unique solution $u^* = A^{-1}f$.

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Many algorithms exist for solving SPD linear systems: Cholesky, Preconditioned Conjugate Gradients, AMG, etc.

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Minimize J(u) = \frac{1}{2} \langle Au, u \rangle - \langle f, u \rangle
subject to Bu = g
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where

- A is $n \times n$, symmetric
- B is $m \times n$, with m < n
- $f \in \mathbf{R}^n$, $g \in \mathbf{R}^m$ are given (either f or g could be 0, but not both)

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Standard approach: Introduce Lagrange multipliers, $p \in \mathbf{R}^m$

• Lagrangian
$$\mathcal{L}(u, p) = \frac{1}{2} \langle Au, u \rangle - \langle f, u \rangle + \langle p, Bu - g \rangle$$

• First-order optimality conditions: $\nabla_u \mathcal{L} = 0$, $\nabla_p \mathcal{L} = 0$

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System (1) is a saddle point problem. Its solutions (u^*, p^*) are saddle points for the Lagrangian $\mathcal{L}(u, p)$:

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Also called a KKT system (Karush-Kuhn-Tucker), or equilibrium equations.

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Gil Strang calls (1) "the fundamental problem of scientific computing."

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- Linear elasticity
- Mixed FEM formulations of 2nd- and 4th-order elliptic PDEs
- PDE-constrained optimization (e.g., variational data assimilation)

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- SQP and IP methods for nonlinear constrained optimization
- Structural analysis
- Resistive networks, power network analysis
- Image processing (e.g., image registration)

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The bibliography in this paper contains 535 items.

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Google Scholar reports over 700 citations to date.

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The emphasis of this lecture (and the next) will be on iterative solvers for large, sparse saddle point problems, with a focus on our own recent work on preconditioners for incompressible flow problems.

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The ultimate goal: to develop robust preconditioners that perform uniformly well independently of discretization details and problem parameters.

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For flow problems, we would like to have solvers that converge fast regardless of mesh size, viscosity, etc. Moreover, the cost per iteration should be linear in the number of unknowns.



Properties of saddle point matrices







2 Examples of saddle point problems











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The following result establishes necessary and sufficient conditions for the unique solvability of the saddle point problem (1).

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Then the coefficient matrix

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In particular, A is invertible if A is SPD and B has full rank ("standard case").

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Generalizations, I

In some cases, a stabilization (or regularization) term needs to be added in the (2,2) position, leading to linear systems of the form

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$$\begin{pmatrix} A & B^{\mathsf{T}} \\ B & -\beta C \end{pmatrix} \begin{pmatrix} u \\ p \end{pmatrix} = \begin{pmatrix} f \\ g \end{pmatrix}$$
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where $\beta > 0$ is a small parameter and the $m \times m$ matrix C is symmetric positive semidefinite, and often singular, with $\|C\|_2 = 1$.

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Another important example is the discretization of the Reissner–Mindlin plate model in linear elasticity. In this case β is related to the thickness of the plate; the limit case $\beta = 0$ can be seen as a reformulation of the biharmonic problem.

In other cases, the matrix A is not symmetric: $A \neq A^T$. In this case, the saddle point system does not arise from a constrained minimization problem.

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The most important examples of this case are linear systems arising from the Picard and Newton linearizations of the steady incompressible Navier–Stokes equations. The following result is applicable to the Picard linearization (Oseen problem):

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Theorem. Assume that

- $H = \frac{1}{2}(A + A^T)$ is symmetric positive semidefinite $n \times n$
- B has full rank: rank (B) = m

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Theorem. Assume that

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Then

- $\operatorname{Null}(H) \cap \operatorname{Null}(B) = \{0\} \Rightarrow \mathcal{A} \text{ invertible}$
- \mathcal{A} invertible \Rightarrow Null $(\mathcal{A}) \cap$ Null $(\mathcal{B}) = \{0\}$.

