Solving the Helmholtz equation at high frequency

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Collaborators:

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Jun Zou (Chinese University of Hong Kong)
and others

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Outline of talk

- A walk around Helmholtz-land
- Very large non-Hermitian indefinite matrices
- Iterative methods and preconditioning
- Convergence theory - absorptive case
- Some examples
- A glimpse of some new results for the propagative case

This is a very active area with many other groups working.
Recent survey: IGG, Spence, Zou, SINUM 58 (2020)

Hermann von Helmholtz 1821–1894:
worked in physiology, physics, philosophy

Reduced wave equation

$$-\Delta U + \frac{\partial^2 U}{\partial t^2} \;=\; F, \quad \text{on} \quad \mathbb{R}^3 \times \mathbb{R}$$

$$F(x,t) = \exp(\mathrm{i}kt) f(x)$$

$$U(x,t) = \exp(\mathrm{i}kt) u(x) \quad \text{separation of variables}$$

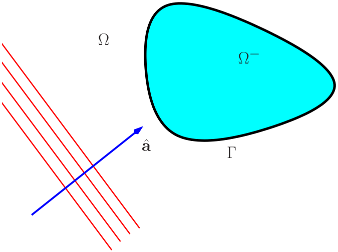
$$-(\Delta u + k^2 u) \;=\; f \quad \text{on} \quad \mathbb{R}^3$$

Helmholtz equation in its simplest form

“Elliptic” but “singularly perturbed” as $k \to \infty$

“Bandlimited data” $\Longrightarrow$ “solve in frequency domain”

Scattering problem: $u^i(x) = \exp(\mathrm{i}k\hat{a}.x)$



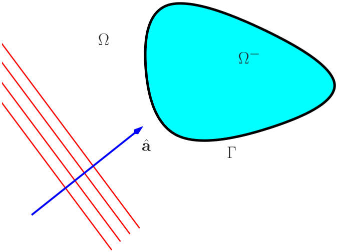
Scattered field u satisfies

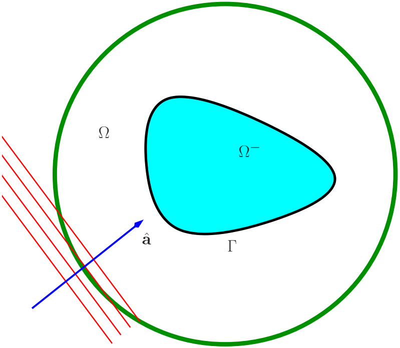
$$-(\Delta u + k^2 u) = 0 \text{ in } \Omega$$

$$u = -u^i \text{ on } \Gamma$$

S.R.C. $$\frac{\partial u}{\partial r} - \mathrm{i}ku = o(r^{-(d-1)/2}),\ r \to \infty \text{ in far field}$$

Scattering problem: $u^i(x) = \exp(ik\hat{a}.x)$





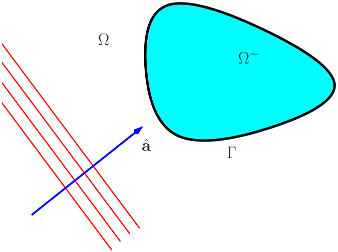
Scattered field u satisfies

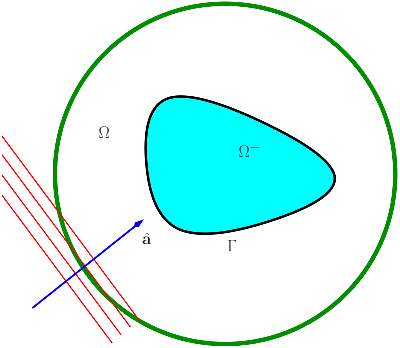
$$-(\Delta u + k^2 u) = 0 \text{ in } \Omega$$

$$u = -u^i \text{ on } \Gamma$$

Simplest $\frac{\partial u}{\partial r} - iku = 0$ Impedance cond. on 'far field boundary'

