ADI iterations for general elliptic problems

John Strain
Mathematics Department
UC Berkeley
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OVERVIEW

Classical alternating direction implicit (ADI) iteration
– Essentially optimal in simple domains
– Applies to narrow class of special elliptic equations
– Useful for variable-coefficient and nonlinear problems

Generalize ADI to arbitrary elliptic systems
– Eliminate symmetry, commutativity, separability, . . .
– Solve Laplace, Helmholtz, Stokes, . . . , with single code

Convert elliptic problems to first-order overdetermined form
– Control computational error via residuals
– Illuminate solvability of boundary value problem

CLASSICAL ALTERNATING DIRECTION IMPLICIT

Separable second-order equations in rectangles

$$-\Delta u = Au + Bu = -\partial_1^2 u - \partial_2^2 u = f$$

efficiently solved by essentially optimal ADI iteration

$$(s+A)(s+B)u^{m+1} = (s-A)(s-B)u^m + 2sf$$

when A and B are commuting positive Hermitian operators

Fast damping over geometric range

$$a \geq 0 \quad \to \quad \left|\frac{s-a}{s+a}\right| \leq 1$$

$$\frac{1}{2} \leq \frac{b}{s} \leq 2 \quad \to \quad \left|\frac{s-b}{s+b}\right| \leq \frac{1}{3}$$

implies $O(\epsilon)$ error reduction in $O(\log N \log \epsilon)$ sweeps

FIRST AND SECOND ORDER ELLIPTIC PROBLEMS

Cauchy-Riemann

$$\partial_x u = \partial_y v \qquad \partial_y u = -\partial_x v$$

Low-frequency time-harmonic Maxwell

$$\nabla \times E = -\frac{i\omega}{c} H \qquad \nabla \cdot E = 4\pi\rho$$

$$\nabla \times H = \frac{i\omega}{c} E + \frac{4\pi}{c} j \qquad \nabla \cdot H = 0$$

Linear elasticity

$$\partial_i \sigma_{ij} + F_j = 0 \qquad \sigma_{ij} - \frac{1}{2} C_{ijkl} \left(\partial_k u_l + \partial_l u_k \right) = 0$$

Laplace/Poisson/Helmholtz/Yukawa/ ...

$$\Delta u + \lambda u = f$$

Stokes

$$-\Delta u + \nabla p = f \qquad \nabla \cdot u = 0$$

CONVERTING TO FIRST-ORDER SYSTEMS

Higher-order system of partial differential equations

$$\cdots + \sum_{ijl} a_{ijkl}\partial_i\partial_j v_l + \sum_{jl} b_{jkl}\partial_j v_l + \sum_{l} c_{kl} v_l = f_k \qquad \text{in } \Omega$$

$$\sum_{l} \alpha_{kl} v_l + \sum_{jl} \beta_{kjl}\partial_j v_l + \cdots = g_k \qquad \text{on } \Gamma = \partial\Omega$$

Seek new solution vector $u = (v, \partial_1 v, \ldots, \partial_d v, \ldots)^T$

Vector u satisfies first-order system

$$Au = \sum_{j} A_j \partial_j u + A_0 u = f \qquad \text{in } \Omega$$

$$Bu = g \qquad \text{on } \Gamma$$

Sparse matrices A_j, A_0, B localize algebraic structure

PITFALL OF CONVERSION

Robin boundary value problem for 2D Poisson equation

$$\Delta v + \lambda v = f \qquad \text{in } \Omega$$

$$\alpha v + \beta \partial_n v = g \qquad \text{on } \Gamma$$

3×3 square system

$$Au = \begin{bmatrix} \partial_1 & -1 & 0 \\ \partial_2 & 0 & -1 \\ \lambda & \partial_1 & \partial_2 \end{bmatrix} \begin{bmatrix} v \\ \partial_1 v \\ \partial_2 v \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ f \end{bmatrix}$$

$$Bu = \begin{bmatrix} \alpha & \beta n_1 & \beta n_2 \end{bmatrix} \begin{bmatrix} v \\ \partial_1 v \\ \partial_2 v \end{bmatrix} = g$$

System not elliptic (in sense of Protter): principal part

$$\sum_j k_j A_j = \begin{bmatrix} k_1 & 0 & 0 \\ k_2 & 0 & 0 \\ 0 & k_1 & k_2 \end{bmatrix} \qquad \text{singular for all } k!$$

