Towards Textbook Multigrid for the Helmholtz Equation

Oliver Ernst

Collaborators: Martin Gander, Ira Livshits Shu-Lin Wu
Howard Elman, Dianne O'Leary

Celebration in Honor of Dianne P. O'Leary
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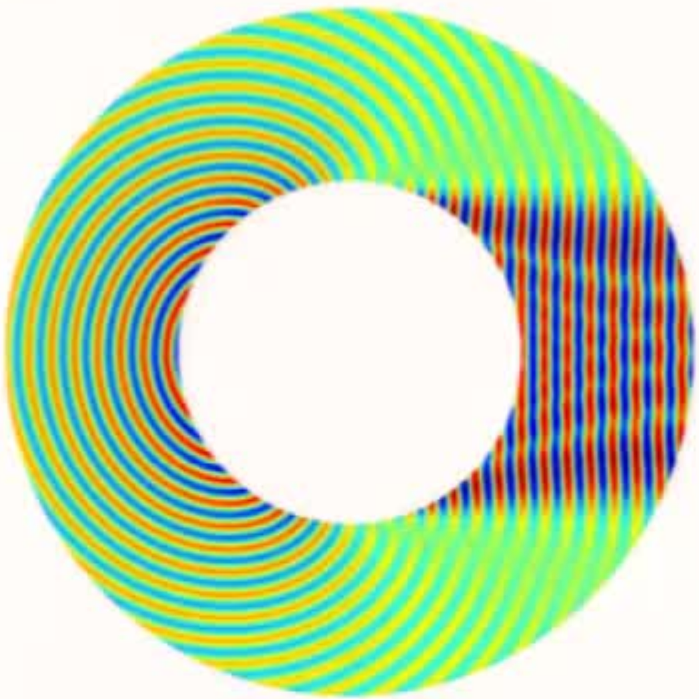
Mathematik!
TU Chemnitz

Prof. O'Leary and Me

- Academic siblings: Gene Golub PhD's #11 and #23.
- The capacitance matrix method.
- Collaboration 1997/98 as postdoctoral fellow at University of Maryland.
- 2 joint papers:
  [Elman, E. & O'Leary, 2001], [Elman, E., & O'Leary, Stewart, 2005]
- the Helmholtz equation ...



Outline

1. Solving the Helmholtz Equation: Some History

2. Dianne O'Leary's Contributions

3. Recent Developments

Helmholtz Equation

The continuous problem

$$-\Delta u - k^2 u = f, \qquad \partial_r u - iku = o(r^{(d-1)/2}),\ r \to \infty.$$

Applications:

- Wave propagation problems: acoustics, EM, elasticity
- Inverse problems: seismic/EM imaging, medical imaging, shape ID
- Control problems: acoustic/EM design, cloaking

Variants:

- Scattering, propagation: k real, constant; exterior BVP.
- Inhomogeneous medium: $k = k(x)$, $\operatorname{Im} k \geq 0$.

Discretization:

- Solutions highly oscillatory for large k: e^{ikx}.
  Resolution with mesh size h necessitates keeping kh small (analogous statements for p-refinement).
- Pollution effect: stability constant (inf-sup) proportional to $1/k$.
  [Ihlenburg & Babuška, 1997], [Melenk & Sauter, 2011]

Helmholtz Equation

The discrete problem

$$\boldsymbol{A}\boldsymbol{u} = \boldsymbol{f}, \qquad \boldsymbol{A} = \boldsymbol{A}(k,h) \in \mathbb{C}^{N\times N}.$$

Properties:

- Resolution dictates fine meshes, i.e., N large.
- Pollution (stability) dictates even larger N.
- Sparse direct solvers of limited applicability.
- $\boldsymbol{A}$ complex-symmetric, not Hermitian (non-normal).
- $\boldsymbol{A}$ increasingly indefinite as $|k|$ grows (many eigenvalues in left half-plane).
- Iterative solvers (Krylov subspace/multigrid/domain decomposition methods) plagued with difficulties, cf. [E. & Gander, 2012].

Helmholtz Equation
The discrete problem

$$\boldsymbol{A}\boldsymbol{u} = \boldsymbol{f}, \qquad \boldsymbol{A} = \boldsymbol{A}(k, h) \in \mathbb{C}^{N \times N}.$$

Compare with evolution of complexity for solving $-\Delta u = f$ with N DOF (on 3D cube to accuracy ϵ):

Method	Complexity	
GE	N^3	
Banded GE	$N^{2+1/3}$	
Jacobi/Gauss-Seidel	$N^{1+2/3} \log \epsilon$	
SOR	$N^{1+1/3} \log \epsilon$	
CG	$N^{1+1/3} \log \epsilon$	
ICCG	$N^{1+1/6} \log \epsilon$	
fast Poisson solvers	$N \log N$	(separable domains only)
iterated multigrid	$N \log \epsilon$	
full multigrid	N	

