Fast Poisson solvers for spectral methods

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Based on: F. & Townsend, “Fast Poisson solvers for spectral methods,” to appear in IMA J. Numer. Anal.

Introduction
A long-standing question

Consider Poisson's equation on $[-1, 1]^2$ with homogeneous Dirichlet conditions,

$$u_{xx} + u_{yy} = f, \quad (x, y) \in [-1, 1]^2, \quad u(\pm 1, \cdot) = u(\cdot, \pm 1) = 0.$$

The classic fast Poisson solver using finite differences:

$$\underbrace{KX + XK^T = F,}_{\text{solve with DST-I, } \mathcal{O}(n^2 \log n)} \qquad K = \frac{1}{h^2}\begin{bmatrix} 2 & -1 & & \\ -1 & \ddots & \ddots & \\ & \ddots & \ddots & -1 \\ & & -1 & 2 \end{bmatrix}$$

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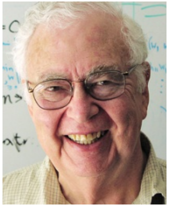
Bill Buzbee



Gene Golub

- Based on **structured eigenvectors**
- Complexity increases with order of accuracy

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breaks down for spectral


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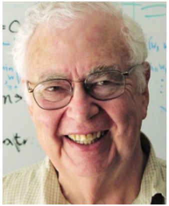
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Can we make a spectrally-accurate Poisson solver with $\mathcal{O}(n^2 \log n)$ complexity?

A sparse identity

The ultraspherical polynomials

Dirichlet on $[-1,1]$ $\longleftrightarrow$ Pick a basis that vanishes at ± 1

The classical orthogonal polynomials, f_k, satisfy

$$A(x)f_k''(x) + B(x)f_k'(x) = q_k f_k(x), \qquad x \in [-1,1].$$

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The ultraspherical polynomials of parameter $\lambda > 0$, $C_k^{(\lambda)}$, satisfy [NIST DLMF, 18.8.1]

$$(1 - x^2) C_k^{(\lambda)''}(x) - (2\lambda + 1) x C_k^{(\lambda)'}(x) = -k(k + 2\lambda) C_k^{(\lambda)}(x), \qquad x \in [-1, 1].$$

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The second derivative of $(1-x^2)C_k^{(\lambda)}(x)$ is given by

$$\frac{\partial^2}{\partial x^2}\left[(1-x^2)C_k^{(\lambda)}(x)\right] = (1-x^2)C_k^{(\lambda)''}(x) - 4xC_k^{(\lambda)'}(x) - 2C_k^{(\lambda)}(x).$$

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Idea: Choose $\lambda = \frac{3}{2}$

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The ultraspherical polynomials

$$\frac{\partial^2}{\partial x^2}\left[(1-x^2)C_k^{(3/2)}(x)\right] = -(k(k+3)+2)C_k^{(3/2)}(x).$$

$$\boxed{C_k^{(3/2)}(x) \text{ is an eigenfunction of the differential operator } u \mapsto \tfrac{\partial^2}{\partial x^2}[(1-x^2)u]}$$

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$$\boxed{C_k^{(3/2)}(x) \text{ is an eigenfunction of the differential operator } u \mapsto \tfrac{\partial^2}{\partial x^2}[(1-x^2)u]}$$

$$\begin{aligned}\nabla^2\left[(1-y^2)(1-x^2)C_j^{(3/2)}(y)C_k^{(3/2)}(x)\right] = &-(j(j+3)+2)(1-x^2)C_j^{(3/2)}(y)C_k^{(3/2)}(x)\\ &-(k(k+3)+2)(1-y^2)C_j^{(3/2)}(y)C_k^{(3/2)}(x)\end{aligned}$$

Therefore, represent the solution in the basis

$$u(x,y) \approx \sum_{j=0}^{m-1}\sum_{k=0}^{n-1} X_{jk}(1-y^2)(1-x^2)C_j^{(3/2)}(y)C_k^{(3/2)}(x), \qquad (x,y)\in[-1,1]^2.$$

A sparse identity
Does it diagonalize Poisson?

$$\nabla^2 u = f$$

A sparse identity
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$$\nabla^2 \left[\sum_{j,k} X_{jk} (1 - y^2)(1 - x^2) C_j^{(3/2)}(y) C_k^{(3/2)}(x) \right] = \sum_{j,k} F_{jk} C_j^{(3/2)}(y) C_k^{(3/2)}(x)$$

