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Is the Helmholtz equation really sign-indefinite?

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Joint work with Euan A. Spence (Bath)

What people say about sign-indefiniteness

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Sure???

The Helmholtz equation

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Why is it interesting?

1. very general: $(k = \omega / c)$

   wave equation $\dfrac{\partial^2 U}{\partial t^2} - c^2 \Delta U = c^2 F$

   time-harmonic regime $U(\mathbf{x}, t) = \Re\{u(\mathbf{x}) e^{-i\omega t}\}$

   $\rightarrow$ Helmholtz equation;

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3. easy to write, difficult to solve numerically (for $k \gg 1$)

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   $\rightarrow$ Helmholtz equation;

2. plenty of applications;
3. easy to write, difficult to solve numerically (for $k \gg 1$):
   - oscillating solutions $\rightarrow$ expensive to approximate;
   - numerical dispersion / pollution effect;
   - sign-indefinite?

Variational formulations

BVPs for (linear elliptic) PDEs are often posed in variational form:

$$\text{(VF)} \quad \text{find} \quad u \in \mathcal{V} \quad \text{such that} \quad a(u,w) = F(w) \quad \forall w \in \mathcal{V},$$

$\mathcal{V}$ Hilbert space,
$a(\cdot,\cdot) : \mathcal{V} \times \mathcal{V} \to \mathbb{R}$ bilinear form,
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They can be approximated using a Galerkin discretisation:

(GD) find $u_N \in \mathcal{V}_N$ s.t. $a(u_N, w_N) = F(w_N) \quad \forall w_N \in \mathcal{V}_N,$

$\mathcal{V}_N \subset \mathcal{V}$ finite dimensional space, $\dim(\mathcal{V}_N) = N$.

Continuity & coercivity

Most desirable properties for (VF), $\exists C_c, \alpha > 0$:

$$|a(u,w)| \le C_c \, \|u\|_{\mathcal{V}} \, \|w\|_{\mathcal{V}} \qquad \forall u, w \in \mathcal{V}, \qquad \text{continuity},$$
$$|a(w,w)| \ge \alpha \, \|w\|_{\mathcal{V}}^2 \qquad \forall w \in \mathcal{V}, \qquad \text{coercivity}.$$

("Sign-definite" := coercive; "sign-indefinite" := not coercive.)

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Consequences of continuity & coercivity (Lax–Milgram, Céa):

- well-posedness of (VF): $\exists!\, u \in \mathcal{V}, \quad \|u\|_{\mathcal{V}} \le \|F\|_{\mathcal{V}'}/\alpha$;
- well-posedness of any (GD): $\exists!\, u_N \in \mathcal{V}_N, \quad \|u_N\|_{\mathcal{V}} \le \|F\|_{\mathcal{V}'}/\alpha$;
- quasi-optimality of any (GD):

$$\|u - u_N\|_{\mathcal{V}} \le \frac{C_c}{\alpha} \inf_{w_N \in \mathcal{V}_N} \|u - w_N\|_{\mathcal{V}};$$

- good properties for (GD) linear system.

Coercivity is a property of the bilinear form—no PDEs here.

Back to PDEs

Typical example:
Standard (VF) of Dirichlet problem for the Laplace equation ($\Delta u = -f$) is continuous + coercive (+ symmetric):
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More interesting example:

Impedance Helmholtz BVP
$$\begin{cases} \Delta u + k^2 u = -f & \text{in } \Omega, \\ \frac{\partial u}{\partial \mathbf{n}} - iku = g & \text{on } \partial\Omega. \end{cases}$$

HVF
$$\begin{cases} a(u,w) := \int_\Omega (-\nabla u \cdot \nabla \overline{w} + k^2 u \overline{w}) \,\mathrm{d}\mathbf{x} + ik \int_{\partial\Omega} u \overline{w} \,\mathrm{d}s, \\ F(w) := -\int_\Omega f \,\overline{w} \,\mathrm{d}\mathbf{x} - \int_{\partial\Omega} g \,\overline{w} \,\mathrm{d}s, \\ \mathcal{V} := H^1(\Omega), \quad \|w\|^2_{1,k,\Omega} := \|\nabla w\|^2_{L^2(\Omega)} + k^2 \|w\|^2_{L^2(\Omega)}. \end{cases}$$

(Note: now everything is complex-valued.)