Helmholtz Equation

Solution strategies

- Capacitance matrix methods
  [Proskurowski & Widlund, '76], [O'Leary & Widlund, '79/81],
  [E., '94/96], [Heikkola, Toivanen & Rossi, '03]
- Krylov method preconditioned with fast solver for nearby operator
  [Bayliss, Goldstein & Turkel, '83/84],
  [E. & Golub, '92], [Elman & O'Leary, '98/99],
  [Laird & Giles, '02]
  [Erlangga, Oosterlee & Vuik, '04/06], [Erlangga, '08], [Erlangga & Nabben, '08]
  [Sheikh, Lahaye & Vuik, '13], [Gander, Graham & Spence, '15]
- Domain decomposition
  [Després, '91], [Toselli, '98], [Gander & al., '02], [Graham, Spence & Vainikko, '15]
- Multigrid
  [Yserentant, '86/88]
  [Brandt & Ta'asan, '86], [Brandt & Livshits, '97, '03/06]
  [Lee & al., '00] [Elman, E. & O'Leary, '01]
- Sweeping preconditioners
  [Engquist & Ying, '11], [PoulsonEtAl, '13]

Outline

Dianne O'Leary's Contributions

Capacitance matrix methods

MATHEMATICS OF COMPUTATION, VOLUME 33, NUMBER 147
JULY 1979, PAGES 849–879

Capacitance Matrix Methods for the Helmholtz Equation on General Three-Dimensional Regions

By Dianne P. O'Leary* and Olof Widlund**

Abstract. Capacitance matrix methods provide techniques for extending the use of fast Poisson solvers to arbitrary bounded regions. These techniques are further studied and developed with a focus on the three-dimensional case. A discrete analogue of classical potential theory is used as a guide in the design of rapidly convergent iterative methods. Algorithmic and programming aspects of the methods are also explored in detail. Several conjugate gradient methods are discussed for the solution of the capacitance matrix equation. A fast Poisson solver is developed which is numerically very stable even for indefinite Helmholtz equations. Variants thereof allow substantial savings in primary storage for problems on very fine meshes. Numerical results show that accurate solutions can be obtained at a cost which is proportional to that of the fast Helmholtz solver in use.

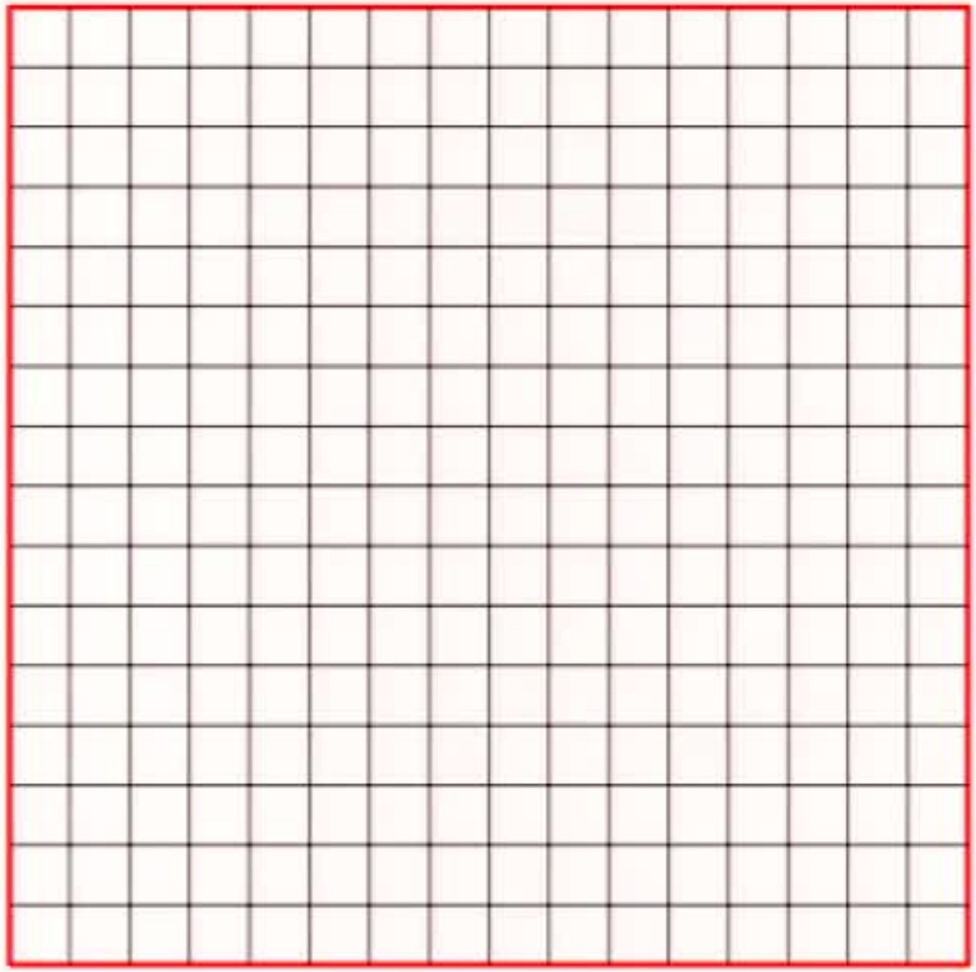
1. Introduction. It is well known that highly structured systems of linear algebraic equations arise when Helmholtz's equation

$$-\Delta u + cu = f, \quad c = \text{constant}, \tag{1.1}$$

p. 876: "Negative values of c lead to more difficult problems."