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We know the action of ∇^2 on this basis:

$$\begin{aligned} \nabla^2 \left[(1 - y^2)(1 - x^2) C_j^{(3/2)}(y) C_k^{(3/2)}(x) \right] = & -(k(k+3)+2)(1 - y^2) C_j^{(3/2)}(y) C_k^{(3/2)}(x) \\ & -(j(j+3)+2)(1 - x^2) C_j^{(3/2)}(y) C_k^{(3/2)}(x) \end{aligned}$$

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Does it diagonalize Poisson?

diagonal

$$MXD^T + DXM^T = F$$

symmetric pentadiagonal

[NIST DLMF, 18.9.7-8]

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$$AX - XB = D^{-1}FD^{-1} \qquad \begin{aligned} A &= D^{-1}M, \\ B &= -M^T D^{-1} \end{aligned}$$

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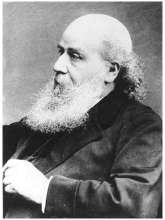

James Sylvester

A pentadiagonal Sylvester equation

Aleksandr Lyapunov

The alternating direction implicit (ADI) method
Solving Sylvester equations

$$AX - XB = F \qquad\qquad A, B, F \in \mathbb{C}^{n\times n}$$

- Based on **structured eigenvalues**


Donald Peaceman


Henry Rachford

$$AX - XB = F \qquad A, B, F \in \mathbb{C}^{n \times n}$$

still works for spectral

- Based on **structured eigenvalues**

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$$AX - XB = F \qquad\qquad A, B, F \in \mathbb{C}^{n\times n}$$

set $X_0 := 0$

choose shift parameters $p_j, q_j \in \mathbb{C}$

for $j = 0, 1, \ldots, J-1$

  solve $X_{j+1/2}(B - p_j I) = F - (A - p_j I)X_j$

  solve $(A - q_j I)X_{j+1} = F - X_{j+1/2}(B - q_j I)$

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2. How many iterations J do we need?

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for $j = 0, 1, \ldots, \boldsymbol{J} - 1$

  solve $X_{j+1/2}(\boldsymbol{B} - \boldsymbol{p_j I}) = F - (A - p_j I)X_j$

  solve $(\boldsymbol{A} - \boldsymbol{q_j I})X_{j+1} = F - X_{j+1/2}(B - q_j I)$

1. What shifts p_j, q_j should we choose?
2. How many iterations J do we need?
3. What is the cost of each iteration?

ADI as a fast direct solver

Three requirements

$$AX - XB = F \qquad\qquad A, B, F \in \mathbb{C}^{n\times n}$$

Three requirements on A and B will help us answer those three questions:

- P1. A and B are normal matrices.
- P2. There are real, disjoint intervals such that $\sigma(A) \subset [a, b]$, $\sigma(B) \subset [c, d]$.
- P3. For any $p \in \mathbb{C}$, $(A - pI)x = f$ and $(B - pI)x = f$ can be solved in $\mathcal{O}(n)$ operations.

ADI as a fast direct solver
Normal matrices

P1. A and B are normal matrices.

Then there is a bound on $\|X - X_J\|_2$ based on the spectra $\sigma(A)$, $\sigma(B)$ and the chosen shifts $p_0, \ldots, p_{J-1}$ and $q_0, \ldots, q_{J-1}$:

$$\frac{\|X - X_J\|_2}{\|X\|_2} \leq \frac{\sup_{z\in\sigma(A)} |r(z)|}{\inf_{z\in\sigma(B)} |r(z)|}, \qquad r(z) = \frac{\prod_{j=0}^{J-1}(z - p_j)}{\prod_{j=0}^{J-1}(z - q_j)}.$$

Goal: choose shifts p_j, q_j so that the rational function $r(z)$ makes the bound as small as possible:

$$\frac{\sup_{z\in\sigma(A)} |r(z)|}{\inf_{z\in\sigma(B)} |r(z)|} = \inf_{s\in\mathfrak{R}_{J,J}} \frac{\sup_{z\in\sigma(A)} |s(z)|}{\inf_{z\in\sigma(B)} |s(z)|}$$

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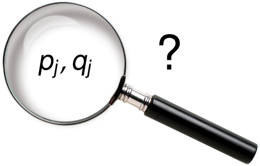
rational functions



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$$\frac{\|X - X_J\|_2}{\|X\|_2} \leq Z_J(\sigma(A), \sigma(B)), \qquad r(z) = \frac{\prod_{j=0}^{J-1}(z - p_j)}{\prod_{j=0}^{J-1}(z - q_j)}.$$