Is Helmholtz sign-indefinite?

For $k^2 \geq \lambda_1 > 0$ (1st Laplace–Dirichlet eigenvalue), $a(\cdot,\cdot)$ is continuous but not coercive in $H^1(\Omega)$.

Other techniques are applicable based on Fredholm alternative (Gårding inequality, Schatz's argument...)

$\Rightarrow$ well-posedness of (HVF),

$\Rightarrow$ well-posedness of (HGD) and quasi-optimality for "N large enough" only.

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$\Rightarrow$ well-posedness of (HVF),
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Does this imply that the Helmholtz equation is sign-indefinite?
NO!
The standard variational formulation (HVF) of the BVP is sign-indefinite, but not the equation itself.

New question: is there any continuous & coercive variational formulation equivalent to the Helmholtz impedance BVP?

How to find a coercive Helmholtz formulation?

- Modus operandi: in general it holds

  coercivity $\Rightarrow$ explicit stability constant $\|u\|_{\mathcal{V}} \leq \alpha^{-1} \|F\|_{\mathcal{V}'}$;

  Fredholm $\Rightarrow$ unknown stability constant $\|u\|_{\mathcal{V}} \leq C \|F\|_{\mathcal{V}'}$.

- A clue: MELENK, CUMMINGS&FENG, HETMANIUK proved

  $?$ $\Rightarrow$ (almost) explicit stability bounds for (HVF).

- A suspicion:
  maybe there's a "hidden coercivity" behind...

- How to find an evidence?
  reverse engineer Melenk's proof to define a variational formulation by applying the main tools used there:
  Rellich identities and multipliers.

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- How to find an evidence?
  reverse engineer Melenk's proof to define a variational formulation by applying the main tools used there:
  Rellich identities and multipliers.

- 1^{st} surprise: it works!

- 2^{nd} surprise: it is derived exactly as the standard (HVF).

How was Helmholtz variational form obtained?

Standard (HVF) was obtained by

1. multiplying $\mathcal{L}u := \Delta u + k^2 u = -f$ with test function w;
2. using Green 1st identity
   $$(\Delta u)\overline{w} = \mathbf{div}[(\nabla u)\overline{w}] - \nabla u \cdot \nabla \overline{w};$$
3. integrating by parts
   $$\int_\Omega \mathrm{div}[\mathbf{A}]\,\mathrm{d}\mathbf{x} \;\mapsto\; \int_{\partial\Omega} \mathbf{A}\cdot\mathbf{n}\,\mathrm{d}s;$$
4. substituting the impedance BC in the boundary term.

Same steps to derive a new formulation:
only 1–2 are changed.

How to derive a new variational formulation – I

1. Multiply $\mathcal{L}u = -f$ with Morawetz-type test function

$$\mathcal{L}u\,\overline{\mathcal{M}w} = (\Delta u + k^2 u)\overline{\left(\mathbf{x}\cdot\nabla w - ik\beta w + \frac{d-1}{2}w\right)} \qquad \beta \in \mathbb{R}.$$

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2. We expand the terms of this product.

2^I Highest order term expanded using Rellich-type identity

$$(\Delta u)(\mathbf{x}\cdot\nabla\overline{w}) = \underbrace{\mathrm{div}}_{\to\partial\Omega}\left[(\nabla u)(\mathbf{x}\cdot\nabla\overline{w})\right] - \underbrace{\nabla u\cdot\nabla\overline{w}}_{\to|\nabla u|^2>0} - \underbrace{\nabla u\cdot\left((\mathbf{x}\cdot\nabla)\nabla\overline{w}\right)}_{\text{don't like this!}}.$$

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To get rid of last term (with Hessian of $w\notin H^2$) we “symmetrise”

$$(\Delta u)(\mathbf{x}\cdot\nabla\overline{w}) + (\mathbf{x}\cdot\nabla u)(\Delta\overline{w}) = \mathrm{div}\left[\ldots\right] + (d-2)\nabla u\cdot\nabla\overline{w}.$$