Scattering problem: $u^i(x) = \exp(ik\hat{a}.x)$





Scattered field u satisfies **Model Problem:**

$$-(\Delta u + k^2 u) = f \text{ in } \Omega$$

$$u = 0 \text{ on } \Gamma$$

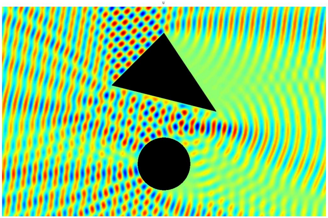
$$\frac{\partial u}{\partial r} - iku = g \quad \text{on 'far field boundary'} \quad \partial\Omega$$

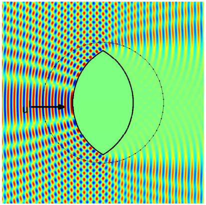
$\Omega^- = \emptyset \quad \longrightarrow \quad$ 'Interior impedance problem'

Oscillatory solutions

Plane wave scattering:

$$u^i(x) = \exp(ik\hat{a}.x)$$

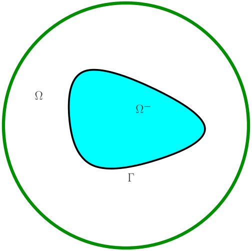




‘Hybrid Numerical - Asymptotic Methods’
Chandler-Wilde, IGG, Langdon, Spence 2012
Groth, Hewett, Langdon, 2019

Here we consider ‘standard’ FEM

Helmholtz stability



For the model problem: Assume
(i) Ω^-, and domain inside $\partial\Omega$ are Lipschitz and star-shaped with respect to a ball.
(ii) $f \in L^2(\Omega)$ and $g \in L^2(\partial\Omega)$.

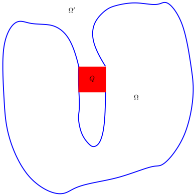
Then $\exists!$ $u \in H^1(\Omega)$ and

$$\underbrace{\|\nabla u\|^2_{L^2(\Omega)} + k^2\|u\|^2_{L^2(\Omega)}}_{=:\|u\|^2_{1,k}} \leq C_{\text{stab}}\{\|f\|^2_{L^2(\Omega)} + \|g\|^2_{L^2(\Gamma)}\}, \quad k \to \infty$$

C_{stab} indept of k. cf. Melenk 95, Cummings & Feng 06...

Not star-shaped - Geometric trapping

Square cavity



$C_{\text{stab}} \gtrsim k$

Chandler-Wilde, Spence, Gibbs, Smyshlyaev 2020

Elliptic cavity

$C_{\text{stab}} \gtrsim \exp(\beta k)$

some $\beta > 0$

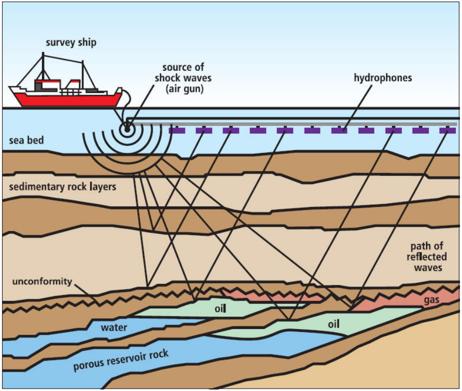
Betcke, Chandler-Wilde, IGG, Langdon and Lindner, 2011

Variable coefficients

$$
\begin{aligned}
-\Delta u - k^2 n u &= f \quad \text{in} \quad \text{bounded polyhedral domain} \quad \Omega \\
u &= 0 \quad \text{on} \quad \Gamma \\
\frac{\partial u}{\partial n} - iku &= g \quad \text{on} \quad \partial\Omega
\end{aligned}
$$

n ‘refractive index’ or ‘squared slowness’

Seismic imaging (Full waveform inversion)



Shaunagh Downing, Silvia Gazzola, Euan Spence and Schlumberger (Cambridge)

Variable coefficients

$$\begin{aligned} -\nabla . A \nabla u - k^2 n u &= f \quad \text{in} \quad \text{bounded polyhedral domain} \quad \Omega \\ u &= 0 \quad \text{on} \quad \Gamma \\ \frac{\partial u}{\partial n} - iku &= g \quad \text{on} \quad \partial\Omega \end{aligned}$$

A ‘diffusion coefficient’