<u>Goal</u>: choose shifts p_j, q_j so that the rational function $r(z)$ makes the bound as small as possible:

$$\underbrace{Z_J(\sigma(A), \sigma(B))}_{\text{Zolotarev number}} = \inf_{s \in \mathfrak{R}_{J,J}} \frac{\sup_{z\in\sigma(A)} |s(z)|}{\inf_{z\in\sigma(B)} |s(z)|}$$

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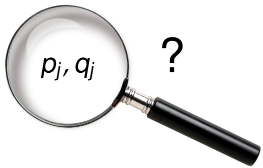

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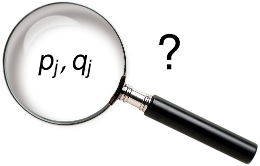

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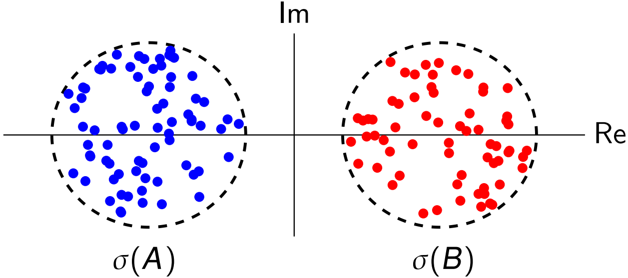
Yegor Zolotarev



P2. There are real, disjoint intervals such that $\sigma(A) \subset [a,b], \ \sigma(B) \subset [c,d]$.

The **Zolotarev problem** is well-studied for real spectra.

1. Optimal shifts are known: for $[a,b] = [-\alpha,-1]$ and $[c,d] = [1,\alpha]$

$$p_j = -\alpha \, \mathrm{dn}\left[\tfrac{2j+1}{2J} K\left(\sqrt{1-\tfrac{1}{\alpha^2}}\right), \sqrt{1-\tfrac{1}{\alpha^2}}\right]$$
$$q_j = \quad \alpha \, \mathrm{dn}\left[\tfrac{2j+1}{2J} K\left(\sqrt{1-\tfrac{1}{\alpha^2}}\right), \sqrt{1-\tfrac{1}{\alpha^2}}\right]$$

[Zolotarev, 1877]
[Lu & Wachspress, 1991]

ADI as a fast direct solver

Real separated spectra

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Jacobi elliptic function

complete elliptic integral of the first kind

[Zolotarev, 1877]
[Lu & Wachspress, 1991]

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1. Optimal shifts are known: Möbius transformations preserve rational functions, so set $\alpha = 2\sqrt{\gamma^2 - \gamma} + 2\gamma + 1$ with $\gamma = \frac{|c-a||d-b|}{|c-b||d-a|}$:

$$p_j = T\left(-\alpha \,\mathrm{dn}\left[\frac{2j+1}{2J} K\left(\sqrt{1-\frac{1}{\alpha^2}}\right), \sqrt{1-\frac{1}{\alpha^2}}\right]\right)$$

$$q_j = \underbrace{T}_{\substack{\text{Möbius transformation} \\ \{-\alpha,-1,1,\alpha\} \mapsto \{a,b,c,d\}}}\left(\ \ \alpha \,\mathrm{dn}\left[\frac{2j+1}{2J} K\left(\sqrt{1-\frac{1}{\alpha^2}}\right), \sqrt{1-\frac{1}{\alpha^2}}\right]\right)$$

[Sabino, 2007]

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The **Zolotarev problem** is well-studied for real spectra.

2. There is an upper bound on $Z_J([a, b], [c, d])$:

$$Z_J([a,b],[c,d]) \leq 4\left[\exp\left(\frac{\pi^2}{2\log(16\gamma)}\right)\right]^{-2J}$$

[Braess & Hackbusch, 2005]
[Beckermann & Townsend, 2017]

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1. Optimal shifts are known.
2. There is an upper bound on $Z_J([a,b],[c,d])$.

Run ADI with the optimal shifts p_j, q_j. The J^{th} iterate has relative error:

$$\frac{\|X - X_J\|_2}{\|X\|_2} \leq 4\left[\exp\left(\frac{\pi^2}{2\log(16\gamma)}\right)\right]^{-2J}$$

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Run ADI with the optimal shifts p_j, q_j. The J^{th} iterate has relative error:

$$\frac{\|X - X_J\|_2}{\|X\|_2} \leq 4 \left[\exp\left(\frac{\pi^2}{2 \log(16\gamma)} \right) \right]^{-2J}$$

a priori error estimate

P2. There are real, disjoint intervals such that $\sigma(A) \subset [a, b]$, $\sigma(B) \subset [c, d]$.

The **Zolotarev problem** is well-studied for real spectra.

