MPE: Numerical Methods

Christmas Lectures

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Sparse linear algebra: motivation

We wish to solve

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

where A is *sparse*, normally coming from the discretisation of a PDE.

- Recall, iterative methods for linear systems *never need A itself.*
- Fixed point iterations and Krylov subspace methods only ever use A in context of matrix-vector product.

Corollaries

- Only need to provide matrix-vector product to solvers.
- If storing A, exploit sparse structure.

Sparse matrix formats

- Rather than storing a dense array (with *many* zeros), store only the non-zero entries, plus their locations.
- Data size becomes $\mathcal{O}(n_{\text{nz}})$ rather than $\mathcal{O}(n_{\text{row}}n_{\text{col}})$.
- For finite stencils (as from mesh-based discretisations) asymptotically save $\mathcal{O}(n_{\text{col}})$.

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Name	Easy insertion	Fast $A\mathbf{x}$	$A + B$
Coordinate (COO)	Yes	No	Easy
CSR	No	Yes	Hard[1]
CSC	No	Yes	Hard[1]
ELLPACK	No	Yes	Hard[1]

Table 1: Common sparse storage types. Saad 2003, § 3.4 provides a nice discussion of various formats.

Name	Language	Fortran?	Python?	Parallel	PCs
PETSc[2]	C	Yes	Yes	Yes	Many
`scipy.sparse`[3]	Python	No	Yes	No	Some
EIGEN[4]	C++	No	No	No	Some
Trilinos[5]	C++	No	Yes	Yes	Many

Table 2: Some sparse libraries

Sparse matrix formats II: a zoo

Many formats

Operations with sparse matrices are bounded by the *memory bandwidth* of the machine. The proliferation of slight variations to the CSR format all attempt to exploit *extra structure* in the matrix to increase performance through *vectorisation* and better cache reuse.

Common interface

Fortunately, you shouldn't have to care. A sparse matrix library should offer a *consistent* interface to insert values, and perform matrix operations, irrespective of the underlying format.

Sparse matrix implementation: libraries

Maxim

The most important part of programming is knowing when not to write your own code.

There are *many* full-featured sparse libraries available (serial and parallel). When you need sparse linear algebra, take the time to learn one.

Some advice

- We've seen already that iterative methods only need $A\mathbf{x}$.
- *But*, it is important to be able to *precondition* the solver.

- Assembled sparse matrix formats give you good performance, *and* access to a wide suite of preconditioners.

Maxim
Always start by implementing problems with assembled operators. Now you can try lots of things quickly and get your model working. Then, *and only then* can you start worrying about further performance optimisations.

Questions upon encountering a matrix

1. What do you want to do with it?
   - Compute $A\mathbf{x}$?
   - Solve linear systems (or eigen-problems)?
2. What does the spectrum look like?
   - Are the eigenvalues all distinct, or clustered?
   - Symmetric positive definite? $\sigma(A) \subset \mathbb{R}^+$
   - Nonsymmetric definite? $\sigma(A) \subset \{z \in \mathbb{C} : \Re(z) > 0\}$
   - Symmetric indefinite? $\sigma(A) \subset \mathbb{R}$
   - Nonsymmetric indefinite? $\sigma(A) \in \mathbb{C}$
3. What is its sparsity?
4. Is there a better way of computing $A\mathbf{x}$ than by starting with A?
5. Is there another matrix whose spectrum is similar, but is "nicer"?
6. *How can we precondition A?*

Krylov methods are not solvers

Assertion 1 (Krylov solvers are not solvers)**.** *Despite guarantees of convergence in exact arithmetic for CG (and GMRES), in actual practical cases a* bare *Krylov method is almost useless.*

- Krylov methods converge fast if:
  1. there is a *low-degree* polynomial with $p(0) = 1$ with $p(\lambda_i) = 0\ \forall \lambda_i$, or
  2. you're lucky and you get a "special" right hand side.

- Convergence to a tolerance requires $p(\lambda_i)$ small. Achievable if eigenvalues are *clustered*.
- For most operators we will encounter, the eigenvalues are typically *not clustered*.

Preconditioning to the rescue

Definition 1 (Preconditioner)**.** A *preconditioner* $\mathcal{P}$ is a *method* for constructing a linear operator $P^{-1} = \mathcal{P}(A, A_p)$ using a matrix A and some extra information A_p, such that the spectrum of $P^{-1}A$ (or AP^{-1}) is well-behaved.

- P^{-1} is *dense*, and P itself is often not available (and not needed).
- Normally, A is not used by $\mathcal{P}$. But often we make the choice $A_p = A$.
- Often $\mathcal{P}$ can be a (matrix-based) "black-box". Things like Jacobi, Gauss-Seidel, (incomplete) factorisations fall into this category.
- If you know something about A, you can often do better than a black-box approach.

If you're writing a simulation

Direct solvers (LU factorisation)
Reasonable for medium-sized problems, *robust* but *not scalable*.

2D $\mathcal{O}(N_{\text{dof}}^{3/2})$ flops, $\mathcal{O}(N_{\text{dof}} \log N_{\text{dof}})$ memory.

3D $\mathcal{O}(N_{\text{dof}}^{2})$ flops, $\mathcal{O}(N_{\text{dof}}^{4/3})$ memory.

1. Develop your problem at small scale, using a (sparse) direct solver. "Get all the maths right".
2. Switch to an iterative method, weep quietly as your problem no longer converges.
3. Read the literature to find a robust h-independent preconditioner (iterations constant irrespective of resolution).
4. ... (implementation).
5. Solve at scale (without waiting until next year).

Choosing a preconditioner: connections to PDEs

- We often think of preconditioning in the context of "I have a matrix system I want to solve".
- However, there is a very deep connection between preconditioning and functional analysis (and the theory of PDEs).
- In particular, figuring out what an appropriate preconditioner is.
- For more details, Kirby (2010) and Málek and Strakoš (2014) provide a good introduction.

A sketch for CG

- We can formulate Krylov methods in Hilbert spaces. Let
$$A : V \to V; \quad b \in V.$$
- A Krylov method seeks an "optimal"
$$x_m \in K_m(A, b) = \text{span}\{b, Ab, A^2b, \ldots, A^{m-1}b\},$$
where K_m is the *Krylov basis*.
- CG is appropriate if A is SPD and finds x_m minimising the A-norm of the error:
$$x_m = \arg\min_{y \in K_m} \langle Ay, y\rangle - 2\langle b, y\rangle$$
- Note that this construction *requires* that $A : V \to V$.

Where's the problem?