Variable coefficients

$$
\begin{aligned}
-\Delta u - k^2 n u &= f \quad \text{in} \quad \text{bounded polyhedral domain} \quad \Omega \\
u &= 0 \quad \text{on} \quad \Gamma \\
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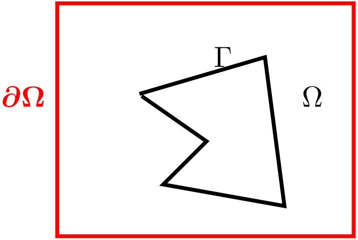
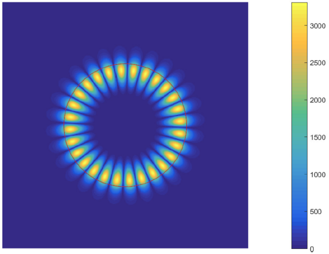


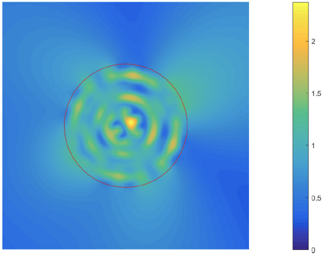
non-trapping condition:
$n(\boldsymbol{x}) + \boldsymbol{x}.\nabla n(\boldsymbol{x}) \geq \mu > 0$

IGG, Pembery, Spence, 2019
IGG, Sauter, 2020
Then stability, with
$C_{\text{stab}} = C_{\text{stab}}(\mu)$

Trapping can occur - but is very delicate



$k_1 = 1.77945199481921$



$k_3 = 1.779451994815$

$n = 2$ inside circle, $n = 1$ outside

Moiola and Spence 2019
Lafontaine, Spence, Wunch 2019

Finite Element Method

Global problem $u \in H^1(\Omega)$,

$$\underbrace{\int_\Omega (\nabla u.\nabla \overline{v} - k^2 n \; u\overline{v}) - \mathrm{i}k \int_{\partial\Omega} u\overline{v}}_{a(u,v)} = \int_\Omega f\overline{v} + \int_{\partial\Omega} g\overline{v}, \quad v \in H^1(\Omega)$$

Finite element discretization (degree p)

$$\mathbf{A}\mathbf{u} := (\mathbf{S} - k^2 \; \mathbf{M}_n - \mathrm{i}k\mathbf{N})\mathbf{u} = \mathbf{f}$$

For existence/error control: $h \sim k^{-1-1/2p}$ Du & Wu, 2015

For quasioptimality need : $h \sim k^{-1-1/p}$ Melenk & Sauter 2011

$\mathbf{A}$ complex symmetric non-Hermitian dimension n.
To accurately compute 100 waves in Ω need n DoFs, with

$$n \sim 10^7 \text{ in 2D}, \quad n \sim 10^{10} \text{ in 3D}$$

Poisson versus Helmholtz (at high frequency)

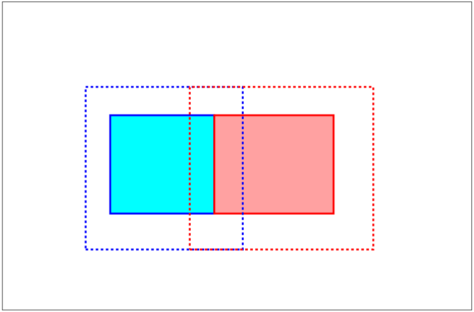
	$-\Delta u = f$ bounded domain + boundary cond.	$-\Delta u - k^2 nu = f$ k large + far field condition
∃! solution?	✓	✓
Solution bounded in terms of data?	✓	NO!
FE solution exists?	✓	$h \sim k^{-(1+1/2p)}$
Quasioptimal?	✓	$h \sim k^{-(1+1/p)}$
Efficient solver for linear systems?	✓	NO!