1. Optimal shifts are known.
2. There is an upper bound on $Z_J([a, b], [c, d])$.

How does γ scale with n?

For a given tolerance $0 < \epsilon < 1$, iterate

$$J = \left\lceil \frac{\log(16\gamma)\log(4/\epsilon)}{\pi^2} \right\rceil$$

times. Then $\|X - X_J\|_2 \leq \epsilon \|X\|_2$.

a priori error estimate

ADI as a fast direct solver

Fast shifted linear solves

P3. For any $p \in \mathbb{C}$, $(A - pI)x = f$ and $(B - pI)x = f$ can be solved in $\mathcal{O}(n)$ operations.

set $X_0 := 0$

choose shift parameters $p_j, q_j \in \mathbb{C}$

for $j = 0, 1, \dots, J-1$

$$\left.\begin{aligned} &\text{solve}\quad X_{j+1/2}(B - p_j I) = F - (A - p_j I)X_j \\ &\text{solve}\quad (A - q_j I)X_{j+1} = F - X_{j+1/2}(B - q_j I) \end{aligned}\right\} \mathcal{O}(n^2)$$

Then the total cost of ADI is $\mathcal{O}(Jn^2)$. (Is $J = \mathcal{O}(\log n)$?)

ADI as a fast direct solver

Three requirements

P1. A and B are normal matrices.

P2. There are real, disjoint intervals such that $\sigma(A) \subset [a, b],\ \sigma(B) \subset [c, d]$.

P3. For any $p \in \mathbb{C}$, $(A - pI)x = f$ and $(B - pI)x = f$ can be solved in $\mathcal{O}(n)$ operations.

1. What shifts p_j, q_j should we choose?
2. How many iterations J do we need?
3. What is the cost of each iteration?

ADI as a fast direct solver

Three requirements

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1. What shifts p_j, q_j should we choose? P1 + P2
2. How many iterations J do we need?
3. What is the cost of each iteration?

ADI as a fast direct solver

Three requirements

- P1. A and B are normal matrices.
- P2. There are real, disjoint intervals such that $\sigma(A) \subset [a, b]$, $\sigma(B) \subset [c, d]$.
- P3. For any $p \in \mathbb{C}$, $(A - pI)x = f$ and $(B - pI)x = f$ can be solved in $\mathcal{O}(n)$ operations.

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2. How many iterations J do we need? P1 + P2
3. What is the cost of each iteration? P3

ADI as a fast direct solver
Three requirements

Back to our spectral discretization:

$$AX - XB = D^{-1}FD^{-1} \qquad \begin{aligned} A &= D^{-1}M, \\ B &= -M^T D^{-1} \end{aligned}$$

ADI as a fast direct solver
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ADI as a fast direct solver
Three requirements

Back to our spectral discretization:

$$\tilde{A}\tilde{X} - \tilde{X}\tilde{B} = D^{-1/2} F D^{-1/2} \qquad \begin{aligned} \tilde{A} &= D^{-1/2} M D^{1/2}, \\ \tilde{B} &= -D^{1/2} M^T D^{-1/2} \end{aligned}$$

P1. A and B are normal matrices.

Transform A and B to normal matrices:

$$\begin{aligned} \tilde{A} &= D^{1/2} A D^{-1/2} \\ \tilde{B} &= D^{-1/2} B D^{1/2} \end{aligned}$$

$\checkmark$

and recover $X = D^{-1/2} \tilde{X} D^{1/2}$.

ADI as a fast direct solver

Three requirements

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ADI as a fast direct solver
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P2. There are real, disjoint intervals such that $\sigma(\tilde{A}) \subset [a, b]$, $\sigma(\tilde{B}) \subset [c, d]$.

We can prove that

$$\sigma(\tilde{A}) \subset \left[-\tfrac{1}{2}, -\tfrac{1}{2n^4}\right], \quad \sigma(\tilde{B}) \subset \left[\tfrac{1}{2n^4}, \tfrac{1}{2}\right]$$

by bounding the zeros of $(1 - x^2)C^{(3/2)}(x)$. ✓

Therefore, $\gamma = \mathcal{O}(n^4)$ and $J = \mathcal{O}(\log \gamma) = \mathcal{O}(\log n)$.

ADI as a fast direct solver
Three requirements

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$$\tilde{A}\tilde{X} - \tilde{X}\tilde{B} = D^{-1/2} F D^{-1/2} \qquad \begin{aligned} \tilde{A} &= D^{-1/2} M D^{1/2}, \\ \tilde{B} &= -D^{1/2} M^T D^{-1/2} \end{aligned}$$

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$(\tilde{A} - pI)$ and $(\tilde{B} - pI)$ are pentadiagonal with zero sub- and super-diagonals.