- For a discretisation of a PDE, we typically have
$$A : V \to V^*.$$
- Consider an H^1 discretisation of the Laplacian. This maps from H^1 (the space of piecewise smooth functions) to its dual H^{-1}. But
$$H^1 \subset L^2 \subset H^{-1}$$
- So now $V^* \neq V$. But CG *requires* that $b, Ab, \ldots, \in V$.
- We can think of preconditioning as fixing this "type-error" by choosing $B : V^* \to V$ and then solving the preconditioned problem
$$BA : V \to V^* \to V.$$
- Analysis of the PDE tells you an appropriate choice of B.

A concrete example

Model problem

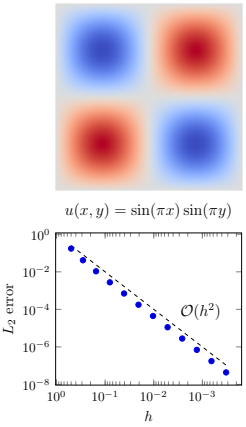
$$\begin{aligned} -\nabla^2 u(x,y) &= f(x,y), && \text{in } \Omega = [-1,1]^2 \\ u(x,y) &= 0. && \text{on } \partial\Omega \end{aligned}$$

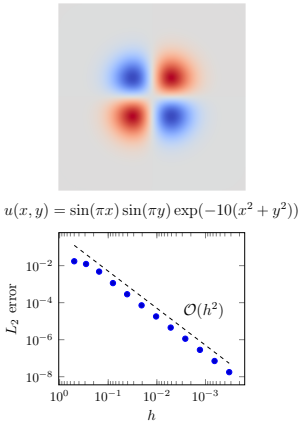
Discretised with 5-point stencil on regular grid (expect $\mathcal{O}(h^2)$ convergence of error).

Is my code correct?

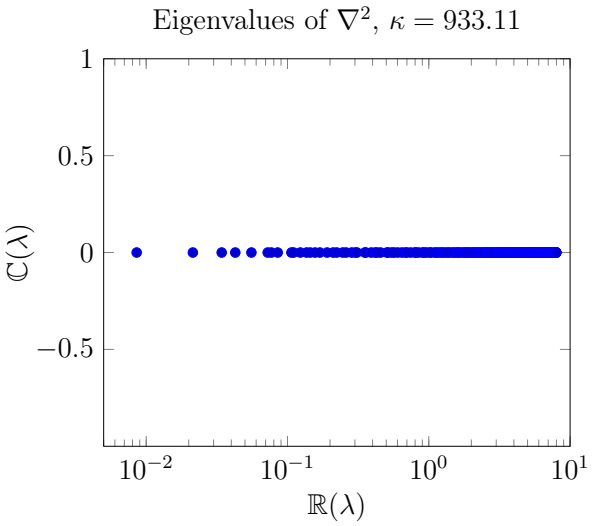
First, I need to check that I have implemented things correctly

Two exact solutions





Spectrum



Expected convergence

Recall that the A-norm of the *error* at the k^{th} iteration is bounded above by

$$||u_* - u_k||_A = ||e_k||_A \leq 2||e_0||_A \left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right)^k.$$

Where $\kappa = |\lambda_{\max}/\lambda_{\min}|$ is the *condition number* of A (or the preconditioned A as appropriate).

Poisson convergence

The Laplacian has an h-dependent condition number:

$$\lim_{h\to 0} \kappa \sim \mathcal{O}(h^{-2})$$

and so we expect CG to converge in $\mathcal{O}(h^{-1})$ iterations.

Stopping criteria (a reminder)

CG minimises the A-norm of the *error*, but we don't have access to that while iterating (we don't know the solution!). However, we can bound the 2-norm of the error.

Theorem 2. *<2->* *If we require* $||r_k||_2 < \lambda_{min}^{-1}\delta$ *then we guarantee* $||u_* - u_k||_2 < \delta$.

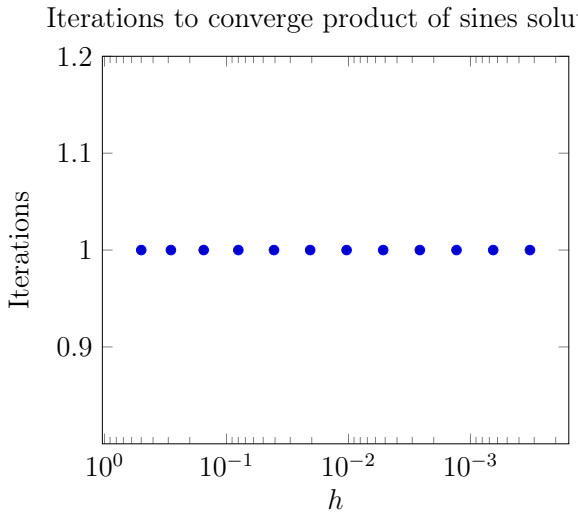
Proof.

$$\begin{aligned} ||u_* - u_k||_2 &= ||A^{-1}A(u_* - u_k)||_2 \leq ||A^{-1}||_2||(b - Au_k)||_2 \\ &= \lambda_{\min}^{-1}||r_k||_2. \end{aligned}$$