How to derive a new variational formulation – II

2^{II} 0+1 order terms symmetrised with

$$u(\mathbf{x} \cdot \nabla \overline{w}) + (\mathbf{x} \cdot \nabla u)\overline{w} = \operatorname{div}[\mathbf{x}\, u\overline{w}] - d\, u\overline{w}.$$

How to derive a new variational formulation – II

2^{II} 0+1 order terms symmetrised with

$$u(\mathbf{x}\cdot\nabla\overline{w}) + (\mathbf{x}\cdot\nabla u)\overline{w} = \mathrm{div}[\mathbf{x}\,u\overline{w}] - d\,u\overline{w}.$$

2^{III} Remaining terms $\mathcal{L}u(\overline{-ik\beta w + \frac{d-1}{2}w})$ with Green identity.

Final identity

$$-\mathcal{L}u\overline{\mathcal{M}w} = +\nabla u\cdot\nabla\overline{w} + k^2 u\overline{w} + \mathcal{M}u\overline{\mathcal{L}w}$$
$$- \mathrm{div}\left[\nabla u\overline{\mathcal{M}w} + \mathcal{M}u\,\nabla\overline{w} + \mathbf{x}(k^2 u\overline{w} - \nabla u\cdot\nabla\overline{w})\right].$$

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$$-\,\mathrm{div}\left[\nabla u\overline{\mathcal{M}w} + \mathcal{M}u\,\nabla\overline{w} + \mathbf{x}(k^2 u\overline{w} - \nabla u\cdot\nabla\overline{w})\right].$$

2^{IV} Add term $\frac{1}{3k^2}\mathcal{L}u\overline{\mathcal{L}w}$ to control $\mathcal{M}u\overline{\mathcal{L}w}$.

3 – 4 Integrate by parts + impose BC.

A new variational formulation

We end up with a variational formulation defined by

$$b(u,w) := \int_\Omega \left(\nabla u \cdot \nabla \overline{w} + k^2 u \overline{w} + \left(\mathcal{M}u + \tfrac{1}{3k^2}\mathcal{L}u\right) \overline{\mathcal{L}w} \right) \mathrm{d}\mathbf{x}$$
$$- \int_{\partial\Omega} \left(iku\,\overline{\mathcal{M}w} + \left(\mathbf{x}\cdot\nabla_T u - ik\beta u + \tfrac{d-1}{2}u\right) \frac{\partial \overline{w}}{\partial \mathbf{n}} \right.$$
$$\left. + (\mathbf{x}\cdot\mathbf{n}) \left(k^2 u \overline{w} - \nabla_T u \cdot \nabla_T \overline{w} \right) \right) \mathrm{d}s,$$
$$G(w) := \int_\Omega f \left(\overline{\mathcal{M}w} - \tfrac{1}{3k^2}\overline{\mathcal{L}w} \right) \mathrm{d}\mathbf{x} + \int_{\partial\Omega} g\, \overline{\mathcal{M}w}\, \mathrm{d}s,$$

in the space $V := \left\{ v:\ v \in H^1(\Omega),\ \Delta v \in L^2(\Omega),\ \nabla v \in \left(L^2(\partial\Omega)\right)^d \right\}$.

(b and G continuous in V.)

$b(u,w) = G(w)\ \forall w \in V$ is equivalent to the impedance BVP:

$$\begin{cases} \Delta u + k^2 u = -f & \text{in } \Omega, \\ \frac{\partial u}{\partial \mathbf{n}} - iku = g & \text{on } \partial\Omega. \end{cases}$$

(Sometimes) Helmholtz is sign-definite!

If Ω is star-shaped with respect to $B_{\gamma L}$, i.e.

$$\mathbf{x} \cdot \mathbf{n}(\mathbf{x}) \geq \gamma L > 0 \quad \text{a.e. } \mathbf{x} \in \partial\Omega \qquad (L := \operatorname{diam}\Omega),$$

and $\beta \geq 3L/\gamma$, then $b(\cdot,\cdot)$ is coercive in V:

$$\operatorname{Re}\{b(w,w)\} \geq \frac{1}{4}\gamma \|w\|_V^2 \qquad \forall w \in V.$$

The norm is weighted with k and L:

$$\|w\|_V^2 := \quad k^2 \|w\|^2_{L^2(\Omega)} \quad + \|\nabla w\|^2_{L^2(\Omega)} + k^{-2} \|\Delta w\|^2_{L^2(\Omega)}$$
$$+Lk^2 \|w\|^2_{L^2(\partial\Omega)} + L \|\nabla w\|^2_{L^2(\partial\Omega)}.$$

Coercivity is proved using the previous identities and Cauchy–Schwarz inequality (only!).