Dianne O'Leary's Contributions

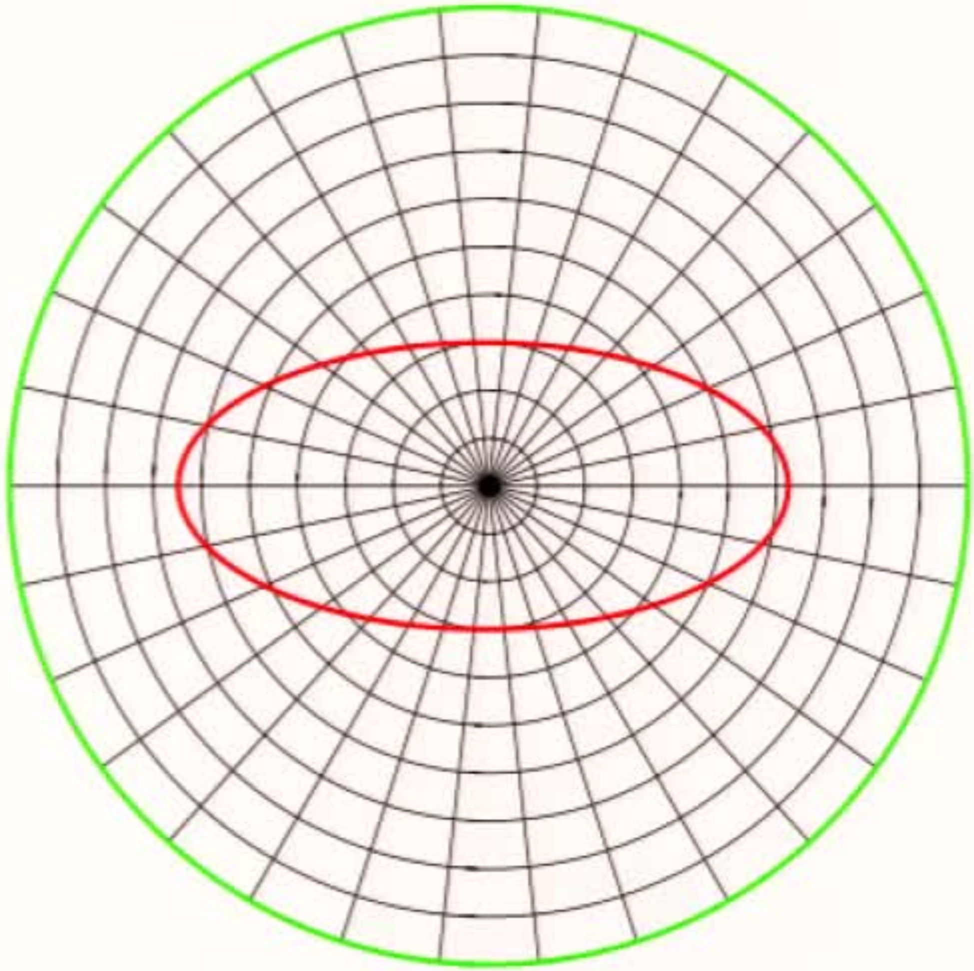
Capacitance matrix methods



[Elman & O'Leary, 1998], [Elman & O'Leary, 1999] (3D)

Dianne O'Leary's Contributions

Capacitance matrix methods



[E., '94,'96]

Dianne O'Leary's Contributions

[Elman, E. & O'Leary, 2001]

(Ideal) Multigrid for $\boldsymbol{Au} = \boldsymbol{f}$

- Smoothing (relaxation): $\tilde{\boldsymbol{u}} \approx \boldsymbol{A}^{-1}\boldsymbol{f}, \quad \boldsymbol{M} \approx \boldsymbol{A}$

$$\boldsymbol{u} = \tilde{\boldsymbol{u}} + \underbrace{(\boldsymbol{u} - \tilde{\boldsymbol{u}})}_{\boldsymbol{e}} = \tilde{\boldsymbol{u}} + \boldsymbol{A}^{-1}\underbrace{(\boldsymbol{f} - \boldsymbol{A}\tilde{\boldsymbol{u}})}_{\boldsymbol{r}} \approx \tilde{\boldsymbol{u}} + \boldsymbol{M}^{-1}(\boldsymbol{f} - \boldsymbol{A}\tilde{\boldsymbol{u}})$$

$$\boldsymbol{u} \leftarrow \boldsymbol{u} + \boldsymbol{M}^{-1}(\boldsymbol{f} - \boldsymbol{Au}), \qquad \boldsymbol{e} \leftarrow (\boldsymbol{I} - \boldsymbol{M}^{-1}\boldsymbol{A})\boldsymbol{e}, \quad \text{leads to smooth } \boldsymbol{e}.$$