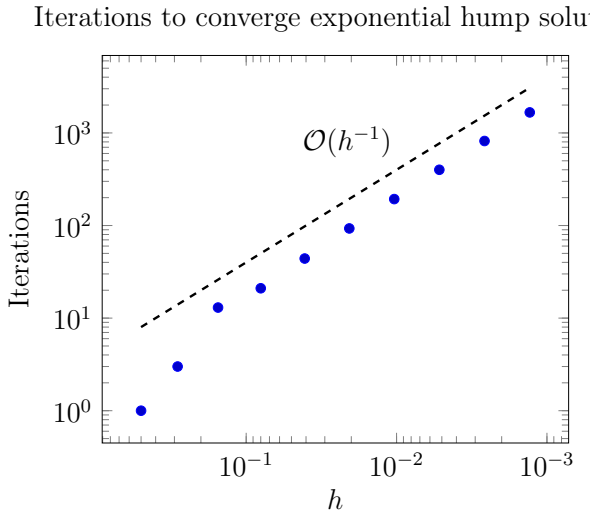
□

Back to the model problem

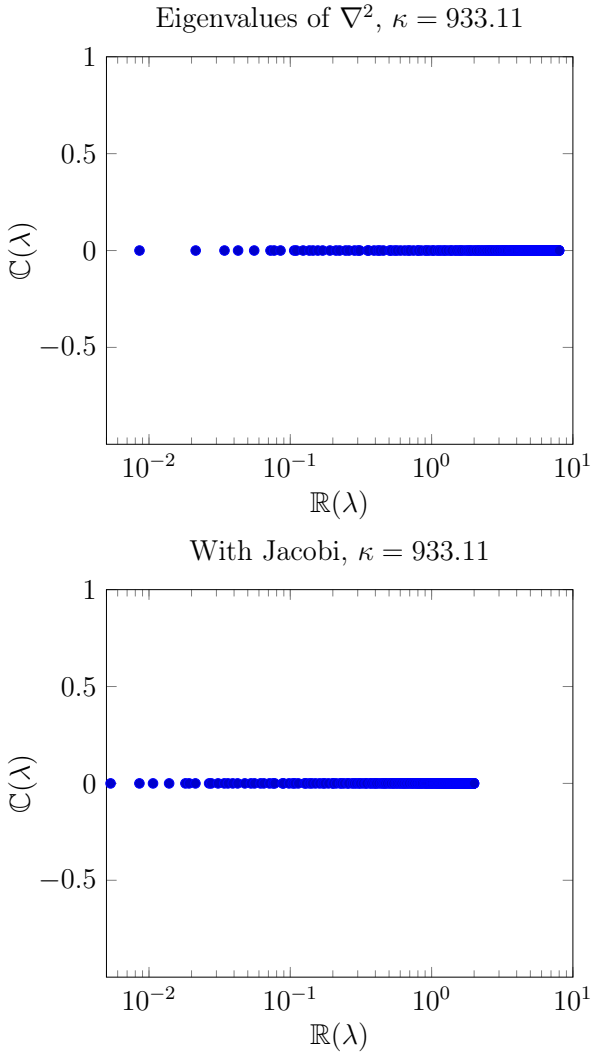
We've seen that the *unpreconditioned* operator has a *bad* spectrum for iterative solvers. Let's try when $u(x, y) = \sin(\pi x)\sin(\pi y)$



