Lecture 2. High Frequency Behaviour of Formulations of Time-Harmonic Scattering

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Focus of Today's Lecture

For

$$\Delta u + k^2 u = 0,$$

and boundary or finite element methods for its solution:

- **1.** How does conditioning depend on k (and the geometry)?
- 2. How can we remove or reduce this dependence?

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What is conditioning? For a linear system

$$Ax = b$$

the condition number is

 $\operatorname{cond} A := \|A\| \|A^{-1}\|$ where $\|A\| := \sup_{x \neq 0} \frac{\|Ax\|}{\|x\|}$. Large condition numbers associated with:

- slow convergence of iterative solution methods;
- magnification of effects of errors, e.g. in entries of A.

For

$$\Delta u + k^2 u = 0,$$

and boundary or finite element methods for its solution:

1. How does conditioning depend on k (and the geometry)?

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What is conditioning? For an operator equation

$$Ax = b$$

 $(A: X \to Y \text{ a continuous linear operator, } x \in X, b \in Y)$ the condition number is

cond $A := ||A||_{X \to Y} ||A^{-1}||_{Y \to X}$ where $||A||_{X \to Y} := \sup_{0 \neq x \in X} \frac{||Ax||_Y}{||x||_X}$.

For

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and boundary or finite element methods for its solution:

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- 2. How can we remove or reduce this dependence?

What is conditioning? For the variational equation: find $u \in X$ such that

$$a(u,v) = f(v), \quad v \in Y,$$

(X and Y Hilbert spaces, $a: X \times Y \to \mathbb{C}$ a continuous sesquilinear form) a relevant **condition number** is that of the associated operator $A: X \to Y'$, defined by

$$Au(v) = a(u, v), \quad u \in X, v \in Y.$$

Since (see Melenk notes, Theorem 3 (Babuška-Brezzi), Hiptmair, 'Fundamental Concepts', §2),

$$\|A\|_{X \to Y'} = M, \quad M := \sup_{0 \neq u \in X, v \in Y} \frac{|a(u, v)|}{\|u\|_X \|v\|_Y},$$
$$\|A^{-1}\|_{Y' \to X} = \gamma^{-1}, \quad \gamma := \inf_{0 \neq u \in X} \sup_{0, \neq v \in Y} \frac{|a(u, v)|}{\|u\|_X \|v\|_Y},$$

M often called the norm of a and γ its $\operatorname{inf-sup}$ constant, it holds that

$$\operatorname{cond} A = \frac{M}{\gamma}.$$

Precise Focus of Today's Lecture

For

$$\Delta u + k^2 u = 0,$$

and integral equation or domain methods for its solution:

- **1.** How does conditioning depend on k (and the geometry)?
- 2. How can we remove or reduce this dependence?

Estimating ||A|| and $||A^{-1}||$ when A is an integral operator, and **norm** and **inf-sup** constants of sesquilinear forms.



Recall from Yesterday ...

a standard weak formulation in Ω_R^+ , that part of Ω^+ inside a ball of radius R, with the exact Dirichlet to Neumann map on the sphere Γ_R truncating the domain.



Let V_R denote the closure of $\{v|_{\Omega_R^+} : v \in C_0^\infty(\Omega^+)\} \subset H^1(\Omega_R^+)$ in the norm of $H^1(\Omega_R^+)$.

u satisfies the scattering problem if and only if the restriction of u to Ω_R^+ satisfies a variational problem of the form: find $u \in V_R$ such that

$$a(u,v) = f(v), \quad v \in V_R.$$

The functional f depends on the incident field. $a(\cdot, \cdot)$ is the sesquilinear form on $V_R \times V_R$ defined by

$$a(u,v) := \int_{\Omega_R^+} (\nabla u \cdot \nabla \bar{v} - k^2 u \bar{v}) \, dx - \int_{\Gamma_R} \gamma \bar{v} T_R \gamma u \, ds$$

where $\gamma: V_R \to H^{1/2}(\Gamma_R)$ is the usual trace operator.

Summary of Known Results

With Markus's norm, i.e. $||u||_{V_R}^2 = \int_{\Omega_R^+} (|\nabla u|^2 + k^2 |u|^2) dx$, ...