- Coarse grid correction: $\boldsymbol{A} = \boldsymbol{A}_h$, $\boldsymbol{e} = \boldsymbol{e}^h \approx \boldsymbol{I}_H^h \boldsymbol{e}^H$

$$\boldsymbol{A}_h \boldsymbol{e}^h = \boldsymbol{r}^h \longrightarrow \boldsymbol{A}_h \boldsymbol{I}_H^h \boldsymbol{e}^H = \boldsymbol{r}^h \longrightarrow \underbrace{\boldsymbol{I}_h^H \boldsymbol{A}_h \boldsymbol{I}_H^h}_{\boldsymbol{A}_H} \boldsymbol{e}^H = \boldsymbol{I}_h^H \boldsymbol{r}^h$$

$$\boldsymbol{u}^h \leftarrow \boldsymbol{u}^h + \boldsymbol{I}_H^h \boldsymbol{A}_H^{-1} \boldsymbol{I}_h^H \boldsymbol{r}^h, \quad \boldsymbol{e}^h \leftarrow (\boldsymbol{I} - \boldsymbol{I}_H^h \boldsymbol{A}_H^{-1} \boldsymbol{I}_h^H \boldsymbol{A}_h)\boldsymbol{e}^h, \quad \text{removes smooth } \boldsymbol{e}.$$

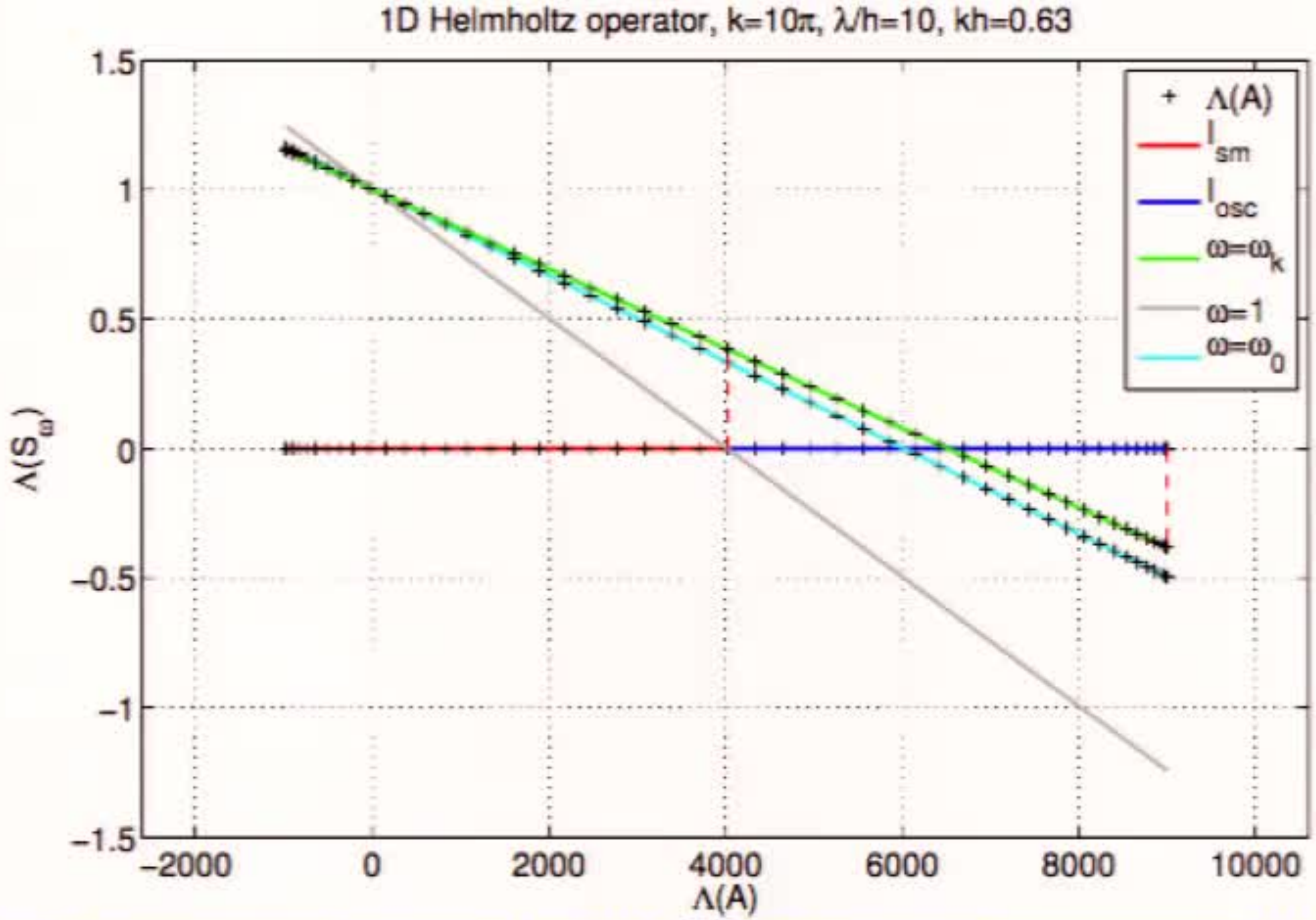
- Recursive application gives multigrid V-cycle iteration.
- Textbook multigrid efficiency: convergence of iteration h-independent.
  Goal for Helmholtz: convergence of iteration h- and k-independent.