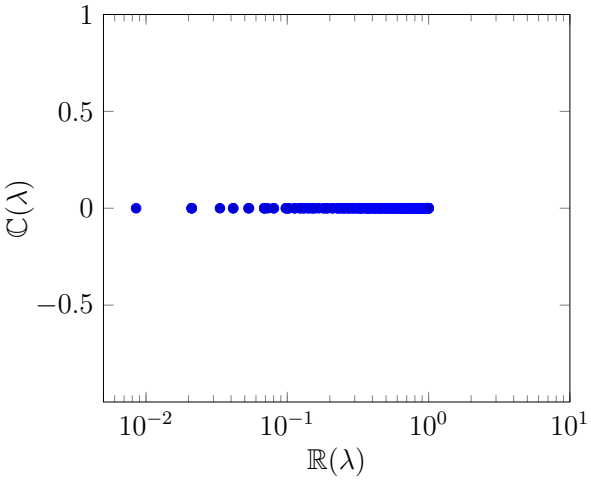
We had a special right hand side



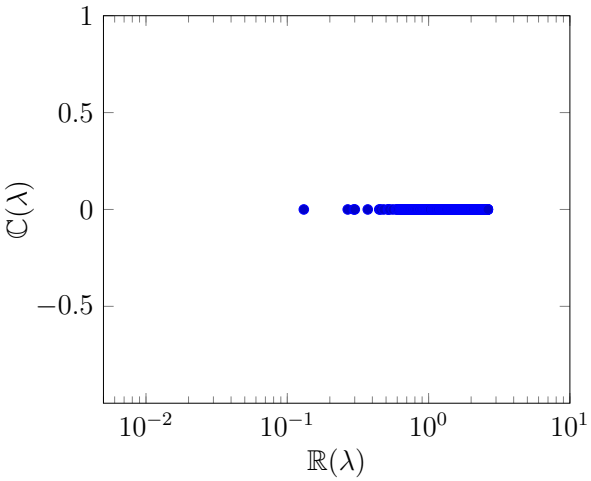
Some preconditioned spectra

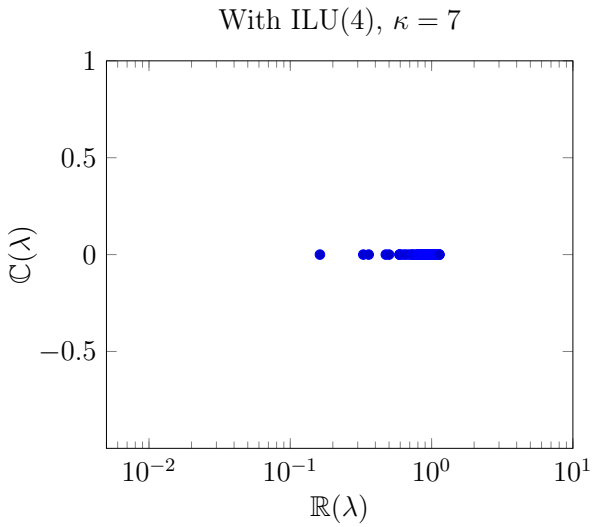


With Gauss-Seidel, $\kappa = 117.5$

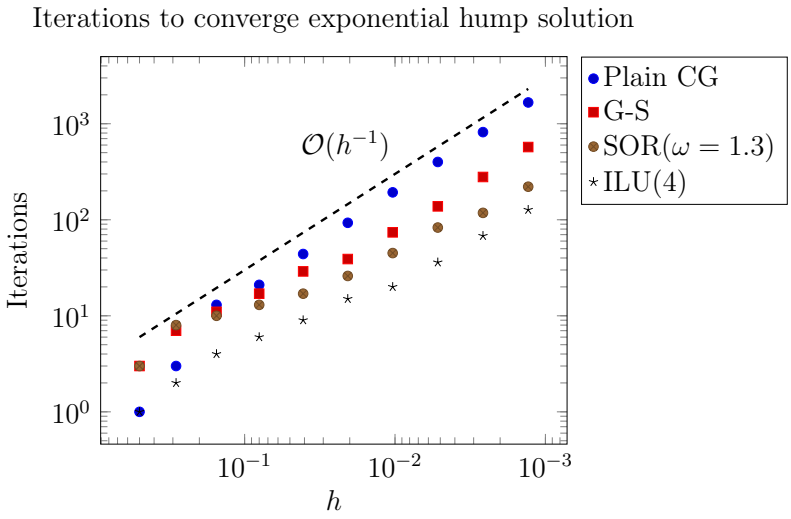