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$$\left(\begin{array}{cc}A & B^{T} \\ -B & O\end{array}\right)\left(\begin{array}{c}u \\ p\end{array}\right) = \left(\begin{array}{c}f \\ -g\end{array}\right)$$

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Theorem. Assume *B* has full rank. If $H = \frac{1}{2}(A + A^T)$ is positive definite, then the spectrum of

$$\mathcal{A}_{-} := \left(\begin{array}{cc} A & B^{\mathsf{T}} \\ -B & O \end{array} \right)$$

lies entirely in the open right-half plane Re(z) > 0. Moreover, if A is SPD and the following condition holds:

 $\lambda_{\min}(A) > 4 \lambda_{\max}(S)$ where $S = BA^{-1}B^T$ ("Schur complement"),

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then \mathcal{A}_{-} is diagonalizable with real positive eigenvalues. In this case, there exists a non-standard inner product on \mathbf{R}^{n+m} in which \mathcal{A}_{-} is self-adjoint and positive definite, and a corresponding conjugate gradient method (B./Simoncini, NM 2006).

Outline



2 Examples of saddle point problems





Let Ω be a domain in \mathbf{R}^d and consider the system



Let Ω be a domain in \mathbf{R}^d and consider the system

 $\mathbf{u} - \nabla p = \mathbf{f}$ in Ω ,

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Let Ω be a domain in \mathbf{R}^d and consider the system

$$\mathbf{u} - \nabla p = \mathbf{f}$$
 in Ω ,

$$\operatorname{div} \mathbf{u} = g \quad \text{in } \Omega,$$

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Let Ω be a domain in \mathbf{R}^d and consider the system

Let Ω be a domain in ${\boldsymbol{\mathsf{R}}}^d$ and consider the system

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\begin{split} \mathbf{u} - \nabla p &= \mathbf{f} \quad \text{in } \Omega, \\ & \text{div } \mathbf{u} = g \quad \text{in } \Omega, \\ & \mathbf{u} \cdot \mathbf{n} = 0 \quad \text{on } \partial \Omega. \end{split}
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Eliminating the vector field \mathbf{u} , the scalar field p must satisfy

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$$\mathbf{u} - \nabla \boldsymbol{p} = \mathbf{f} \quad \text{in } \Omega,$$
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Eliminating the vector field \mathbf{u} , the scalar field p must satisfy

$$-\Delta p = \operatorname{div} \mathbf{f} - g$$
 in Ω , $\frac{\partial p}{\partial \mathbf{n}} = -\mathbf{f} \cdot \mathbf{n}$ on $\partial \Omega$.

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Weak formulation: Find $(\mathbf{u}, p) \in (L^2(\Omega))^d \times H^1(\Omega) \cap L^2_0(\Omega)$ such that

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$$\langle \mathbf{u}, \mathbf{v} \rangle - \langle \nabla p, \mathbf{v} \rangle = \langle \mathbf{f}, \mathbf{v} \rangle, \quad \mathbf{v} \in (L^2(\Omega))^d,$$

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abla q
angle = \langle g,q
angle, \quad q\in H^1(\Omega)\cap L^2_0(\Omega), \end{aligned}$$

where $\langle\cdot,\cdot\rangle$ denotes the L^2 inner product.

Discretization using LBB-stable finite element pairs leads to an algebraic saddle point problem:

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Discretization using LBB-stable finite element pairs leads to an algebraic saddle point problem:

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Here M is a mass matrix, B the discrete divergence, and B^{T} the discrete (negative) gradient.

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- The convergence rate is independent of discretization parameters
- The cost of each iteration is linear in the number of unknowns

Let Ω be a domain in \mathbf{R}^d and let $\alpha \geq 0$, $\nu > 0$. Consider the system

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 $\alpha \mathbf{u} - \nu \Delta \mathbf{u} + \nabla p = \mathbf{f} \quad \text{in } \ \Omega,$

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 ${\rm div}\, {\boldsymbol u}=0 \quad {\rm in} \ \Omega,$

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Weak formulation: Find $(\mathbf{u}, p) \in (H_0^1(\Omega))^d \times L_0^2(\Omega)$ such that

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angle = \langle \mathbf{f}, \mathbf{v}
angle, \quad \mathbf{v} \in \left(H_0^1(\Omega)\right)^d, \ &\langle q, \operatorname{div} \mathbf{u}
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The standard Stokes problem is obtained for $\alpha = 0$ (steady case). In this case we can assume $\nu = 1$.

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Introduction to Saddle Point Problems Examples of saddle point problems

Example 2: the generalized Stokes problem (cont.)

Discretization using LBB-stable finite element pairs or other div-stable scheme leads to an algebraic saddle point problem:

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If an unstable FEM pair is used, then a regularization term $-\beta C$ is added in the (2,2) block of A. The specific choice of β and C depends on the particular discretization used.