1. An **upper bound** on the **inf-sup constant**

$$\gamma := \inf_{\|u\|_{V_R} = 1} \sup_{\|v\|_{V_R} = 1} |a(u, v)|, \text{ that "a}$$

$$\gamma \le \frac{C_1}{kR} + \frac{C_2}{k^2 R^2}.$$

2. That, if the scatterer Υ is starlike (i.e. $x \in \Upsilon \Rightarrow \theta x \in \Upsilon$, for $0 \le \theta \le 1$), then the **lower bound** holds that

$$\frac{1}{5 + 4\sqrt{2}\,kR} \le \gamma.$$

^aThis upper bound also holds for Markus Melenk's example on his page 11, yesterday. 3. An example where Υ is not starlike (two parallel plates) for which

$$\gamma \le \frac{C}{k^2 R^2}.$$

for an unbounded sequence of (nearly resonant) wavenumbers k.

Details: see the blackboard and www.rdg.ac.uk/~sms03snc/monk_bounded_submitted.pdf and the references therein.

Lemma 2.1 Suppose $w \in V_R \cap H^2(\Omega_R^+)$ is such that $\gamma w = \gamma \nabla w = 0$ and w is non-zero. Then the inf-sup constant γ is bounded above by

$$\gamma \le \frac{C_1}{kR} + \frac{C_2}{k^2 R^2},$$

where $C_1 := 2R \left\| \frac{\partial w}{\partial x_1} \right\|_2 / \|w\|_2$, $C_2 := R^2 \|\Delta w\|_2 / \|w\|_2$ and $C_1 \ge 2\sqrt{2} \approx 2.83$.

Lemma 2.1 Suppose $w \in V_R \cap H^2(\Omega_R^+)$ is such that $\gamma w = \gamma \nabla w = 0$ and w is non-zero. Then the inf-sup constant γ is bounded above by

$$\gamma \le \frac{C_1}{kR} + \frac{C_2}{k^2 R^2},$$

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For Markus's interior impedance/Robin problem (p.11 of his notes), the same bound holds if his bounded domain Ω contains a ball of radius R, with

$$C_1 = 2\sqrt{24 + 3d}/3 \approx 3.7$$

Where do the lower bounds on the inf-sup constant come from?

I.e. the lower bound I just showed or the lower bound Markus showed yesterday.

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The main ingredients are:

1. A rephrasing of Markus's Theorem 3 gives us the following general result:

If there exists C > 0 such that, for every $u \in V_R$ and $f \in V'_R$ satisfying

$$a(u,v) = f(v), \quad v \in V_R,$$

it holds that

$$||u||_{V_R} \le C ||f||_{V'_R}, \quad (*)$$

then

 $\gamma \ge C^{-1}.$

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then $\gamma \ge C^{-1}$. $\|u\|_{V_R} \le C \|f\|_{V_R'}, \quad (*)$

2. If there exists $\tilde{C} > 0$ such that, for every $u \in V_R$ and $g \in L^2(\Omega_R^+)$ satisfying

$$a(u,v) = -(g,v)_2 := -\int_{\Omega_R^+} g\bar{v} \, dx, \quad v \in V_R,$$

it holds that

 $||u||_{V_R} \le k^{-1} \tilde{C} ||g||_{L^2(\Omega_R^+)},$

then (*) holds with $C = 1 + 2\tilde{C}$.

3. To establish this last bound, Green's theorem and a Rellich(-Payne-Weinberger-Nečas) type identity.

Such identities, useful for obtaining explicit a prioiri bounds and regularity estimates for strongly elliptic systems, follow from the divergence theorem, and date back to Rellich (1943).

See Chapter 5 of Nečas (1967) or McLean (2000). Our particular version of the identity is essentially that from the PhD of Melenk (1995).

Lemma 2.2. Suppose that $\Omega \subset \mathbb{R}^d$ is a bounded Lipschitz domain and that $v \in H^2(G)$. Then, for every $k \ge 0$, where $g := \Delta v + k^2 v$ and the unit normal vector n is directed into Ω , it holds that

$$\int_{\Omega} \left(|\nabla v|^2 - k^2 |v|^2 + g\bar{v} \right) \, dx = -\int_{\partial\Omega} \bar{v} \, \frac{\partial v}{\partial n} \, ds$$

and

$$\int_{\Omega} \left((2-d) |\nabla v|^2 + dk^2 |v|^2 + 2\Re \left(gx \cdot \nabla \bar{v} \right) \right) \, dx = \\ - \int_{\partial \Omega} \left(x \cdot n \left(k^2 |v|^2 + \left| \frac{\partial v}{\partial n} \right|^2 - |\nabla_T v|^2 \right) + 2\Re \left(x \cdot \nabla_T \bar{v} \, \frac{\partial v}{\partial n} \right) \right) \, ds.$$