With SSOR($\omega = 1.3$), $\kappa = 20.06$



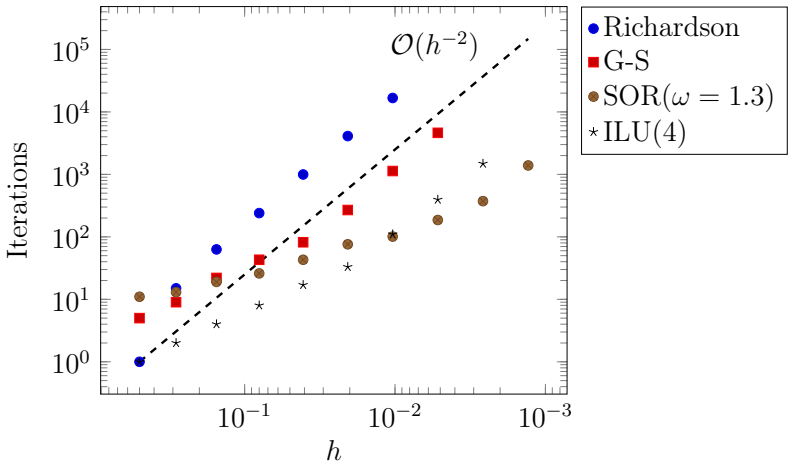


Back to convergence



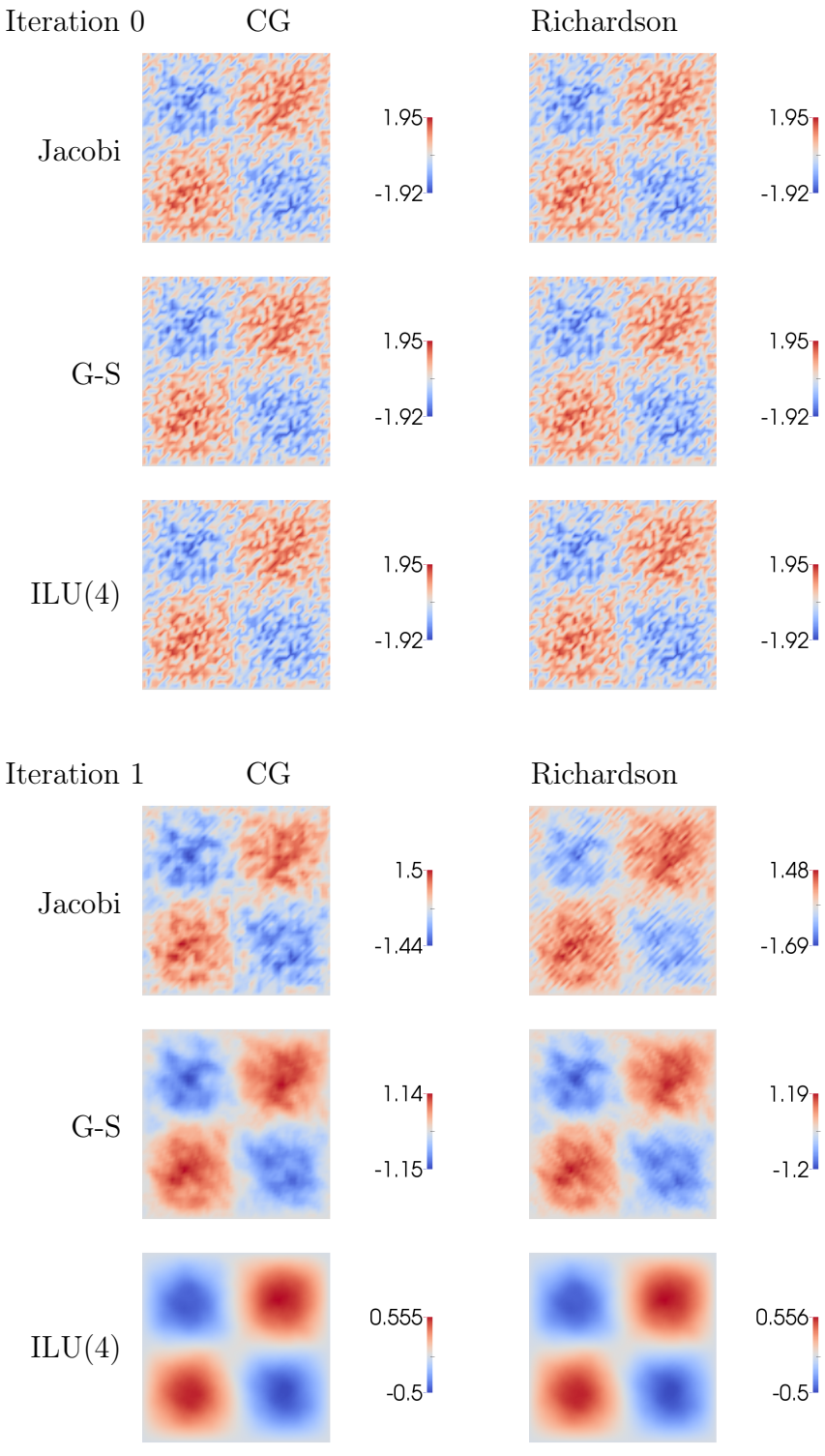
Compare (damped) Richardson

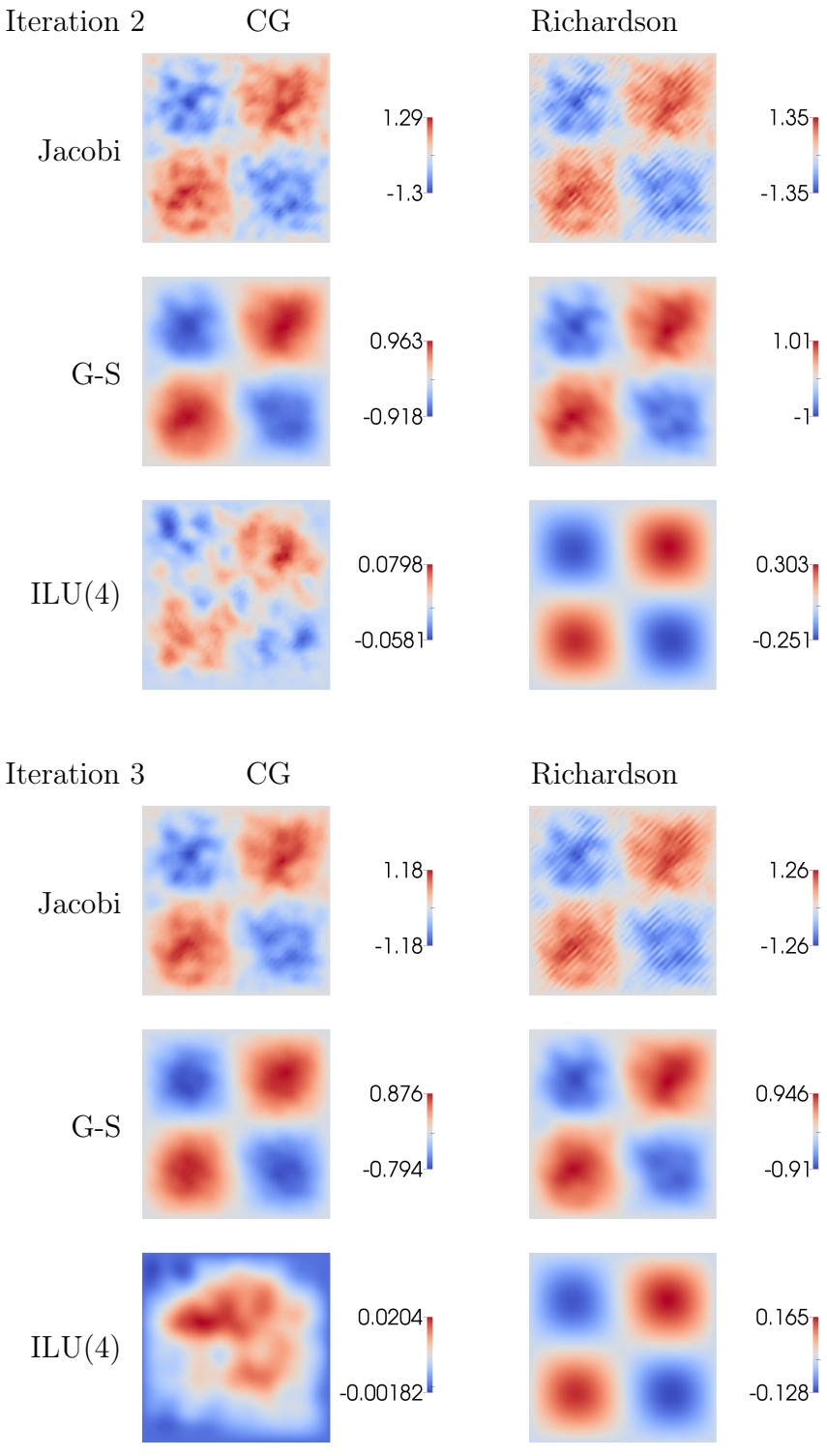
Iterations to converge exponential hump solution