We can use a variant of the Thomas algorithm to solve in $\mathcal{O}(n)$. ✓

A fast spectral Poisson solver on the square

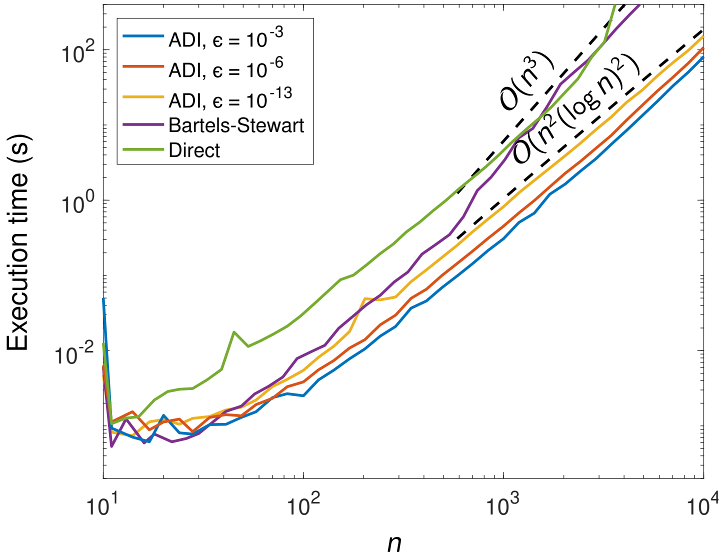
Recipe

For a given error tolerance $0 < \epsilon < 1$: **Cost**

1. Compute $C^{(3/2)}$ coefficients of f — $\mathcal{O}(n^2(\log n)^2 \log 1/\epsilon)$ [Townsend, Webb, & Olver, 2018]
2. Solve matrix equation using ADI — $\mathcal{O}(n^2 \log n \log 1/\epsilon)$
   - $\mathcal{O}(n^2)$ per iteration
   - $\mathcal{O}(\log n \log 1/\epsilon)$ iterations
3. Convert solution to Chebyshev — $\mathcal{O}(n^2(\log n)^2 \log 1/\epsilon)$ [Townsend, Webb, & Olver, 2018]

$$\mathcal{O}(n^2(\log n)^2 \log 1/\epsilon)$$

A fast spectral Poisson solver on the square
Comparison



ADI as a rank-revealing algorithm
Solutions can have low numerical rank

Theorem (F. & Townsend)

The numerical rank of the solution is bounded by

$$\mathrm{rank}_\epsilon(X) \leq \left\lceil \frac{\log(4n^4)\log(4/\epsilon)}{\pi^2} \right\rceil \mathrm{rank}(F),$$

where $\mathrm{rank}_\epsilon(X)$ *is the smallest* k *such that* $\sigma_{k+1}(X)/\sigma_1(X) \leq \epsilon$.

ADI as a rank-revealing algorithm

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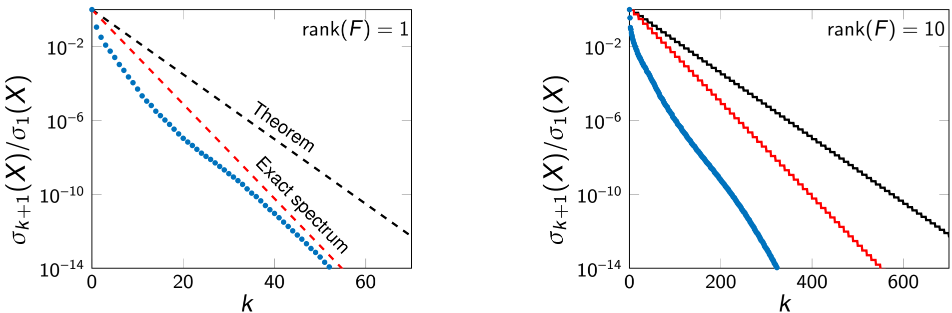
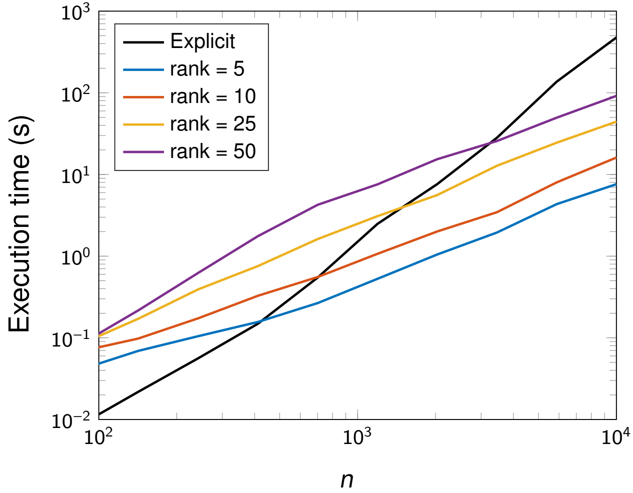