4. To complete the proof for the scattering problem, a subtle property of radiating solutions of the Helmholtz equation, that, if v is radiating and Γ_R is the boundary of the sphere of radius R, then

$$\Re \int_{\Gamma_R} \bar{v} \frac{\partial v}{\partial r} \, ds + R \int_{\Gamma_R} \left(k^2 |v|^2 + \left| \frac{\partial v}{\partial r} \right|^2 - |\nabla_T v|^2 \right) \, ds \le 2kR \, \Im \int_{\Gamma_R} \bar{v} \frac{\partial v}{\partial r} \, ds.$$

Proof. Expand everything in Bessel functions and use the monotonicity property that $|H_{\nu}^{(1)}(z)|^2$ is decreasing for $\nu \ge 0$, $|H_{\nu}^{(1)}(z)|^2 z$ for $\nu \ge 1/2$. (Cf. proof of Lemma 1.13 yesterday.)

The Standard 2nd Kind Integral Equations When the Domain is Lipschitz (Brakhage-Werner and its adjoint)

$$\Delta u + k^2 u = 0$$

$$\Omega^+$$

$$u = 0$$

$$\Gamma$$

$$U = 0$$

$$\Omega^+$$

$$\Omega^+$$

$$\Omega^-$$

$$\Omega^-$$

$$\Omega^+$$

$$\Omega^-$$

$$\Omega^+$$

$$\Omega^+$$

$$\Omega^+$$

$$U(x) = u^i(x) - \int_{\Gamma} G(x, y) \gamma_N^+ u(y) ds(y), \quad x \in \Omega^+,$$

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$$\begin{array}{c} \Delta u + k^2 u = 0 \\ & & & \\ & u^i, \text{ incident wave} & & u = 0 \\ & & & \\ & & & \\ & &$$

$$\begin{array}{c} \Delta u+k^2u=0\\ & & & \\ & &$$

$$V\gamma_N^+ u = 2\gamma_D^+ u^i, \quad \gamma_N^+ u + K'\gamma_N^+ u = 2\gamma_N^+ u^i,$$
$$\Rightarrow A'\gamma_N^+ u = f,$$

where

$$A' := I + K' - i\eta V,$$

I is the identity operator, $\eta \in \mathbb{R}$ the **coupling parameter**, $f := 2\gamma_N^+ u^i - 2i\eta\gamma_D^+ u^i$, and, for $\varphi \in L^2(\Gamma)$ and (almost all) $x \in \Gamma$, $V\varphi(x) = 2\int_{\Gamma} G(x, y)\varphi(y) ds(y), \quad K'\varphi(x) = 2\int_{\Gamma} \frac{\partial G(x, y)}{\partial n(x)}\varphi(y) ds(y).$ Alternatively ..., following Brakhage & Werner (1965) we find that an ansatz for u^s as a combined single and double-layer potential, with density φ and coupling parameter $\eta \in \mathbb{R}$ satisfies the scattering problem iff

$$A\varphi = -2\gamma_D^+ u^i,$$

where

$$A := I + K - i\eta V,$$

and, for $\varphi \in L^2(\Gamma)$ and (almost all) $x \in \Gamma$,

$$V\varphi(x) = 2\int_{\Gamma} G(x,y)\varphi(y)\,ds(y), \quad K\varphi(x) = 2\int_{\Gamma} \frac{\partial G(x,y)}{\partial n(y)}\varphi(y)ds(y).$$

N.B., where $(\phi, \psi) := \int_{\Gamma} \phi \psi ds$, $(A\phi, \psi) = (\phi, A'\psi), \quad \phi, \psi \in C^{\infty}(\Gamma).$

$$A' := I + K' - i\eta V, \quad A := I + K - i\eta V$$

$$V\varphi(x) = 2\int_{\Gamma} G(x,y)\varphi(y)\,ds(y), \quad K'\varphi(x) = 2\int_{\Gamma} \frac{\partial G(x,y)}{\partial n(x)}\varphi(y)ds(y),$$
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$$K\varphi(x) = 2 \int_{\Gamma} \frac{\partial G(x,y)}{\partial n(y)} \varphi(y) ds(y).$$