Iterative solver for linear systems

Iterative method : GMRES (Generalized minimum residual)

$$\mathbf{A}\mathbf{u} = \mathbf{f} \qquad \Longleftrightarrow \qquad \mathbf{B}^{-1}\mathbf{A}\mathbf{u} = \mathbf{B}^{-1}\mathbf{f}$$

Domain decomposition: overlapping subdomains Ω_ℓ



Iterative solver for linear systems

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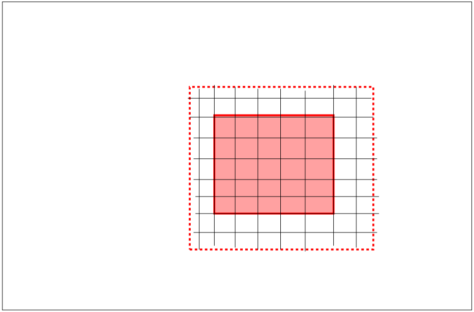


'Local' impedance matrices

$$\mathbf{A}_\ell \sim \int_{\Omega_\ell} (\nabla u . \nabla \overline{v} - k^2 u \overline{v}) - \mathrm{i}k \int_{\partial\Omega_\ell} u \overline{v}$$

Preconditioners based on Ω_ℓ:

'SORAS': $\mathbf{B}^{-1} := \sum_\ell \mathbf{R}_\ell^\top \mathbf{D}_\ell \mathbf{A}_\ell^{-1} \mathbf{D}_\ell \mathbf{R}_\ell$

'ORAS': $\mathbf{B}^{-1} := \sum_\ell \mathbf{R}_\ell^\top \mathbf{D}_\ell \mathbf{A}_\ell^{-1} \mathbf{R}_\ell$

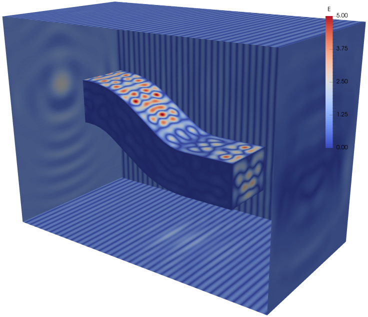
$\mathbf{R}_\ell, \mathbf{R}_\ell^\top$ Restriction and prolongation:

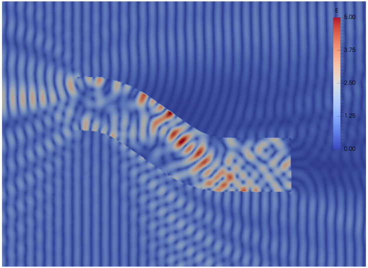
$\sum_\ell \mathbf{D}_\ell \equiv 1$ partition of unity

Enhance performance by adding solve in a coarse space

3D Maxwell (“cobra cavity” at 10 GHz):

with M. Bonazzoli, P.-H. Tournier, V. Dolean, E. Spence





Nédélec elements, degree 2:

Fine grid: 10 pts/wavelength $\Longrightarrow \sim 107,000,000$ DOFs

Coarse grid: 3.3 pts/wavelength (inner GMRES, $\varepsilon_{\rm prec} = k$)

cores	outer GMRES iterations	Total time
1536	31	515.8
3072	32	285.0

Convergence theory for GMRES

GMRES for preconditoned system $\mathbf{B}^{-1}\mathbf{A}\mathbf{u} = \mathbf{B}^{-1}\mathbf{f}$

(Eisenstadt, Elman, Schulz, 1983)...

$\mathbf{B}^{-1}$ is a good preconditioner for $\mathbf{A}$ if

$$\|\mathbf{B}^{-1}\mathbf{A}\| \lesssim 1, \qquad \text{(norm)}$$

and

$$\mathrm{dist}(0, \mathbf{fov}(\mathbf{B}^{-1}\mathbf{A})) \gtrsim 1 \qquad \text{(fov)}$$

where $\mathbf{fov}(\mathbf{C}) := \{\mathbf{x}^*\mathbf{C}\mathbf{x} : \|\mathbf{x}\| = 1\}$

[Sufficient is: $\|\mathbf{I} - \mathbf{B}^{-1}\mathbf{A}\|$ small] .

An approach to the theory:

- Introduce absorption $k^2 \rightsquigarrow k^2 + \mathrm{i}\varepsilon, \quad \varepsilon > 0$
- Fundamental solution now decays:

$$\Phi_k(\boldsymbol{x},\boldsymbol{y}) \rightsquigarrow \Phi_k(\boldsymbol{x},\boldsymbol{y}) \exp(-(\varepsilon/2k)|\boldsymbol{x}-\boldsymbol{y}|)$$