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If an unstable FEM pair is used, then a regularization term $-\beta C$ is added in the (2,2) block of A. The specific choice of β and C depends on the particular discretization used.

Robust, optimal solvers have been developed for this problem: Cahouet–Chabard for $\alpha > 0$; Silvester–Wathen for $\alpha = 0$. Introduction to Saddle Point Problems Examples of saddle point problems

Sparsity pattern: 2D stokes (Q1-P0)



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Introduction to Saddle Point Problems Examples of saddle point problems

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Let Ω be a domain in \mathbf{R}^d and let $\alpha \ge 0$ and $\nu > 0$. Also, let \mathbf{w} be a divergence-free vector field on Ω . Consider the system

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 $\mathbf{u}=\mathbf{0}\quad\text{on }\partial\Omega.$

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Note that for $\mathbf{w} = \mathbf{0}$ we recover the generalized Stokes problem.

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The standard Oseen problem is obtained for $\alpha = 0$ (steady case).

Introduction to Saddle Point Problems Examples of saddle point problems

Example 3: the generalized Oseen problem (cont.)

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Now A is a discrete reaction-convection-diffusion operator. For $\alpha = 0$, A is just a discrete vector convection-diffusion operator. Note that now $A \neq A^T$.

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The Oseen problem arises from Picard iteration applied to the steady incompressible Navier–Stokes equations, and from fully implicit schemes applied to the unsteady NSE. The 'wind' \mathbf{w} represents an approximation of the solution \mathbf{u} obtained from the previous Picard step, or from time-lagging.

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As we will see, this problem can be very challenging to solve, especially for small values of the viscosity ν and on stretched meshes.

Eigenvalues of discrete Oseen problem ($\nu = 0.01$), indefinite form

Eigenvalues of Oseen matrix
$$\mathcal{A} = \begin{pmatrix} A & B^T \\ B & O \end{pmatrix}$$
, MAC discretization.



Note the different scales in the x and y axes.

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Eigenvalues of discrete Oseen problem ($\nu = 0.01$), positive definite form

Eigenvalues of Oseen matrix
$$A_{-} = \begin{pmatrix} A & B^{T} \\ -B & O \end{pmatrix}$$
, MAC discretization.



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2 Examples of saddle point problems

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Version Strain Strai

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Two main classes of solvers exist:

- $\textcircled{O} \text{ Direct methods: based on factorization of } \mathcal{A}$
 - High-quality software exists (Duff et al.; Demmel et al.)
 - Quite popular in some areas
 - Stability issues (indefiniteness)
 - Large amounts of fill-in
 - Not feasible for 3D problems
 - Difficult to parallelize

Version Strain Strai

- Appropriate for large, sparse problems
- Tend to converge slowly
- Number of iterations increases as problem size grows
- Effective preconditioners a must

Much effort has been put into developing preconditioners, with optimality and robustness w.r.t. parameters as the ultimate goals. Parallelizability also needs to be taken into account.

Preconditioners

 $\mbox{Preconditioning:}$ Find an invertible matrix ${\cal P}$ such that Krylov methods applied to the preconditioned system

$$\mathcal{P}^{-1}\mathcal{A}\,\mathbf{x}=\mathcal{P}^{-1}\mathbf{b}$$

will converge rapidly (possibly, independently of the discretization parameter h).

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To be effective, a preconditioner must significantly reduce the total amount of work:

- \bullet Setting up ${\mathcal P}$ must be inexpensive
- Evaluating $\mathbf{z} = \mathcal{P}^{-1}\mathbf{r}$ must be inexpensive
- Convergence must be rapid

Introduction to Saddle Point Problems Some solution algorithms

Preconditioners

Options include:

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Introduction to Saddle Point Problems Some solution algorithms

Preconditioners

Options include:

ILU preconditioners

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Options include:

- ILU preconditioners
- Oupled multigrid methods (geometric and algebraic; Vanka-type)

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Schur complement-based methods ('segregated' approach)

Options include:

- ILU preconditioners
- Oupled multigrid methods (geometric and algebraic; Vanka-type)

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 - Block diagonal preconditioning

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- ILU preconditioners
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- Schur complement-based methods ('segregated' approach)
 - Block diagonal preconditioning
 - Block triangular preconditioning (Elman, Silvester, Wathen et al.)

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Augmented Lagrangian-based techniques (AL)

The choice of an appropriate preconditioner is highly problem-dependent.