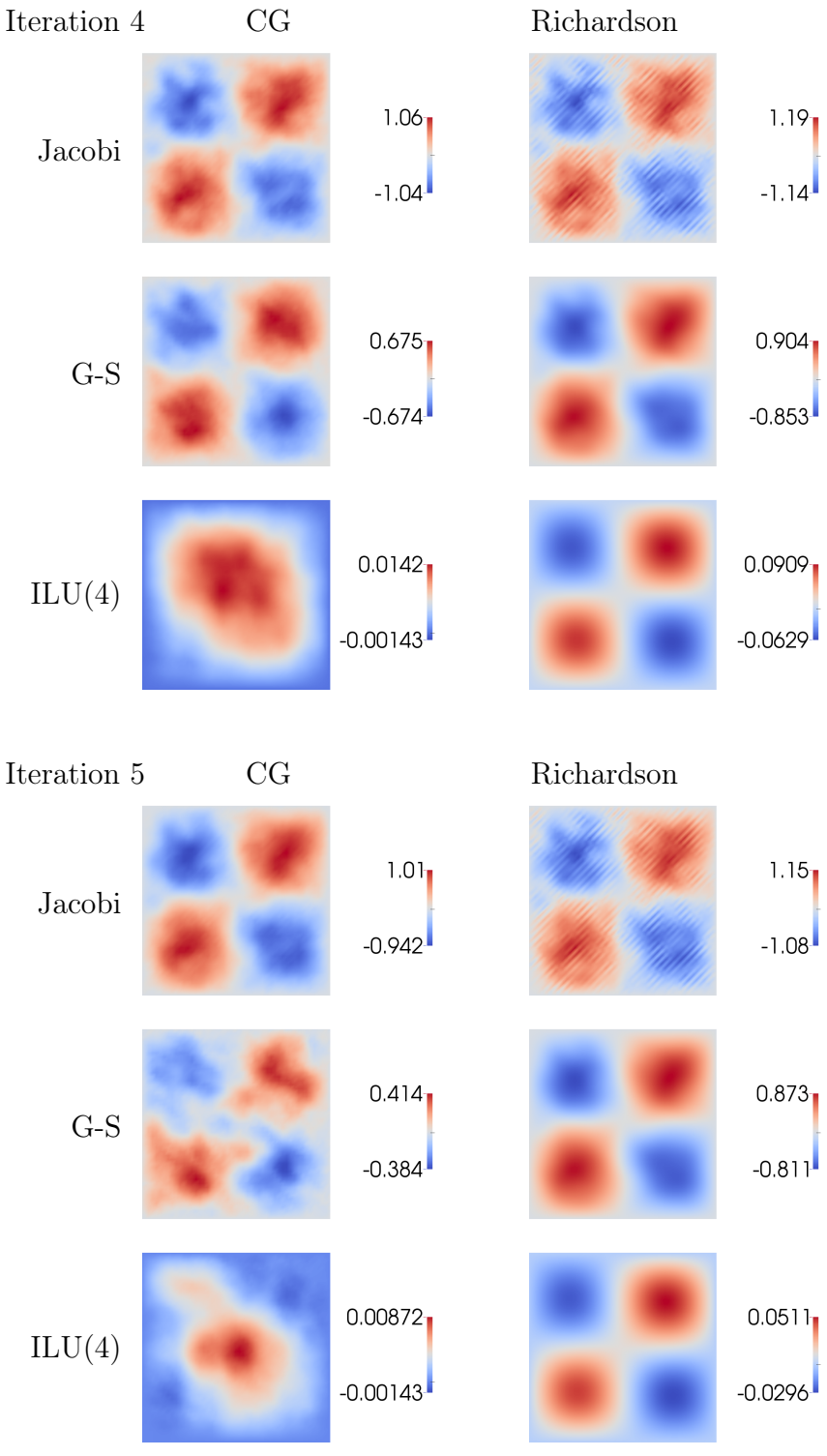


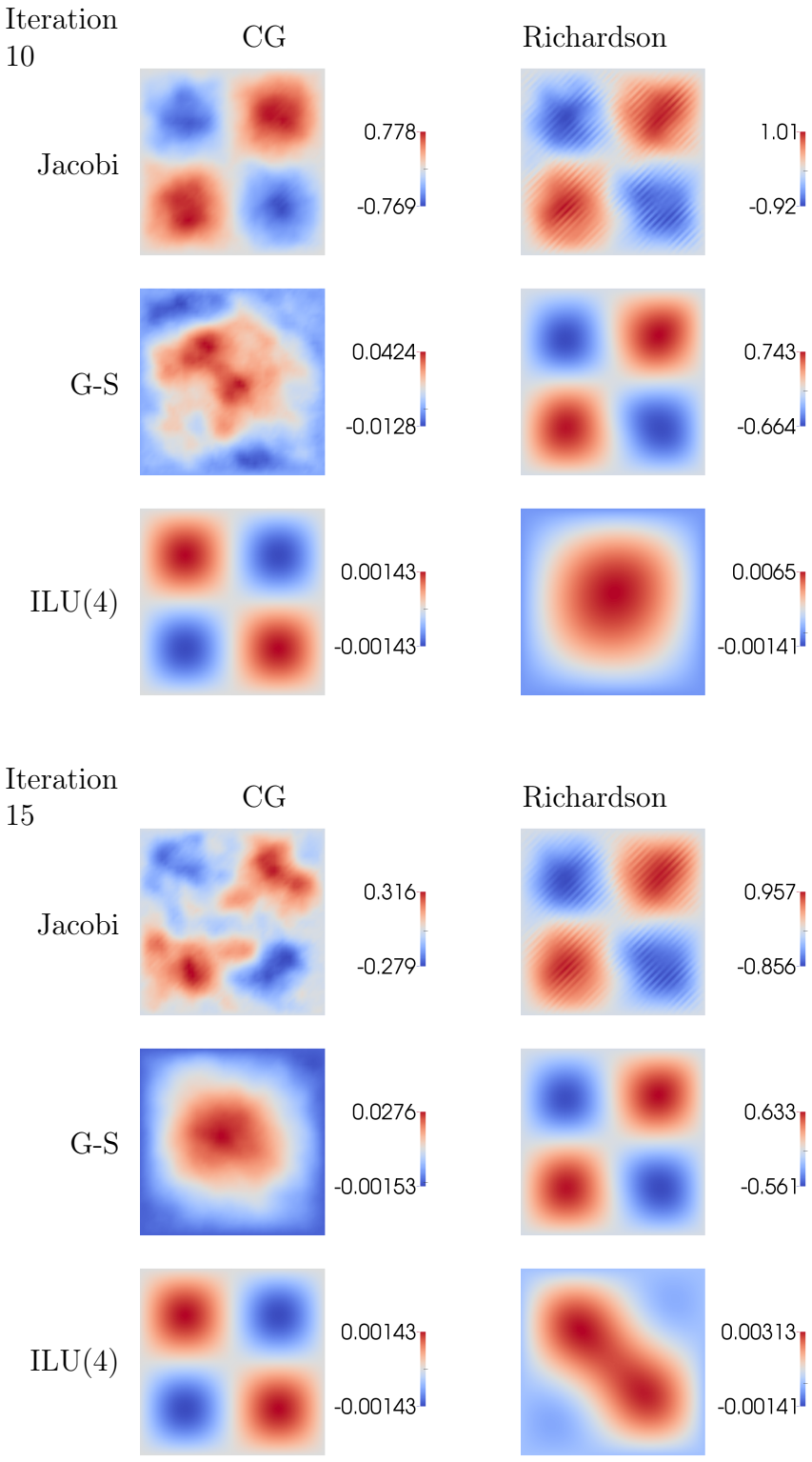
What is going wrong?

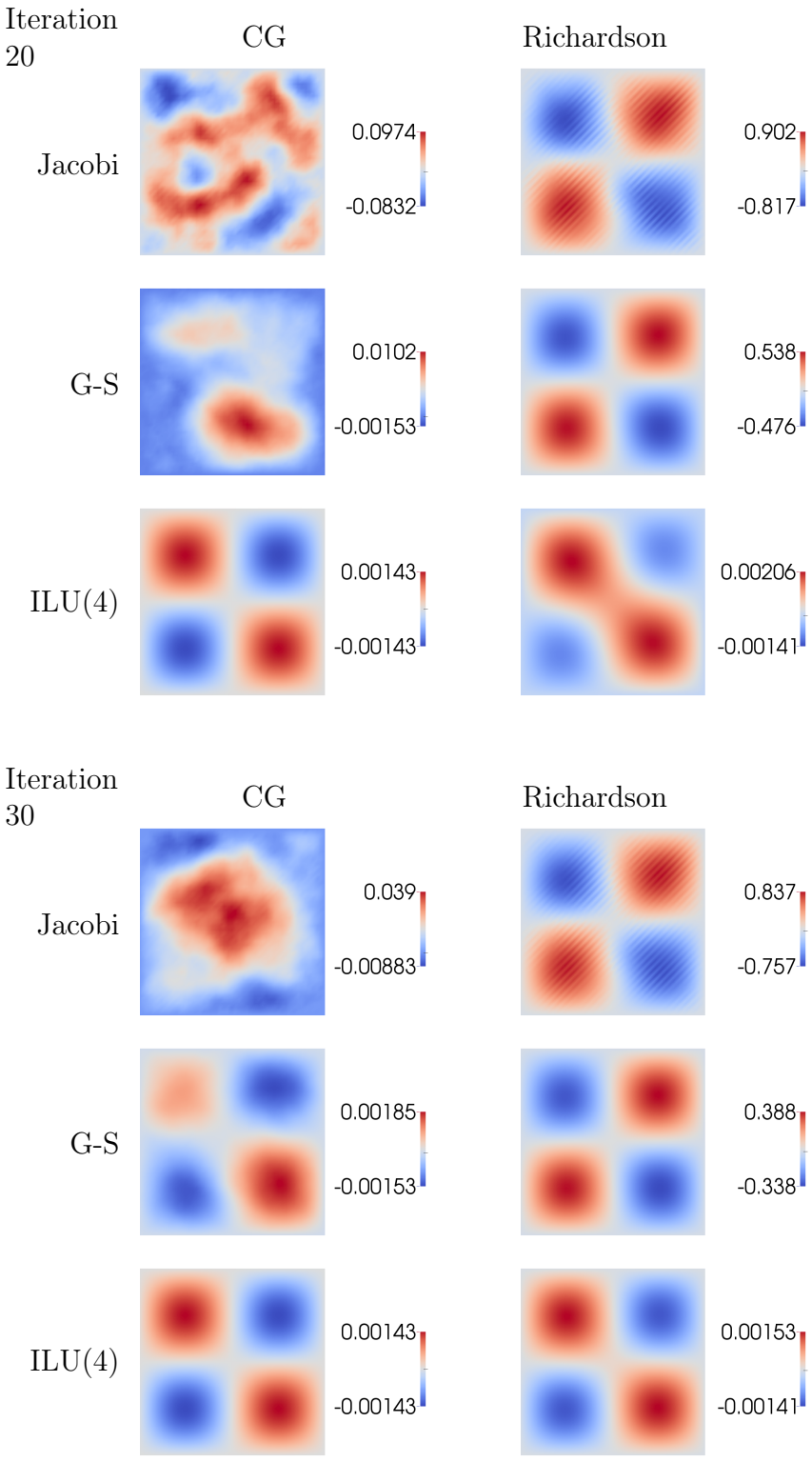
- The asymptotic convergence rate is as expected, can we gain an intuition for why we get this behaviour?
- It's instructive to look at what happens to the error.
- Let's choose the forcing such that $u_* = \sin(\pi x)\sin(\pi y)$
- Initial guess, randomly choose $u_0(x, y) \in [-1, 1]$ satisfying the zero Dirichlet conditions.