Dianne O'Leary's Contributions

[Elman, E. & O'Leary, 2001]

Smoothing: e.g. damped Jacobi in 1D,

$$\boldsymbol{u} \leftarrow \boldsymbol{u} + \omega \boldsymbol{D}^{-1}(\boldsymbol{f} - \boldsymbol{A}\boldsymbol{u}), \qquad \boldsymbol{D} = \frac{2-(kh)^2)}{h^2}\boldsymbol{I}.$$



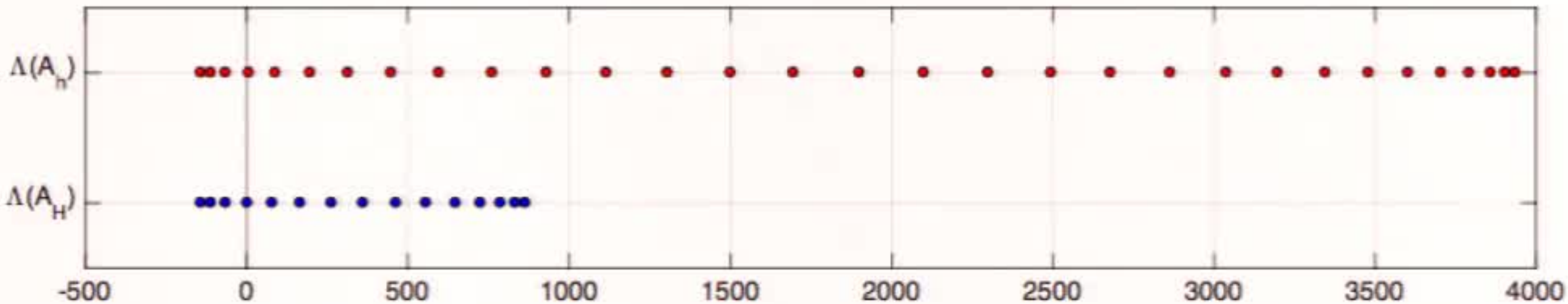
Dianne O'Leary's Contributions

[Elman, E. & O'Leary, 2001]

Coarse grid correction: acting on smooth fine-grid eigenmode $\boldsymbol{v}^h$

$$(\boldsymbol{I} - \boldsymbol{I}_H^h \boldsymbol{A}_H^{-1} \boldsymbol{I}_h^H \boldsymbol{A}_h)\boldsymbol{v}^h \approx \left(1 - \frac{\lambda^h}{\lambda^H}\right) \boldsymbol{v}^h$$

Example: Dirichlet problem on $(0,1)$, $k = 3.93\pi$, $h = 1/32$, $H = 2h$.



$$\left(1 - \frac{\lambda_1^h}{\lambda_1^H}\right) = 0.00017, \qquad \left(1 - \frac{\lambda_4^h}{\lambda_4^H}\right) = 2.4.$$

Dianne O'Leary's Contributions
[Elman, E. & O'Leary, 2001]