Why does it work?

Only one extra ingredient from standard formulation:

Morawetz multiplier $\mathcal{M}(w) = \mathbf{x} \cdot \nabla w + (-ik\beta + \frac{d-1}{2})w$.

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$\mathcal{M}(w)$ and Rellich multiplier ($\mathbf{x} \cdot \nabla w$) already been used in:

- Spectral theory, since RELLICH 1940...
- Scattering theory, k-explicit stability for exterior Helmholtz, wave eq., MORAWETZ, LUDWIG, 1961-75...
- k-explicit stability for interior Helmholtz BVPs (our "clue"), MELENK; CUMMINGS, FENG; HETMANIUK; CHANDLER-WILDE, MONK.
- Coercive BIEs, star-combined operator, SPENCE, CHANDLER-WILDE, GRAHAM, SMYSHLYAEV; SPENCE, KAMOTSKY, SMYSHLYAEV.
- ...
- k-explicit BVP stability for Maxwell, HIPTMAIR, M., PERUGIA; HADDAR, LECHLEITER.

Other coercive formulations

$\exists$ other coercive formulations but very different from standard one:

- Boundary integral equation: combined potential op. (large k, smooth&convex), star-combined op., flat screens...
- Trefftz-discontinuous Galerkin methods (TDG), UWVF: consistency&coercivity in mesh-dependent Trefftz spaces:

$$T(\mathcal{T}_h) = \left\{ v \in H^2(\mathcal{T}_h) \ : \ \Delta v + k^2 v = 0 \text{ in each } K \in \mathcal{T}_h \right\} .$$

- Least squares methods, e.g.:

$$k^{-2} \int_\Omega \mathcal{L}u \mathcal{L}\overline{w} \, \mathrm{d}\mathbf{x} + L \int_{\partial\Omega} \left(\frac{\partial u}{\partial \mathbf{n}} - iku \right) \overline{\left(\frac{\partial w}{\partial \mathbf{n}} - ik \right)} \, \mathrm{d}s = F_{LS}(w).$$

- T-coercivity (Ciarlet) : $\forall$ well-posed VF

  $a(u, w) = F(w) \quad \forall w \in \mathcal{V}$

  admits a coercive reformulation

  $a_T(u, w) := a(u, Tw) = F(Tw) =: F_T(w) \quad \forall w \in \mathcal{V};$

  the operator $T : \mathcal{V} \to \mathcal{V}$ is (usually) not explicit.

Properties of possible Galerkin discretisations

- "Unconditional well-posedness": $\forall V_N \subset V$, $\forall k > 0$, $\Rightarrow \exists! u_N$ Galerkin solution and

$$\|u_N\|_V \leq C(1 + k^{-1})\big(\|f\|_{L^2(\Omega)} + \|g\|_{L^2(\partial\Omega)}\big).$$

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- Quasi-optimality constant is (only!) linear in k:

$$\|u - u_N\|_V \le C\big(k + k^{-1}\big) \inf_{w_N \in V_N} \|u - w_N\|_V .$$

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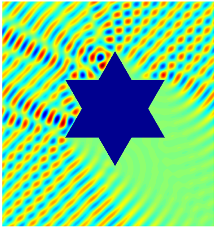
- $V_N \subset V$ ($\Rightarrow \Delta v \in L^2$), piecewise C^2 on a mesh $\Rightarrow$ $V_N \subset C^1(\Omega)$:
  $C^1(\Omega)$-conformal FEM discretisation required!
  Possible alternatives to standard C^1-FEM:
  PUM, VEM, isogeometric, non conformal C-DG/CIP...
  any idea?

Extensions: done&todo

- (Star-shaped) Dirichlet scatterer
  + exterior impedance bc $\rightarrow$ same result.
- Neumann scatterer doesn´t work, why?