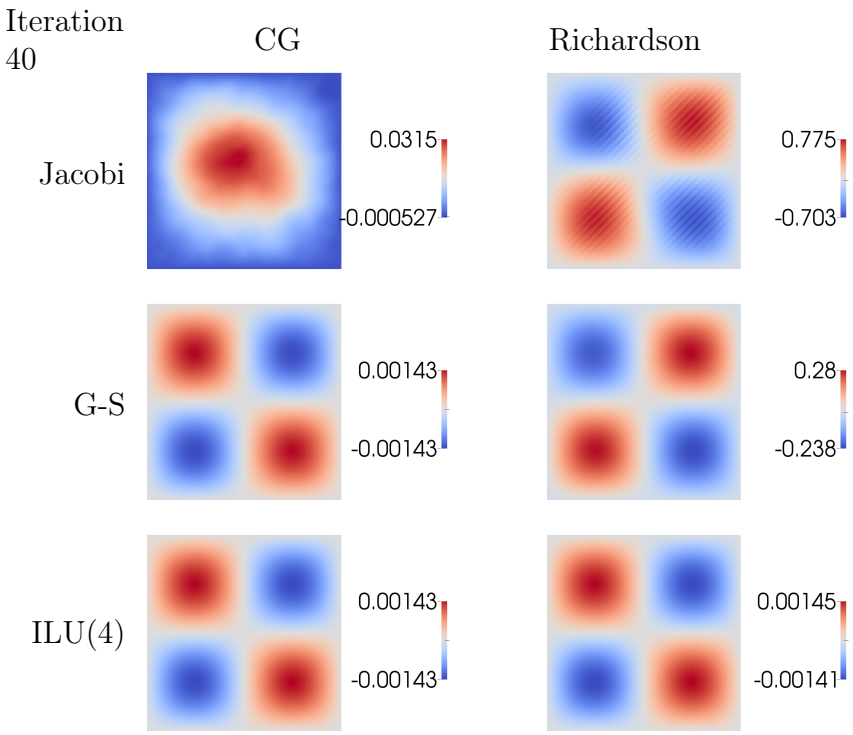

Iteration 0
CG
Richardson
Jacobi
1.95
-1.92
1.95
-1.92
G-S
1.95
-1.92
1.95
-1.92
ILU(4)
1.95
-1.92
1.95
-1.92
Iteration 1
CG
Richardson
Jacobi
1.5
-1.44
1.48
-1.69
G-S
1.14
-1.15
1.19
-1.2
ILU(4)
0.555
-0.5
0.556
-0.5


Iteration 2
CG
Richardson
Jacobi
1.29
-1.3
1.35
-1.35
G-S
0.963
-0.918
1.01
-1
ILU(4)
0.0798
-0.0581
0.303
-0.251
Iteration 3
CG
Richardson
Jacobi
1.18
-1.18
1.26
-1.26
G-S
0.876
-0.794
0.946
-0.91
ILU(4)
0.0204
-0.00182
0.165
-0.128


Iteration 4
CG
Richardson
Jacobi
1.06
-1.04
1.19
-1.14
G-S
0.675
-0.674
0.904
-0.853
ILU(4)
0.0142
-0.00143
0.0909
-0.0629
Iteration 5
CG
Richardson
Jacobi
1.01
-0.942
1.15
-1.08
G-S
0.414
-0.384
0.873
-0.811
ILU(4)
0.00872
-0.00143
0.0511
-0.0296


Iteration 10
CG
Richardson
Jacobi
0.778
-0.769
1.01
-0.92
G-S
0.0424
-0.0128
0.743
-0.664
ILU(4)
0.00143
-0.00143
0.0065
-0.00141
Iteration 15
CG
Richardson
Jacobi
0.316
-0.279
0.957
-0.856
G-S
0.0276
-0.00153
0.633
-0.561
ILU(4)
0.00143
-0.00143
0.00313
-0.00141


Iteration 20
CG
Richardson
Jacobi
0.0974
-0.0832
0.902
-0.817
G-S
0.0102
-0.00153
0.538
-0.476
ILU(4)
0.00143
-0.00143
0.00206
-0.00141
Iteration 30
CG
Richardson
Jacobi
0.039
-0.00883
0.837
-0.757
G-S
0.00185
-0.00153
0.388
-0.338
ILU(4)
0.00143
-0.00143
0.00153
-0.00141



Intuition: what's going on

- Poisson problem is *globally coupled*
- But splitting-based solvers only propagate information *locally*
- So as we increase the resolution more and more, everything takes longer
- Stationary iterations like Jacobi, G-S, SOR are often called smoothers
- They remove *high frequency* error very well, but take a long time to damp the *low frequency* error.

Multilevel methods

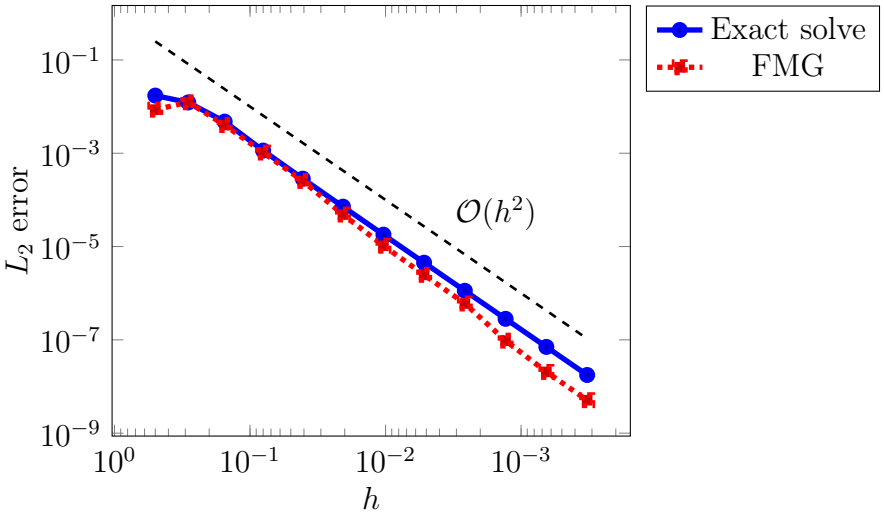
- Use a *hierarchy of scales*
- Use cheap smoothers to get a smooth error
- Move to a coarser grid (where the error looks rough again)
- Rinse and repeat

Optimality

Multigrid methods can be algorithmically *optimal*. Requiring $\mathcal{O}(N_{\text{dof}})$ work to reduce the error to within *discretisation error*.