Coarse grid correction: acting on smooth fine-grid eigenmode $\boldsymbol{v}^h$

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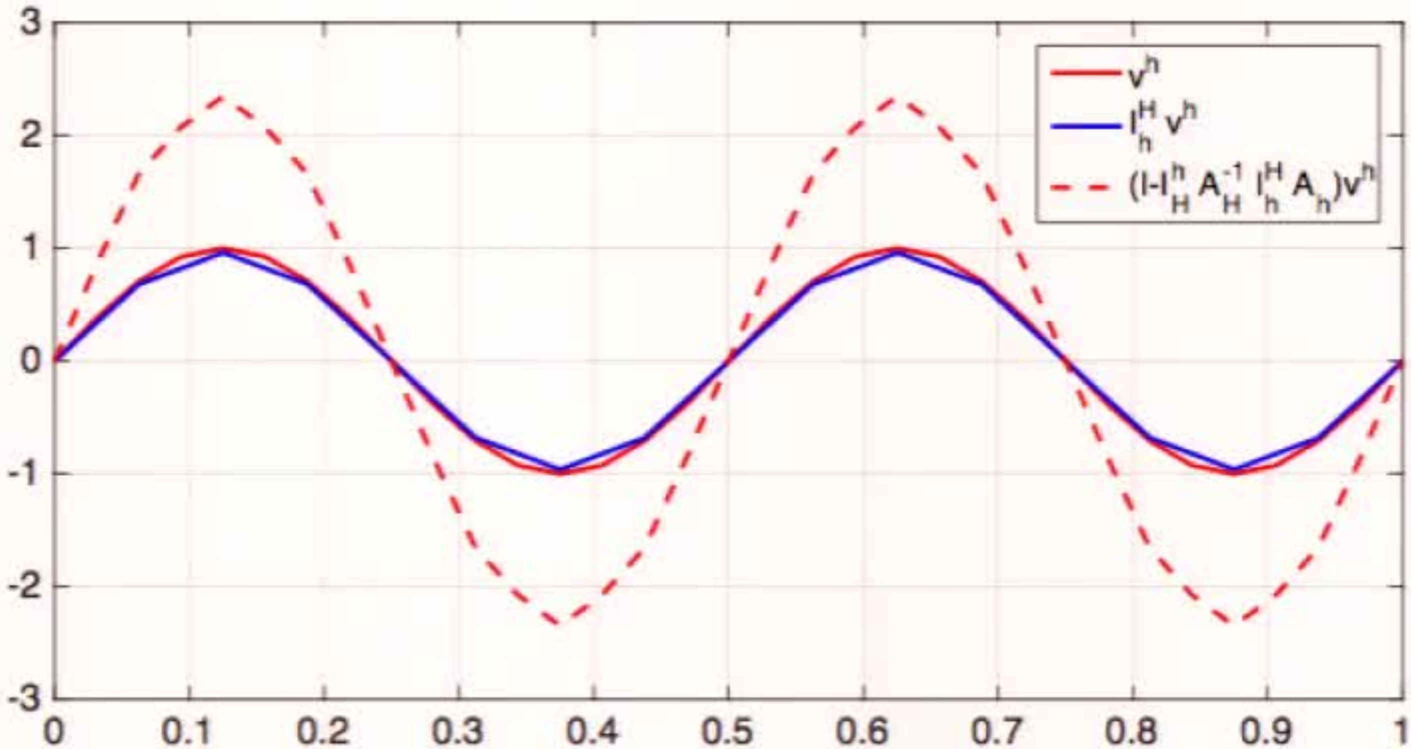

CGC acting on mode 4

Dianne O'Leary's Contributions

[Elman, E. & O'Leary, 2001]

How many eigenvalues cross the imaginary axis during coarsening?

Theorem (Elman, E. & O'Leary, 2001)

For 2nd order finite difference discretization of the Helmholtz equation with Dirichlet boundary conditions on the unit cube in d dimensions ($d = 1, 2, 3$), the number of eigenvalues that undergo a change in sign during the multigrid coarsening process is bounded above by

$$\begin{cases} k\left(\frac{1}{2} - \frac{1}{\pi}\right), & d = 1, \\ k^2\left(\frac{1}{8} - \frac{1}{4\pi}\right), & d = 2, \\ k^3\left(\frac{1}{24\sqrt{3}} - \frac{1}{6\pi^2}\right), & d = 3. \end{cases}$$

Similar bounds for bilinear finite element discretization.

Proof: For FD EV's move left; # known for $h = 0$;
no more movement once discrete problem negative definite.

Dianne O'Leary's Contributions

[Elman, E. & O'Leary, 2001]

Designing a method from this:

- GMRES as smoother on coarse grids; adaptive smoothing schedule.
- FGMRES as outer iteration.
- Reasonably (for the time) robust multigrid-based Helmholtz solver for general finite element discretizations using standard building blocks.

k	Size $E[\lambda]$	$(kh_{\max})_{\text{fine}}$	# Levels	MG	FGMRES
Dirichlet problem					
2π	1	.10	6	36	13
		.21	5	27	12
		.42	4	26	12
4π	2	.21	6	38	16
		.42	5	27	14
8π	4	.42	6	41	20
			5	—	28
			4	100	26
			3	41	16
			2	41	13

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3. Recent Developments

Recent Developments

Dispersion Correction

[E. & Gander, '12/13]

- Fourier modes $e^{ik^h x_j}$ of discrete (1D centered FD) Helmholtz operator possess discrete wave number k^h characterized by

$$\frac{k^h(k)}{k} = \frac{1}{kh} \arccos\left(1 - \frac{k^2 h^2}{2}\right) > 1,$$

resulting in a phase lead relative to continuous counterparts.

- **Idea:** Use modified wave number $\tilde{k}$ in coarse grid discretization such that