- $\mathbf{A} \rightsquigarrow \mathbf{A}_\varepsilon, \qquad \mathbf{B}^{-1} \rightsquigarrow \mathbf{B}_\varepsilon^{-1}$
- Analyse: $\mathbf{B}_\varepsilon^{-1}$ as a preconditioner for $\mathbf{A}_\varepsilon$ coercivity!
- Reasonable because: $\|\mathbf{I} - \mathbf{A}_\varepsilon^{-1}\mathbf{A}\| \ \leq \ C|\varepsilon|/k$

Gander, IGG, Spence, 2015
IGG, Spence, Vainikko, 2017

Rigorous theory for SORAS

Assumptions include:

- $kH \to \infty$
- finite cover Λ, generous overlap,
- $\| \cdot \|_{D_k}$ = norm induced by Helmholtz 'energy':

Theorem: (IGG, Spence, Zou, 2020)

$$\|\mathbf{B}_\varepsilon^{-1}\mathbf{A}_\varepsilon\|_{D_k} \leq C_1 \Lambda \quad \forall \varepsilon$$

$$\inf_{\boldsymbol{V}\neq\mathbf{0}} \frac{|\langle \boldsymbol{V}, \mathbf{B}_\varepsilon^{-1}\mathbf{A}_\varepsilon \boldsymbol{V}\rangle_{D_k}|}{\|\boldsymbol{V}\|_{D_k}^2} \geq \Lambda^{-1} \left(1 - C_2 \Lambda^2 \min\left\{1, \frac{k}{|\varepsilon| H}\right\}\right)$$

GMRES iterates for $B^{-1}A$, $\varepsilon = 0$

$$\Omega = (0,1)^2, \quad p = 1, \quad h \sim k^{-3/2}, \quad n \sim k^3, \quad H \sim k^{-\alpha}$$

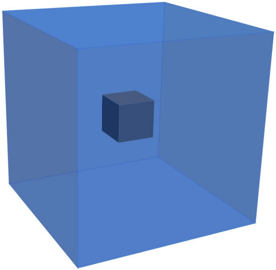
$k \backslash \alpha$	0.2	0.3	0.4	0.5
40	5	8	11	19
60	5	7	14	25
80	4	10	15	24
100	7	9	15	27
120	6	9	17	29
140	6	8	16	31

Robust one level method for ‘pure’ Helmholtz
but have to solve on relatively large subdomains.

(Multilevel) Approximations?

Idea! Subdomain problems are again Helmholtz impedance problems, but with effective wavenumber kH instead of k

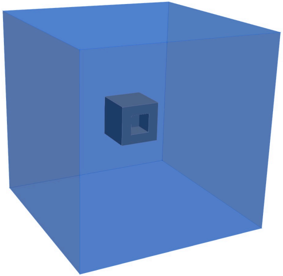
Scattering of plane wave by a cube - 10 grdpts/wavelength
First level: $H = k^{-0.4}$, generous overlap
Second level: $H \sim k^{-0.8}$, minimal overlap.
Outer/Inner GMRES iterates (tolerances = 10^{-6}, 10^{-2})



k	$p = 1$	$p = 2$	$p = 3$
20	15(7)	16(7)	15(7)
30	21(9)	21(9)	20(9)
40	24(9)	25(10)	24(10)
50	28(11)	29(11)	28(12)

Scattering of plane wave by a cube with a cavity

First level: $H = k^{-0.4}$, generous overlap



k	$p=1$	$p=2$	$p=3$ GMRES
20			22
25.1327			29
30			29
40			31
50			35
50.2655			35

$*$ ‘Resonant’ frequencies

Iteration numbers unaffected by resonance

Adding a coarse grid

with M. Bonazzoli, P.-H. Tournier, V. Dolean and E. Spence

$\Omega = (0,1)^3 \qquad p = 1$

$h \sim k^{-3/2}, \qquad n \sim k^{9/2}, \qquad H_{\text{sub}} \sim k^{-0.5} \qquad H_{\text{coarse}} \sim k^{-1}$

two level hybrid preconditioner

k	n	dim Coarse	# GMRES	Time
10	3.9(+4)	1.3(+3)	12	8.9
20	7.0(+5)	9.3(+3)	17	42.2
30	5.0(+6)	3.0(+4)	21	177.1
40	1.6(+7)	6.9(+4)	29	414.8
		$\sim n^{0.6}$	$\sim n^{0.1}$	$\sim n^{0.6}$

"Weak scaling"

Heterogeneity A, n, dependence on degree p?