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where \widehat{A}^{-1} is given by a multigrid V-cycle applied to linear systems with coefficient matrix A and \widehat{M}_p is the diagonal of the pressure mass matrix.

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- \bullet MINRES preconditioned with $\mathcal P$ converges at a rate independent of the mesh size h
- Each preconditioned MINRES iteration costs O(n + m) flops
- Efficient parallelization is possible

Example: Silvester-Wathen preconditioner

Number of MINRES iterations needed for 10^{-6} reduction in residual for locally stabilized Q1 - P0 mixed finite elements for Stokes flow in a cavity. Block diagonal preconditioner: \hat{A} is one multigrid V-cycle with 1,1 relaxed Jacobi smoothing and \hat{M}_p is the diagonal pressure mass matrix. The cpu time (in seconds) is on a Sun sparcv9 502 MHz processor with 1024 Mb of memory. The cpu time is also given for a sparse direct solve (UMFPACK in MATLAB).

grid	n	т	iterations	cpu time	sparse direct cpu
64×64	8450	4096	38	14.3	6.8
128 imes 128	33282	16384	37	37.7	48.0
256 imes256	132098	65536	36	194.6	897
512 imes 512	526339	263169	35	6903	out of memory

Note: the lack of scalability for finer meshes is caused by memory management issues.

But what about more difficult problems?

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- The spectrum of $\mathcal{P}_{\mathcal{T}}^{-1}\mathcal{A}$ is $\sigma(\mathcal{P}_{\mathcal{T}}^{-1}\mathcal{A}) = \{1\}$
- GMRES converges in three iterations with \mathcal{P}_D , and in two iterations with \mathcal{P}_T .

In practice, it is necessary to replace A and S with easily invertible approximations:

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Â should be spectrally equivalent to A: that is, we want cond(Â⁻¹A) ≤ c for some constant c independent of h

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- For the Oseen problem this does not work, except for very small Reynolds.

Recall that $S = -BA^{-1}B^T$ is a discretization of the operator

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A plausible (if non-rigorous) approximation of the inverse of this operator is

$$\widehat{\mathcal{S}}^{-1} := \Delta^{-1} (-\nu \Delta + \mathbf{w} \cdot \nabla)_{\rho}$$

where the subscript p indicated that the convection-diffusion operator acts on the pressure space. Hence, the action of S^{-1} can be approximated by a matrix-vector multiply with a discrete pressure convection-diffusion operator, followed by a Poisson solve.

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This preconditioner performs well for small or moderate Reynolds numbers.
Test problems: steady Oseen, homogeneous Dirichlet BCs, two choices of the wind function.

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A preconditioning step requires two convection-diffusion solves (three in 3D) and one Poisson solve at each iteration, plus some mat-vecs.

Results for KLW preconditioner.

mesh size <i>h</i>	viscosity $ u$							
	1	0.1	0.01	0.001	0.0001			
constant wind								
1/16	6 / 12	8 / 16	12 / 24	30 / 34	100 / 80			
1/32	6/10	10 / 16	14 / 24	24 / 28	86 / 92			
1/64	6/10	8/14	16/24	22 / 32	64 / 66			
1/128	6/10	8/12	16 / 26	24 / 36	64 / 58			
rotating vortex								
1/16	6/8	10 / 12	30 / 40	>400/188				
1/32	6/8	10 / 12	30 / 40	> 400 / 378				
1/64	4/6	8/12	26 / 40	> 400 / > 400				
1/128	4/6	8/10	22 / 44	228 / > 400				

Number of Bi-CGSTAB iterations

(Note: exact solves used throughout. Stopping criterion: $\|\mathbf{b} - A\mathbf{x}_k\|_2 < 10^{-6} \|\mathbf{b}\|_2$).

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Results with Vanka-type MG preconditioner

Results for Vanka-MG-BiCGStab approach, isoP2-P0 FEM.

mesh size <i>h</i>	viscosity $= \nu$					
	1	0.1	0.01	10^{-3}	10^{-4}	
constant wind						
1/16	4	4	3	4	5	
1/32	4	4	3	4	4	
1/64	4	4	4	3	5	
1/128	4	4	4	3	4	
rotating vortex						
1/16	4	5	5	8	14	
1/32	4	4	6	9	17	
1/64	4	4	5	8	40	
1/128	4	4	4	9	> 400	

Better than KLW preconditioner, but still not robust for low viscosity. Can we do better than this?

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