SOLVED BY OVERDETERMINATION

$$\Delta v + \lambda v = f \qquad \textbf{in } \Omega$$

Overdetermined 4×3 **elliptic system**

$$Au = \begin{bmatrix} \partial_1 & -1 & 0 \\ \partial_2 & 0 & -1 \\ 0 & -\partial_2 & \partial_1 \\ \lambda & \partial_1 & \partial_2 \end{bmatrix} \begin{bmatrix} v \\ \partial_1 v \\ \partial_2 v \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ f \end{bmatrix}$$

Compatibility conditions $\Rightarrow$ **overdetermined but elliptic**

$$\sum_j k_j A_j = \begin{bmatrix} k_1 & 0 & 0 \\ k_2 & 0 & 0 \\ 0 & -k_2 & k_1 \\ 0 & k_1 & k_2 \end{bmatrix}$$

full-rank $\Rightarrow$ **injective for** $k \neq 0$

Analytical benefit: controls derivatives $\partial_j u$ **in terms of** u **and** f

Computational advantage: controls error via residuals

CONVERSION OF 2D STOKES

Stokes for 2-vector u and scalar p

$$-\Delta u + \nabla p = f \qquad \nabla \cdot u = 0$$

Converts to 13×9 sparse system with

$$u = \begin{bmatrix} u_1 \\ u_{1,1} \\ u_{1,2} \\ u_2 \\ u_{2,1} \\ u_{2,2} \\ p \\ \color{red}{p_{,1}} \\ \color{red}{p_{,2}} \end{bmatrix} \qquad \sum_j k_j A_j = \begin{bmatrix} k_1 & & & & & & & & \\ k_2 & & & & & & & & \\ & k_2 & -k_1 & & & & & & \\ & k_1 & k_2 & & & & k_1 & & \\ & & & k_1 & & & & & \\ & & & k_2 & & & & & \\ & & & & k_2 & -k_1 & & & \\ & & & & k_1 & k_2 & k_2 & & \\ k_1 & & & k_2 & & & & & \\ & & & & & & \color{red}{k_1} & & \\ & & & & & & \color{red}{k_2} & & \\ & & & & & & & \color{red}{k_2} & \color{red}{-k_1} \\ & & & & & & & \color{red}{k_1} & \color{red}{k_2} \end{bmatrix}$$

Elliptic (in sense of Protter) with Laplace equation $\Delta p = \nabla \cdot f$

BOUNDARY CONDITIONS FOR DERIVATIVES?

Example: Dirichlet $v = g \to Bu = g$ with rank-1 matrix B

Intuitively, the system $Au = f$ includes compatibility conditions

Analytically, Fourier transform in half space $\to$ well-posed

Computational methods enforce compatibility conditions up to boundary $\to$ stable

Overdetermined interior $\leftrightarrow$ underdetermined boundary

LOCAL SOLVABILITY FOR NORMAL DERIVATIVE

Ellipticity of first-order system

$$Au = \sum_j A_j \partial_j u + A_0 u = f \qquad \text{in } \Omega$$

implies any normal part $A_n = \sum_j n_j A_j$ is left-invertible

$$A_n^\dagger = (A_n^* A_n)^{-1} A_n^* \qquad \longrightarrow \qquad A_n^\dagger A_n = I$$

Determines any directional derivative

$$\partial_n u = \sum_i n_i \partial_i u = A_n^\dagger \left(f - A_T \partial_T u - A_0 u\right)$$

in terms of tangential derivatives

$$A_T \partial_T u = \sum_j A_j \partial_j u - A_n \partial_n u = \sum_{ij} A_i \left(\delta_{ij} - n_i n_j\right) \partial_j u$$

and zero-order data

SOLVE BOUNDARY VALUE PROBLEM

With full tangential data plus elliptic system can integrate

$$\partial_n u = A_n^{\dagger}\,(f - A_T \partial_T u - A_0 u)$$

inward to solve boundary value problem

Boundary conditions

$$Bu = \left[\begin{array}{ccc} \alpha & \beta n_1 & \beta n_2 \end{array}\right] \left[\begin{array}{c} v \\ \partial_1 v \\ \partial_2 v \end{array}\right] = g \qquad BB^* = I$$

determine local projection $B^*Bu = B^*g$ on the boundary

Boundary value problem constrains $(I - B^*B)u$ on boundary

Contrast: hyperbolic systems blind $\perp$ characteristics

GENERALIZED ADI FOR POISSON SYSTEM

Choose arbitrary sweep direction n and normalize

$$\sum_j A_j \partial_j u = \sum_{ij} A_i (n_i n_j + \delta ij - n_i n_j) \partial_j u = A_n \partial_n u + A_T \partial_T u$$