Theorem: (IGG, Spence, Zou, 2018)

$$\|\mathbf{B}_\varepsilon^{-1}\mathbf{A}_\varepsilon\|_{D_k} \leq C_1\,\Lambda \qquad \forall\,\varepsilon$$

$$\inf_{\boldsymbol{V}\neq\mathbf{0}} \frac{|\langle \boldsymbol{V}, \mathbf{B}_\varepsilon^{-1}\mathbf{A}_\varepsilon \boldsymbol{V}\rangle_{D_k}|}{\|\boldsymbol{V}\|_{D_k}^2} \geq \Lambda^{-1}\left(1 - C_2\,\Lambda^2 \min\left\{1, \frac{k}{|\varepsilon| H}\right\}\right)$$

Heterogeneity A, n, dependence on degree p?

Theorem: (Gong IGG, Spence, 2020)

$$\|\mathbf{B}_\varepsilon^{-1}\mathbf{A}_\varepsilon\|_{D_k} \;\leq\; C_1(A,n)\,\Lambda \quad \forall\,\varepsilon$$

$$\inf_{\boldsymbol{V}\neq\mathbf{0}} \frac{|\langle \boldsymbol{V}, \mathbf{B}_\varepsilon^{-1}\mathbf{A}_\varepsilon \boldsymbol{V}\rangle_{D_k}|}{\|\boldsymbol{V}\|_{D_k}^2} \;\geq\; \Lambda^{-1}\left(1 - C_2(A,n)\,\Lambda^2\,\min\left\{1, \frac{k}{|\varepsilon|H}\right\}\right)$$

'local dependence' on contrast of A, n

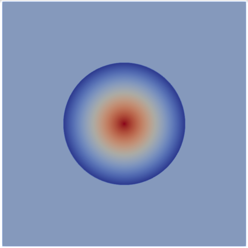
Independent of polynomial degree p as $k \to \infty$

Robust to polynomial degree p

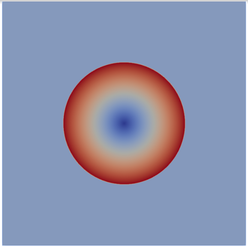
constant A and n, # GMRES iterations

$k \backslash p$	1	2	3	4
40	17	18	17	16
60	16	16	16	15
80	15	16	15	14
100	14	15	14	14
150	14	15	14	14

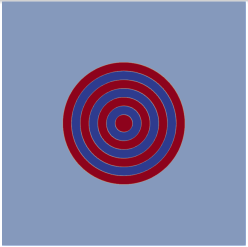
Local dependence on contrast in refractive index n



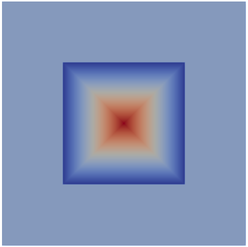
(a) (nontrapping)



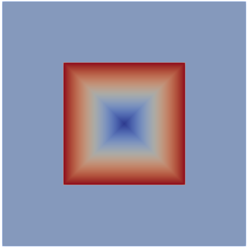
(b) (trapping)



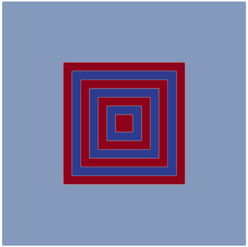
(c) c oscillates



(d) (nontrapping)



(e) (trapping)



(f) c oscillates

$A = I$ and n varying, $p = 1$

$k \backslash n$	$n = 1$	Fig 1a	Fig 1b	Fig 1c	Fig 1d	Fig 1e	Fig 1f
40	14	18	17	34	16	19	24
60	13	19	18	25	14	18	22
80	13	17	19	27	13	15	28
100	13	15	19	26	13	15	27

Robust to ‘trapping’ (empirically)

Current work

Gong, Gander, IGG, Lafontaine, Spence

$$\begin{aligned}\mathbf{u} &= \mathbf{u} + \mathbf{B}^{-1}(\mathbf{f} - \mathbf{A}\mathbf{u}) \\ &= (\mathbf{I} - \mathbf{B}^{-1}\mathbf{A})\mathbf{u} + \mathbf{B}^{-1}\mathbf{f} \quad \text{Richardson iteration..}\end{aligned}$$

error $\quad \mathbf{e}^{n+1} = \underbrace{(\mathbf{I} - \mathbf{B}^{-1}\mathbf{A})}_{=:\mathbf{E}} \mathbf{e}^n$