Mapping Properties. (Follows from Ralf, Thm 2.1.9)

$$A': H^{s-1/2}(\Gamma) \to H^{s-1/2}(\Gamma), \quad A: H^{s+1/2}(\Gamma) \to H^{s+1/2}(\Gamma)$$

and these mappings are bounded, for $|s| \le 1/2$. (See Costabel (1988), McLean (2000), Meyer & Coifmann (2000).)

$$A' := I + K' - i\eta V, \quad A := I + K - i\eta V$$

$$V\varphi(x) = 2\int_{\Gamma} G(x,y)\varphi(y)\,ds(y), \quad K'\varphi(x) = 2\int_{\Gamma} \frac{\partial G(x,y)}{\partial n(x)}\varphi(y)ds(y),$$

$$K\varphi(x) = 2 \int_{\Gamma} \frac{\partial G(x,y)}{\partial n(y)} \varphi(y) ds(y).$$

Injectivity. (Ralf, Thm 2.1.16) If $\eta \neq 0$, $A' : H^{-1/2}(\Gamma) \rightarrow H^{-1/2}(\Gamma)$ is injective. (See C-W & Langdon, preprint, but same standard argument as for smooth boundaries, see e.g. Colton & Kress (1983).)

$$A' := I + K' - i\eta V, \quad A := I + K - i\eta V$$

$$\begin{split} V\varphi(x) &= 2\int_{\Gamma} G(x,y)\varphi(y)\,ds(y), \ \ K'\varphi(x) = 2\int_{\Gamma} \frac{\partial G(x,y)}{\partial n(x)}\varphi(y)ds(y), \\ K\varphi(x) &= 2\int_{\Gamma} \frac{\partial G(x,y)}{\partial n(y)}\varphi(y)ds(y). \end{split}$$

Invertibility. If $\eta \neq 0$, then

$$A': H^{s-1/2}(\Gamma) \to H^{s-1/2}(\Gamma), \quad A: H^{s+1/2}(\Gamma) \to H^{s+1/2}(\Gamma)$$

are bijections, for $|s| \leq 1/2$. (See C-W & Langdon, preprint: follows since A is Fredholm of index zero on $H^1(\Gamma)$ and $L^2(\Gamma)$; Verchota (1985), Elschner (1992).)

$$A' := I + K' - i\eta V, \quad A := I + K - i\eta V$$

$$\begin{split} V\varphi(x) &= 2\int_{\Gamma}G(x,y)\varphi(y)\,ds(y), \ \ K'\varphi(x) = 2\int_{\Gamma}\frac{\partial G(x,y)}{\partial n(x)}\varphi(y)ds(y), \\ K\varphi(x) &= 2\int_{\Gamma}\frac{\partial G(x,y)}{\partial n(y)}\varphi(y)ds(y). \end{split}$$

Coercivity. (Ralf, Lemmma 2.1.17) A is coercive (elliptic + compact) as an operator on $H^{1/2}(\Gamma)$ (and A' as an operator on $H^{-1/2}(\Gamma)$), in fact in the 3D case (with the right choice of norm) $\frac{1}{2}A = I - (\frac{1}{2}I - K)$ and $\frac{1}{2}I - K$ is a contraction when k = 0. (Corollary of results in Steinbach & Wendland (2001).) (Ralf, p. 33, not great for discretization as inner products non-local.)

$$A' := I + K' - i\eta V, \quad A := I + K - i\eta V$$

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Wave Number Dependence. But how do ||A|| and $||A^{-1}||$ depend on k, especially as $k \to \infty$, and how should we choose η ?

Theorem. (See Dominguez, Graham, and Smyshlyaev, preprint, and cf. Buffa & Sauter, to appear SISC.)

If Γ is a circle, and $\eta = k$, then, for all sufficiently large k, A is elliptic on $L^2(\Gamma)$, precisely

$$\Re(A\phi, \bar{\phi}) \ge \frac{1}{2} \|\phi\|_2^2,$$

so that $||A^{-1}||_2 \le 2$. Further $||A||_2 = O(k^{1/3})$ as $k \to \infty$.