ADI as a rank-revealing algorithm

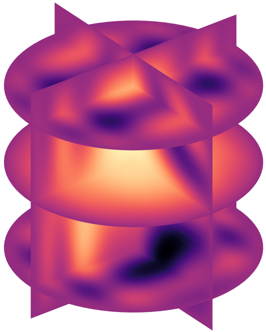
Computing low rank solutions

Factored ADI: given $F = MN^*$, rewrite ADI in terms of low rank factors $X = ZDY^*$

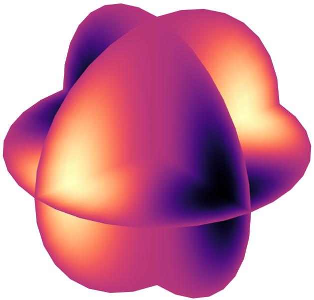


Fast spectral Poisson solvers on more domains

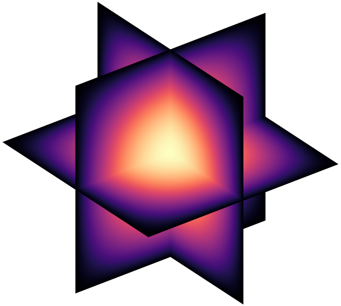
Cylinder, sphere, cube



Chebyshev–Fourier–Chebyshev
Double Fourier sphere
Partial regularity
N decoupled ADI solves
$\mathcal{O}(n^3(\log n)^2)$

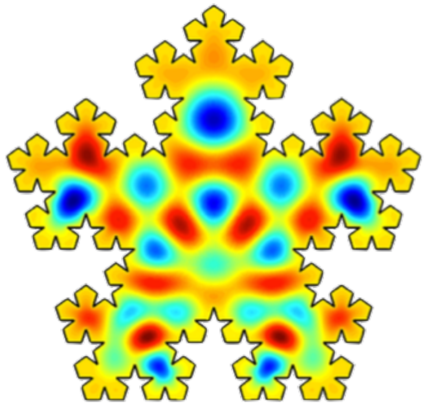


Chebyshev–Fourier–Fourier
Double Fourier sphere
Partial regularity
N decoupled ADI solves
$\mathcal{O}(n^3(\log n)^2)$



Chebyshev–Chebyshev–Chebyshev
Nested ADI iteration
$\mathcal{O}(n^3(\log n)^3)$

Towards more complex geometry
Spectral elements methods and *hp*-adaptivity



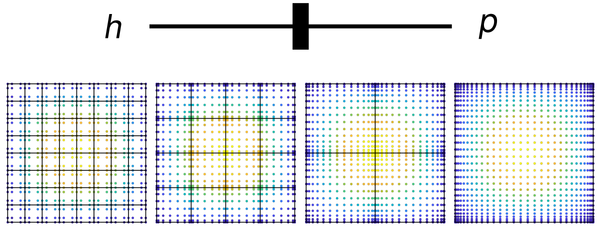
?

Towards more complex geometry

Spectral elements methods and *hp*-adaptivity

SEMs combine:

- the flexibility of finite element methods
- the convergence properties of global spectral methods



Towards more complex geometry
Spectral elements methods and *hp*-adaptivity

SEMs combine:

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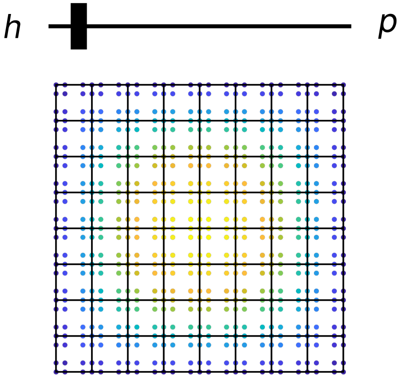

Towards more complex geometry
Spectral elements methods and *hp*-adaptivity

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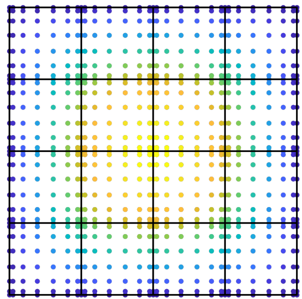