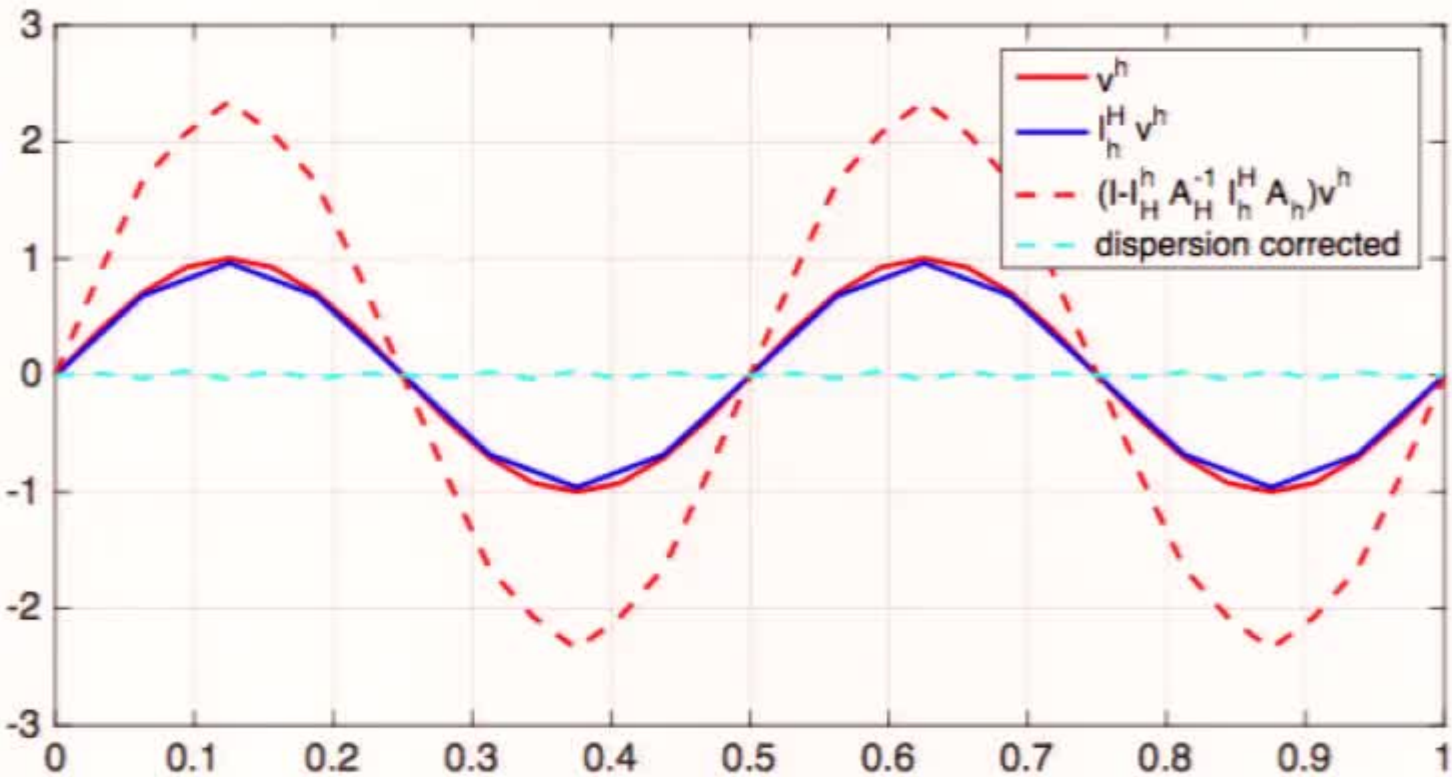
$$k^H(\tilde{k}) = k \qquad \text{or} \qquad k^H(\tilde{k}) = k^h$$

to offset phase lead in coarse grid correction.

- Similar ideas in [Stolk, Ahmed & Bhowmik, '14], [Stolk, '15]

Recent Developments
Dispersion Correction

In previous example: (coarse grid correction acting on smooth mode).