Left-invert A_n by ellipticity and damp on scale $1/s$

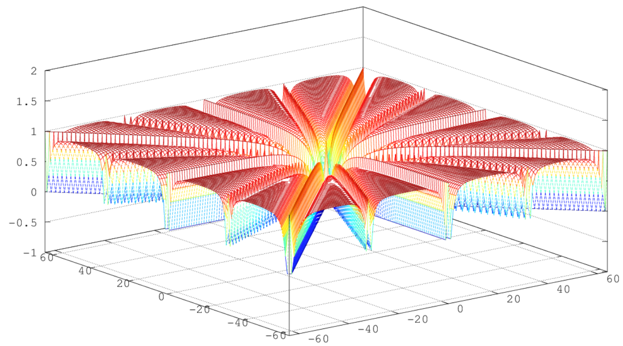
$$s u^{m+1} + \partial_n u^{m+1} + B_0 u^{m+1} = s u^m - B_T \partial_T u^m + A_n^\dagger f$$

Error mode $\mathrm{e}^{\mathrm{i}k^T x}$ damped by matrix symbol

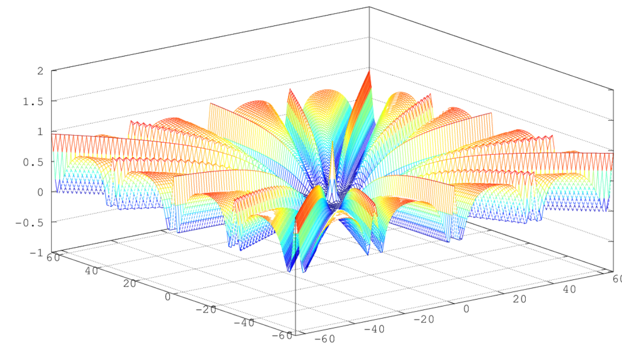
$$\rho(k) = \prod_s \prod_n (s + \mathrm{i}k_n + B_0)^{-1} (s - \mathrm{i}k_T B_T)$$

Spectral radius 0.9^S with $S = O(\log N)$ sweeps

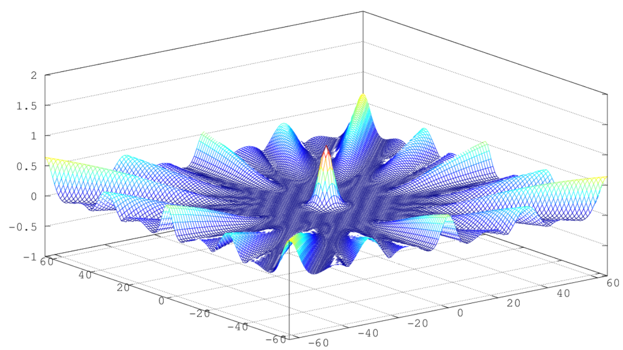
SPECTRAL RADIUS FOR POISSON SYSTEM



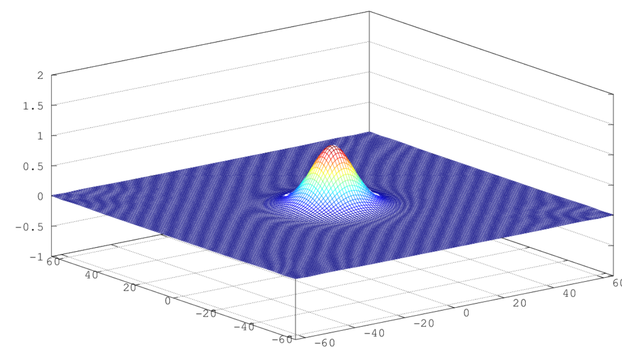
$s = 1$



$s = 4$



$s = 16$



$s = 64$

GENERALIZED ADI FOR YUKAWA SYSTEM

Yukawa as first-order system

$$\Delta u - \lambda u = f \qquad \longrightarrow \qquad A_j u_j + A_0 u = f$$

introduces nonzero eigenvalues $\pm\sqrt{\lambda}$ **of** $B_0 = A_n^\dagger A_0$

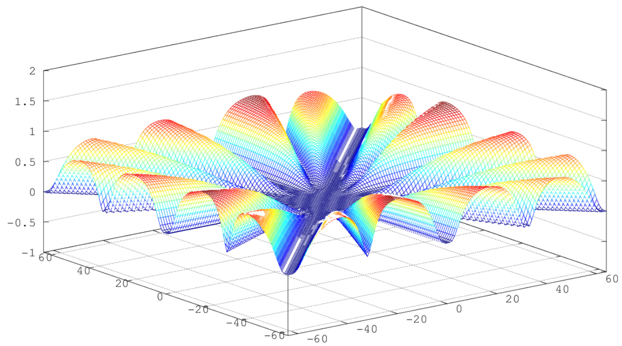
Divide by zero when $s = \sqrt{\lambda}$