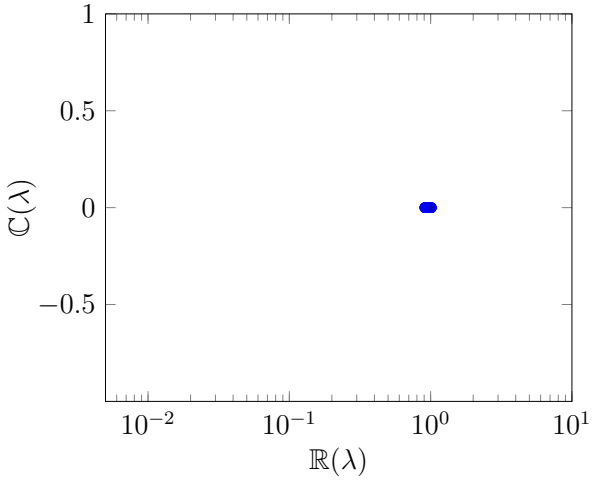
If you're interested in this, the classic text on multigrid is Brandt 1977, but there is a *huge* literature on this.

Error after one "full multigrid" cycle

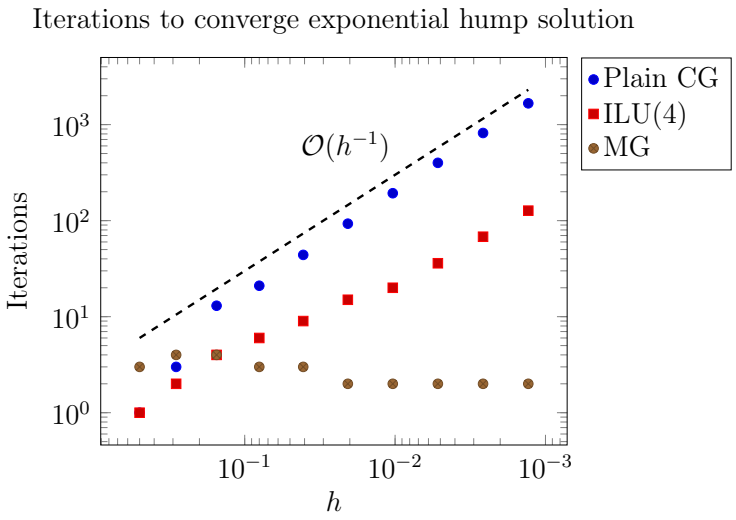


Our favourite spectrum

Eigenvalues of ∇^2 preconditioned by multigrid V-cycle, $\kappa = 1.11$



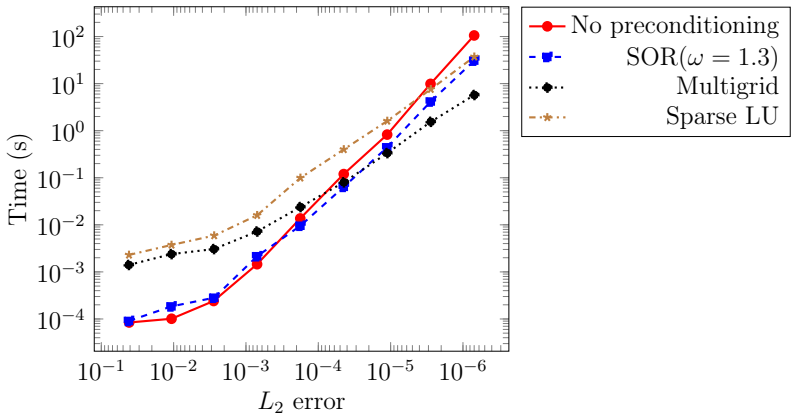
And convergence



What is best for me?

Work precision diagrams

To judge which method to use for your problem, it is important to consider the regime you're interested in. *Work precision* diagrams are useful for this.



Use libraries in your software

Maxim

The most important part of programming is knowing when not to write your own code.

- You should not, except maybe for interest, implement all these iterative methods (and preconditioners) yourself!
- There are many high-quality libraries available. Pick one, and use it.

- I used PETSc to develop the example that produced the results in these slides.

What to do

- CG (Hestenes and Stiefel 1952) minimises the $A-$norm of the error. If A is not SPD, it doesn't define a norm, so we can't do that
- Instead, minimise $2-$norm of residual: $||b - Ax||_2$.
- If A is symmetric (but indefinite), use MINRES or SYMMLQ (Paige and Saunders 1975).
- If A is not symmetric, probably use GMRES (Saad and Schultz 1986).

Asymmetry makes everything worse

- MINRES uses short recurrences and, like CG, uses bounded memory
- GMRES needs to reorthogonalise the current subspace at every step, therefore memory use grows with iteration count.
- Other non-symmetric methods (BICGSTAB, CGS, ...) have worse convergence properties (or no guarantees).

GMRES issues

- Convergence very operator-dependent, see, for example Nachtigal, Reddy, and Trefethen (1992) and Greenbaum, Pták, and Strakoš (1996).
- Restarted GMRES makes things more complex, see Embree (2003) for a nice review.
- Much harder to find good preconditioners for non-symmetric systems.

What about multiple variables?

- Often, we need to solve a problem of more than one variable. Stokes, Navier-Stokes, Cahn-Hilliard, MHD, combinations thereof.
- "black-box" preconditioning is even less likely to work than for single-variable systems.
- Many of the state-of-the art preconditioners for such problems rely on *block factorisations* of the operator.

Block systems

Theorem 3. *If a block matrix*

$$\mathcal{A} = \begin{pmatrix} A & B^T \\ C & 0 \end{pmatrix}$$

is preconditioned by

$$\mathcal{P} = \begin{pmatrix} A & 0 \\ 0 & CA^{-1}B^T \end{pmatrix}$$

then the preconditioned matrix $\mathcal{P}^{-1}\mathcal{A}$ has at most four distinct eigenvalues.

Murphy, Golub, and A. J. Wathen (2000). Writing

$$\mathcal{T} = \begin{pmatrix} I & A^{-1}B^T \\ (CA^{-1}B^T)^{-1}C & 0 \end{pmatrix},$$

then

$$(\mathcal{T} - I/2)^2 = \begin{pmatrix} I/4 + A^{-1}B^T(CA^{-1}B^T)^{-1}C & 0 \\ 0 & I/4 \end{pmatrix}.$$

Since $A^{-1}B^T(CA^{-1}B^T)^{-1}C$ is a projection

$$\left[(\mathcal{T} - I/2)^2 - I/4\right]^2 = (\mathcal{T} - I/2)^2 - I/4$$

and so

$$\mathcal{T}(\mathcal{T} - I)(\mathcal{T}^2 - T - I) = 0.$$

□

Some pointers

- Saad (2003) is good on stationary and Krylov iterations.
- Benzi, Golub, and Liesen (2005) is quite exhaustive on saddle point systems $\left(\begin{smallmatrix} A & B_1^T \\ B_2 & -C \end{smallmatrix}\right)$.
- A. J. Wathen (2015) is a recent (gentle) review article.
- Elman, Silvester, and A. Wathen (2014) covers saddle point solvers in the context of fluid dynamics.
- Kirby (2010) and Mardal and Winther (2011) present an interesting approach to designing preconditioners based on ideas from functional analysis.

Questions?

References

References

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