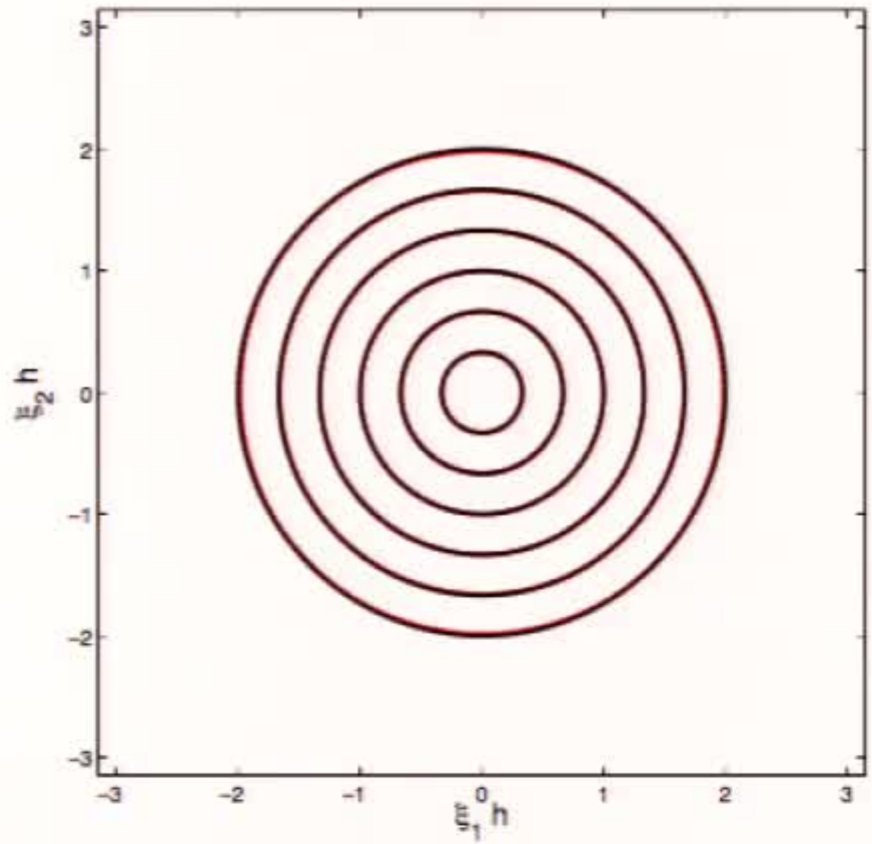


Used in [E. & Gander, '13] to prove convergence for modified V-cycle multigrid method for 1D Helmholtz equation that scales like $O(h^{-4/3})$.

Recent Developments
Dispersion Correction

2D/3D: more than one direction, but higher order discretizations have more isotropic dispersion relations. (cf. [Ainsworth, '04])

Slowness curves:



biquadratic FE

Recent Developments

Shifted Laplacian Preconditioning

- [Erlangga, Vuik & Oosterlee, '04], . . . :
  Standard multigrid works for Helmholtz problems with sufficient absorption.
- Large literature, solver (preconditioner) of choice in geosciences.
- For bounded domain Ω, consider discretizations (linear FE)

$$\boldsymbol{A}: \begin{cases} -\Delta u - k^2 u = f & \text{in } \Omega \\ \partial_n u - iku = g & \text{on } \partial\Omega \end{cases} \qquad \boldsymbol{A}_\epsilon: \begin{cases} -\Delta u - (k + i\epsilon)^2 u = f & \text{in } \Omega \\ \partial_n u - i\mu(k,\epsilon) u = g & \text{on } \partial\Omega \end{cases}$$

$\boldsymbol{B}_\epsilon^{-1} \approx \boldsymbol{A}_\epsilon^{-1}$: multigrid V-cycle applied to $\boldsymbol{A}_\epsilon$.

- Solve $\boldsymbol{A}\boldsymbol{u} = \boldsymbol{f}$ by GMRES preconditioned by $\boldsymbol{A}_\epsilon$, applying $\boldsymbol{A}_\epsilon$ inexactly using $\boldsymbol{A}_\epsilon^{-1} \approx \boldsymbol{B}_\epsilon^{-1}$.

  Sufficient for convergence (exact): $\|\boldsymbol{I} - \boldsymbol{A}_\epsilon^{-1}\boldsymbol{A}\|_2 \lesssim C < 1$.

$$\boldsymbol{I} - \boldsymbol{B}_\epsilon^{-1}\boldsymbol{A} = \boldsymbol{I} - \boldsymbol{B}_\epsilon^{-1}\boldsymbol{A}_\epsilon + \boldsymbol{B}_\epsilon^{-1}\boldsymbol{A}_\epsilon(\boldsymbol{I} - \boldsymbol{A}_\epsilon^{-1}\boldsymbol{A})$$

  $\Rightarrow$ need $\boldsymbol{A}_\epsilon^{-1}$ to be good preconditioner for $\boldsymbol{A}$ and $\boldsymbol{B}_\epsilon^{-1}$ for $\boldsymbol{A}_\epsilon$.

Recent Developments

Shifted Laplacian Preconditioning

- Recently, [Gander, Graham & Spence, '15] have shown:

  For Lipschitz, star-shaped domains using quasi-uniform meshes (easy extension to shape-regular meshes)

  $$\|\boldsymbol{I} - \boldsymbol{A}_\epsilon^{-1}\boldsymbol{A}\| \lesssim \frac{\epsilon}{k}.$$

  Implies k-independent GMRES convergence for ϵ/k sufficiently small.

- [Graham, Spence & Vainikko, '15] have shown $\boldsymbol{B}_\epsilon^{-1} \approx \boldsymbol{A}_\epsilon^{-1}$ for $\boldsymbol{B}_\epsilon^{-1}$ a classical additive Schwarz domain decomposition preconditioner for $\boldsymbol{A}_\epsilon$ ($H \sim k^{-1}$). In this case

  $$\boldsymbol{B}_\epsilon^{-1} \text{ is optimal for } \boldsymbol{A}_\epsilon \text{ when } \epsilon \sim k^2.$$

- Question $\boldsymbol{B}_\epsilon^{-1} \approx \boldsymbol{A}_\epsilon^{-1}$ for multigrid V-cycle still open. Initial steps (1D) in [Coquet & Gander, '15].

Recent Developments
Wave-Ray Multigrid

In 1D: error and residual

$$e(x) = v_+(x)e^{ikx} + v_-(x)e^{-ikx}, \qquad r(x) = w_+(x)e^{ikx} + w_-(x)e^{-ikx}.$$

Obtain v_+ and v_- by solving ray equations

$$v_+''(x) + 2ikv_+(x) = w_+(x), \qquad v_-''(x) - 2ikv_-(x) = w_-(x).$$