Use matrix sign function $K = s\,\textbf{sgn}(B_0)$
computed by Schur decomposition $B_0 = UTU^*$

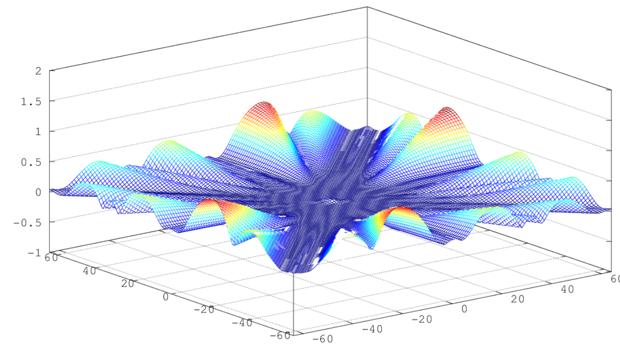
$$Ku^{m+1} + \partial_n u^{m+1} + B_0 u^{m+1} = Ku^m - B_T \partial_T u^m + A_n^\dagger f$$

Spectral radius 0.9^S **with** $\lambda = 10$

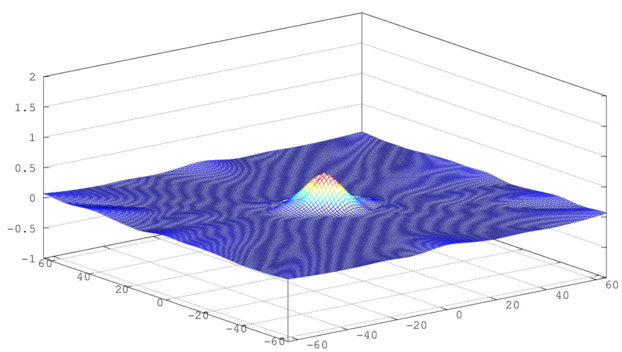
SPECTRAL RADIUS FOR YUKAWA WITH $\lambda = 10$



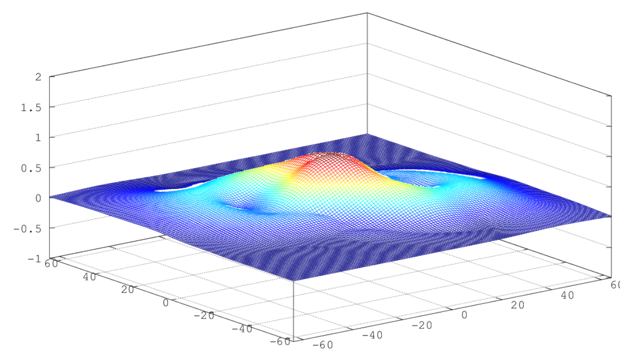
$s = 1$



$s = 4$



$s = 16$



$s = 64$

GENERAL STRUCTURE

Given operators A and B with
cheap resolvents $(sI - A)^{-1}$ and $(sI - B)^{-1}$
find an efficient scheme for the solution of

$$(A + B)u = f$$

Underlies many computational problems where
– A is sparse and B is low-rank
– A and B are both sparse but in different bases
– fast schemes deliver A^{-1} and B^{-1}

Challenging when A and B don't commute

Solution very unlikely in this generality

ADI^2 APPROACH

1. A and B may not be invertible (or even square): square

$$(A+B)^*(A+B)u = (A+B)^* f = g$$

2. Solve corresponding heat equation

$$\partial_t u = -(A+B)^*(A+B)u + g$$

to get u as $t \to \infty$

3. Discretize time and split

$$(I + sA^*A)\,(I + sB^*B)\,u^{m+1} = (I - s(A^*B + B^*A))\,u^m + sg$$

to get u as $t \to \infty$

4. Alternate directions for symmetric symbol

$$\rho = (I + sB^*B)^{-1}(I + sA^*A)^{-1}(I - 2s(A^*B + B^*A))(I + sA^*A)^{-1}(I + sB^*B)^{-1}$$

Similar with more operators A, B, C, D, . . .