Towards more complex geometry
Spectral elements methods and *hp*-adaptivity

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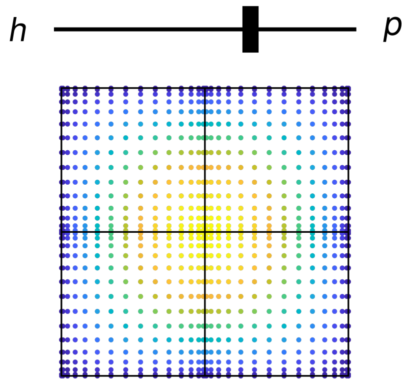

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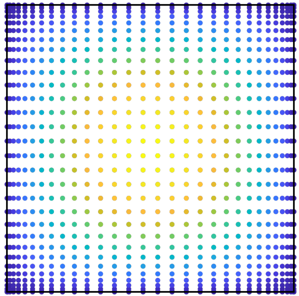

Towards more complex geometry
Spectral elements methods and *hp*-adaptivity

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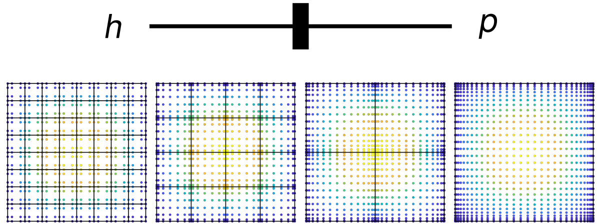


Most SEMs cost $\mathcal{O}(p^6/h^2) = \mathcal{O}(N p^4)$, so the slider is biased.

"In practice, hp-adaptivity means p $\lesssim$ 6." [Sherwin, 2014]

Hierarchical Poincaré–Steklov method

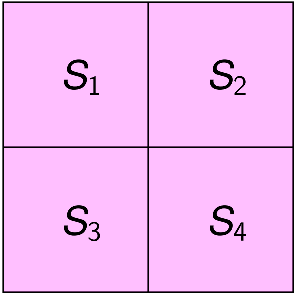
- Patch operators by imposing C^1 continuity across interface
- Merge squares up the tree

Gunnar Martinsson

Adrianna Gillman

[Martinsson, 2013]

[Gillman & Martinsson, 2014]



Hierarchical Poincaré–Steklov method

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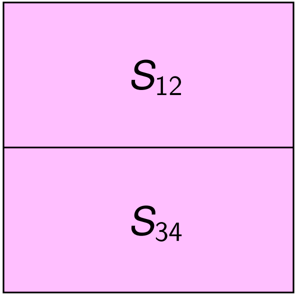

[Martinsson, 2013]

[Gillman & Martinsson, 2014]

Towards more complex geometry
A spectral element method for very high p

Hierarchical Poincaré–Steklov method

- Patch operators by imposing C^1 continuity across interface
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Gunnar Martinsson


Adrianna Gillman

[Martinsson, 2013]

[Gillman & Martinsson, 2014]

Hierarchical Poincaré–Steklov method

- Patch operators by imposing C^1 continuity across interface
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Gunnar Martinsson

Adrianna Gillman

$$+ \quad \text{ADI} \quad = \quad \mathcal{O}(p^3)$$

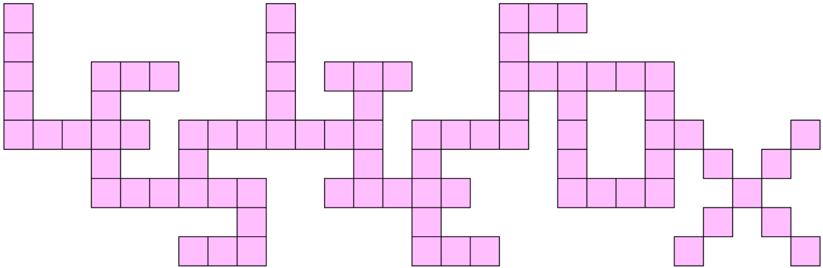
on squares

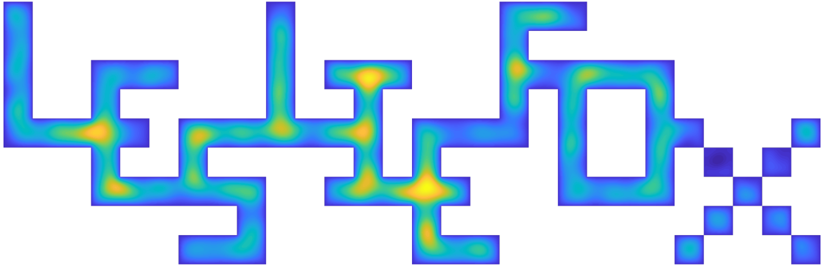
[Martinsson, 2013]