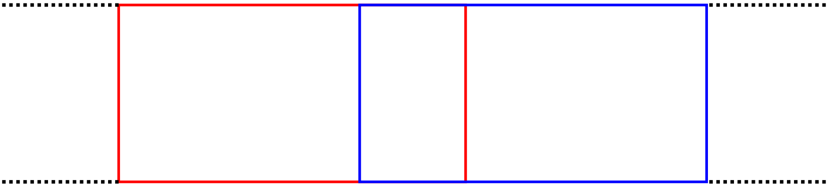
without absorption $(\varepsilon = 0)$:
$\mathbf{B}^{-1}\mathbf{A}$ does not have a 'good' field of values But it can be 'power contractive':

$$\|\mathbf{E}^s\| \ll 1, \quad \text{for some} \quad s$$

Theorem for 'one-way decompositions' (with N subdomains) and ORAS,

$\exists$ norm such that $\|E^N\| \;\leq\; C(N-1)\rho + \mathcal{O}(\rho^2)$

$\rho =$ norm of 'left to right impedance map' (small for large enough overlap)



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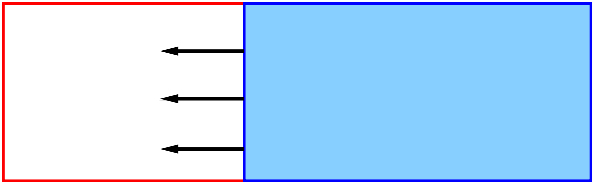

power contractivity

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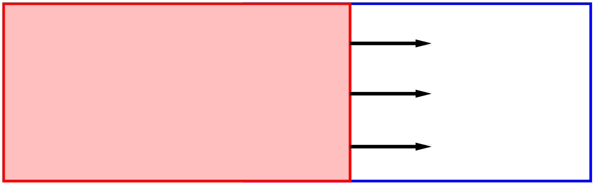

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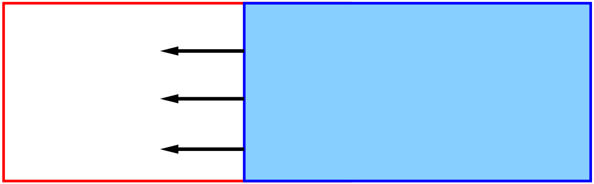
$\exists$ norm such that $\|E^N\| \;\leq\; C(N-1)\rho + \mathcal{O}(\rho^2)$

$\rho =$ norm of 'left to right impedance map' (small for large enough overlap)

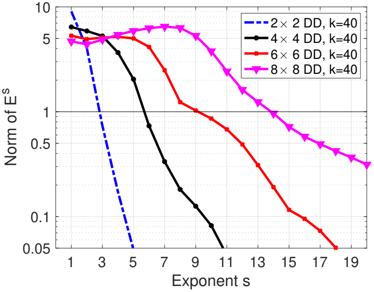


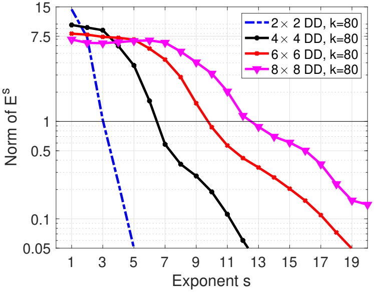
Overview of proof

- When h small, ORAS (for FEM) is close to a simple iterative method formulated at PDE level
- Iterating the simple method is like iterating the impedance map
- The impedance map is contractive (using semiclassical analysis or rigorous computation)

The proof is only for one-way decompositions but....

$\|E^s\|$ - for square domain, square subdomains





Results for 8×8 case:

k	Iterative	GMRES
40	46	28
80	31	26
160	28	24

Summary

- A walk around Helmholtz-land
- Very large non-Hermitian indefinite matrices
- Iterative methods and preconditioning
- Convergence theory - absorptive case
- Some examples
- A glimpse of some new results

Thanks for listening!