ADI^2 FOR POISSON/YUKAWA/HELMHOLTZ

Second-order equation $\rightarrow$ overdetermined first-order system

$$\Delta u + \lambda u = f \quad \rightarrow \quad (A + B + C)u = A_1 \partial_1 u + A_2 \partial_2 u + A_0 u = f$$

with high-frequency zero-order operator $C = O(\lambda)$

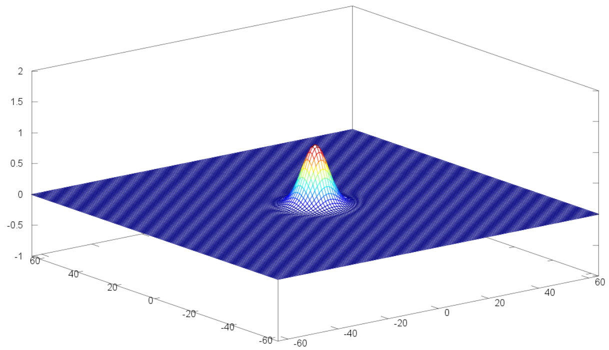
Fourier mode (k_1, k_2) **of error damped with symbol**

$$\begin{aligned}
\rho &= (I + sC^*C)^{-1} (I + sB^*B)^{-1} (I + sA^*A)^{-1} \cdot \\
&\quad (I - 2s(A^*B + A^*C + B^*A + B^*C + C^*A + C^*B)) \cdot \\
&\quad (I + sA^*A)^{-1} (I + sB^*B)^{-1} (I + sC^*C)^{-1} \\
\widehat{\rho} &= \frac{1}{(1 + sk_1^2)^2 (1 + sk_2^2)^2 (1 + s\lambda^2)^2} \begin{bmatrix} 1 & is(\lambda + 1)bk_1 & is(\lambda + 1)bk_2 \\ -is(\lambda + 1)bk_1 & b^2 & 0 \\ -is(\lambda + 1)bk_2 & 0 & b^2 \end{bmatrix}
\end{aligned}$$

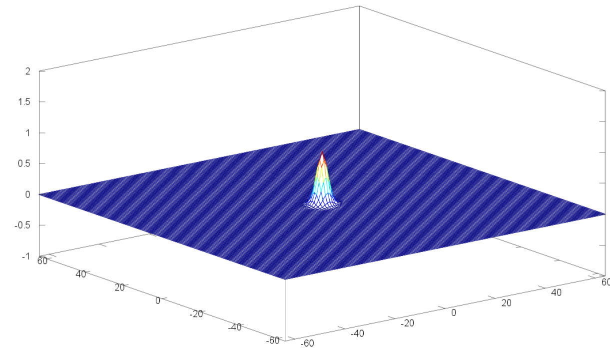
where $b = (1 + s\lambda^2)/(1 + s)$

Eigenvalues of $\widehat{\rho}$ **bounded by 1, controlled by** s **for all** λ

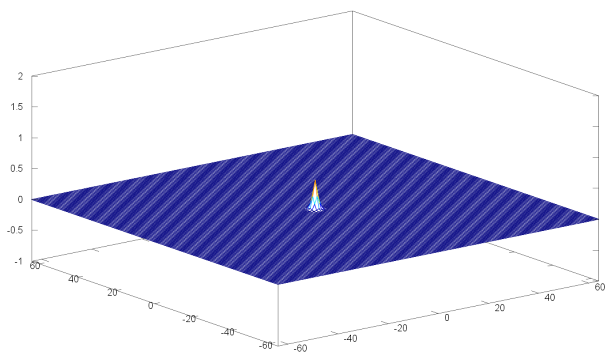
SPECTRAL RADIUS FOR HELMHOLTZ WITH $\lambda = 1$



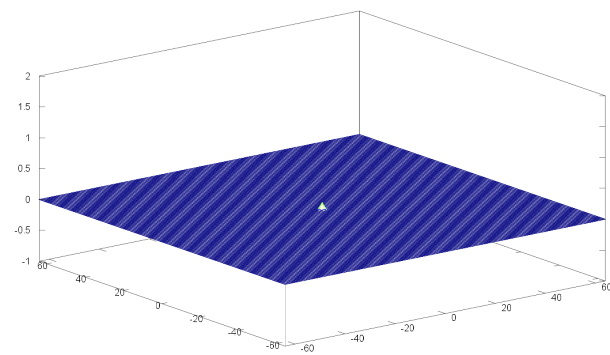
$s = 1/64$



$s = 1/16$



$s = 1/4$



$s = 1$

CONCLUSIONS

Conversion to first-order overdetermined systems yields
– analytical understanding of elliptic structure
– well-posed computational formulations
– fast iterations for numerical solution

Coming attractions:
– fast spectral boundary integral methods
– efficient implicit methods for elliptic moving interfaces
– nonuniform fast Fourier transforms for geometric data
– optimized post-Gaussian quadrature methods