[Gillman & Martinsson, 2014]

Towards more complex geometry

A spectral element method for very high p





$p = 50$

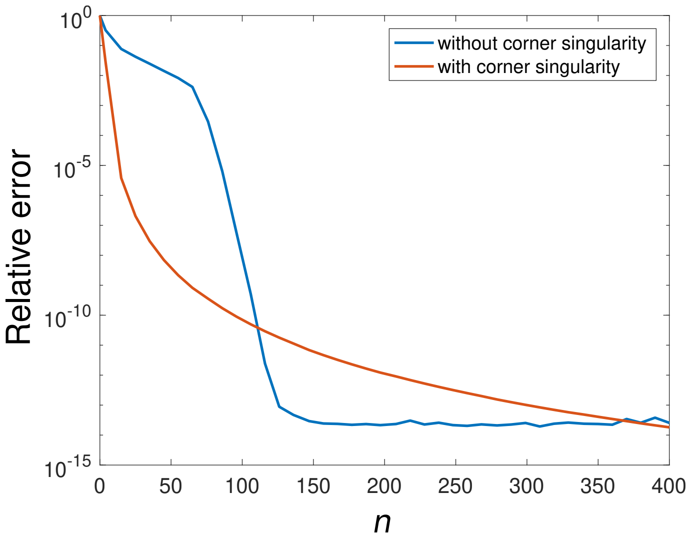
$\sim$6 sec

Thank you

More information in: F. & Townsend, "Fast Poisson solvers for spectral methods," to appear in IMA J. Numer. Anal.

Code publicly available:
`https://github.com/danfortunato/fast-poisson-solvers`

Corner singularities



A connection to finite differences

Exploiting structured eigenvalues

$$KX + XK^T = F, \qquad K = \frac{1}{h^2}\begin{bmatrix} 2 & -1 & & \\ -1 & \ddots & \ddots & \\ & \ddots & \ddots & -1 \\ & & -1 & 2 \end{bmatrix}$$

A connection to finite differences
Exploiting structured eigenvalues

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P1. A and B are normal matrices.

$$KX + XK^T = F, \qquad K = \frac{1}{h^2}\begin{bmatrix} 2 & -1 & & \\ -1 & \ddots & \ddots & \\ & \ddots & \ddots & -1 \\ & & -1 & 2 \end{bmatrix}$$

P1. A and B are normal matrices.

$A = K$ and $B = -K^T$ are real and symmetric, so are normal.

✓

A connection to finite differences
Exploiting structured eigenvalues

$$KX + XK^T = F, \qquad K = \frac{1}{h^2}\begin{bmatrix} 2 & -1 & & \\ -1 & \ddots & \ddots & \\ & \ddots & \ddots & -1 \\ & & -1 & 2 \end{bmatrix}$$

P2. There are real, disjoint intervals such that $\sigma(A) \subset [a, b]$, $\sigma(B) \subset [c, d]$.

A connection to finite differences
Exploiting structured eigenvalues

$$KX + XK^T = F, \qquad K = \frac{1}{h^2}\begin{bmatrix} 2 & -1 & & \\ -1 & \ddots & \ddots & \\ & \ddots & \ddots & -1 \\ & & -1 & 2 \end{bmatrix}$$

P2. There are real, disjoint intervals such that $\sigma(A) \subset [a, b]$, $\sigma(B) \subset [c, d]$.

The eigenvalues of K are

$$-n^2 \sin^2(\pi k/2n), \qquad 1 \leq k \leq n-1$$

✓

Since $(2/\pi)x \leq \sin(x) \leq 1$ for $x \in [0, \pi/2]$, we have:

$$\sigma(A) \subset [-n^2, -1], \qquad \sigma(B) \subset [1, n^2].$$

$$KX + XK^T = F, \qquad K = \frac{1}{h^2}\begin{bmatrix} 2 & -1 & & \\ -1 & \ddots & \ddots & \\ & \ddots & \ddots & -1 \\ & & -1 & 2 \end{bmatrix}$$

P3. For any $p \in \mathbb{C}$, $(A - pI)x = f$ and $(B - pI)x = f$ can be solved in $\mathcal{O}(n)$ operations.

A connection to finite differences

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$(A - pI)$ and $(B - pI)$ are tridiagonal. Solve with Thomas algorithm in $\mathcal{O}(n)$.

✓

A connection to finite differences

Exploiting structured eigenvalues