(picture by T. Betcke)

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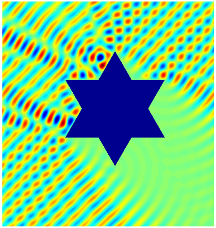
- Maxwell equations: coercive formulation in divergence-free space: bad!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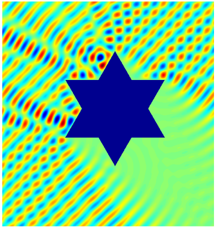

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- Non star-shaped domains/scatterers?
  Need to substitute $\mathbf{x}$ in $\mathcal{M}$ with special fields $\mathbf{Z}(\mathbf{x})$. How?
- Penetrable scatterers, rough surfaces, screens. . .

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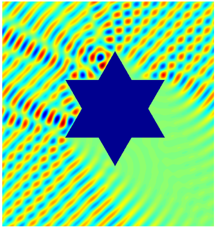

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- Bounds on condition number and GMRES iterations for piecewise-polynomial discretisations.

The message

The Helmholtz impedance BVP is often claimed to be sign-indefinite as its standard variational formulation is.

We showed a new variational formulation of the same problem that is sign-definite and is derived in a very similar way.

More details in our preprint, to appear in SiRev:
Moiola, Spence, *Is the Helmholtz equation really sign-indefinite?*
`http://www.reading.ac.uk/maths-and-stats/research/maths-preprints.aspx`

Thank you!

Identity table (d=dimension)

		Green 1^{st}:	
$(\Delta u)\overline{w}$		$= \text{div}\left[(\nabla u)\overline{w}\right]$	$-\nabla u\cdot\nabla\overline{w}$
		Green 2^{nd}:	
$(\Delta u)\overline{w}$	$-u(\Delta\overline{w})$	$= \text{div}\left[(\nabla u)\overline{w} - u(\nabla\overline{w})\right]$	
		"Helmholtz 1^{st}":	
$(\mathcal{L}u)\overline{w}$		$= \text{div}\left[(\nabla u)\overline{w}\right]$	$-\nabla u\cdot\nabla\overline{w} + k^2 u\overline{w}$
		"Rellich 1^{st}":	
$(\Delta u)(\mathbf{x}\cdot\nabla\overline{w})$		$= \text{div}\left[(\mathbf{x}\cdot\nabla\overline{w})\nabla w\right]$	$-\nabla u\cdot\nabla\overline{w}$ $-\nabla u\cdot\left((\mathbf{x}\cdot\nabla)\nabla\overline{w}\right)$
		"Rellich 2^{nd}":	
$(\Delta u)(\mathbf{x}\cdot\nabla\overline{w})$	$+(\mathbf{x}\cdot\nabla u)(\Delta\overline{w})$	$= \text{div}\left[-\mathbf{x}(\nabla u\cdot\nabla\overline{w}) + \nabla u(\mathbf{x}\cdot\nabla\overline{w}) + (\mathbf{x}\cdot\nabla u)\nabla\overline{w}\right]$	$+(d-2)\nabla u\cdot\nabla\overline{w}$
		"Melenk 2^{nd}":	
$u(\mathbf{x}\cdot\nabla\overline{w})$	$+(\mathbf{x}\cdot\nabla u)\overline{w}$	$= \text{div}\left[\mathbf{x}\, u\overline{w}\right]$	$-d\, u\overline{w}$
		"Morawetz 2^{nd}":	
$\mathcal{L}u\overline{\mathcal{M}w}$	$+\mathcal{M}u\overline{\mathcal{L}w}$	$= \text{div}\left[\nabla u\overline{\mathcal{M}w} + \mathcal{M}u +\nabla\overline{w} + \mathbf{x}(k^2 u\overline{w} - \nabla u\cdot\nabla\overline{w})\right]$	$-\nabla u\cdot\nabla\overline{w} - k^2 u\overline{w}$
	symmetric term	div term	non-div term

Symmetrisation trick R1→R2:

$$\nabla u\cdot\left((\mathbf{x}\cdot\nabla)\nabla\overline{w}\right) + \nabla\overline{w}\cdot\left((\mathbf{x}\cdot\nabla)\nabla u\right) = \text{div}\left[\mathbf{x}(\nabla u\cdot\nabla\overline{w})\right] - d\,\nabla u\cdot\nabla\overline{w}.$$