Proof. Explicit calculation of spectrum of A (this dates back to Kress and Spassov 1983), and clever estimates of Bessel functions uniform in argument and order.

N.B. In the circle case A = A'.

N.B. Suggests variational formulation in $L^2(\Gamma)$ attractive and natural!? (cf. Ralf, p.33)

Let n(x) denote the outward unit normal at $x \in \Gamma$, and

$$R_0 := \max_{x \in \Gamma} |x|, \quad \delta_- := \text{ess. inf} \ x \cdot n(x).$$

Theorem. (C-W & Monk, preprint.) If Ω^- is a polyhedron which is starlike with respect to the origin (i.e. $\delta_- > 0$), or a more general piecewise smooth, Lipschitz, starlike domain, $\eta = k$ and $kR_0 \ge 1$, then

$$||A^{-1}||_2 = ||A'^{-1}||_2 \le \frac{1}{2} \left(1 + 13\theta + 4\theta^2\right),$$

where $\theta := R_0 / \delta_-$.

Examples.

Circle/sphere: $\theta = 1$, $||A^{-1}||_2 = ||A'^{-1}||_2 \le 9$. Cube: $\theta = \sqrt{3}$, $||A^{-1}||_2 = ||A'^{-1}||_2 \le 18$.

The Main Ingredients in the Proof

1. Green's theorem and a Rellich(-Payne-Weinberger-Nečas) type identity.

Such identities, useful for obtaining explicit a priori bounds and regularity estimates for strongly elliptic systems, follow from the divergence theorem, and date back to Rellich (1943).

See Chapter 5 of Nečas (1967) or McLean (2000). Our particular version of the identity is essentially that from the PhD of Melenk (1995).

Lemma 2.2. Suppose that $\Omega \subset \mathbb{R}^d$ is a bounded Lipschitz domain and that $v \in H^2(G)$. Then, for every $k \ge 0$, where $g := \Delta v + k^2 v$ and the unit normal vector n is directed into Ω , it holds that

$$\int_{\Omega} \left(|\nabla v|^2 - k^2 |v|^2 + g\bar{v} \right) \, dx = -\int_{\partial\Omega} \bar{v} \, \frac{\partial v}{\partial n} \, ds$$

and

$$\int_{\Omega} \left((2-d) |\nabla v|^2 + dk^2 |v|^2 + 2\Re \left(gx \cdot \nabla \bar{v} \right) \right) \, dx = -\int_{\partial\Omega} \left(x \cdot n \left(k^2 |v|^2 + \left| \frac{\partial v}{\partial n} \right|^2 - |\nabla_T v|^2 \right) + 2\Re \left(x \cdot \nabla_T \bar{v} \frac{\partial v}{\partial n} \right) \right) \, ds.$$

Corollary 2.3. Suppose that $\Omega \subset \mathbb{R}^d$ is a bounded Lipschitz domain and that $v \in C^2(\Omega) \cap C^1(\overline{\Omega})$ and $\Delta v + k^2 v = 0$ in Ω . Then, where the unit normal vector n is directed into Ω , it holds that

$$\int_{\Omega} \left(|\nabla v|^2 - k^2 |v|^2 \right) \, dx = -\int_{\partial\Omega} \bar{v} \, \frac{\partial v}{\partial n} \, ds \tag{1}$$

and

$$\int_{\Omega} \left((2-d) |\nabla v|^2 + dk^2 |v|^2 \right) dx = -\int_{\partial\Omega} \left(x \cdot n \left(k^2 |v|^2 + \left| \frac{\partial v}{\partial n} \right|^2 - |\nabla_T v|^2 \right) + 2\Re \left(x \cdot \nabla_T \bar{v} \frac{\partial v}{\partial n} \right) \right) ds.$$

N.B. This is applied in Ω^- and in Ω^+_R to $v := \Psi_{SL}\varphi$, where $\varphi = A'^{-1}\psi$, in order to bound $(\gamma_N^+ - \gamma_N^-)v = \varphi$ in terms of ψ , starting from

$$\varphi = {A'}^{-1}\psi \Rightarrow \gamma_N^- v - i\eta\gamma_D^- v = \frac{1}{2}\psi.$$

2. Once again, the property of radiating solutions of the Helmholtz equation, that, if v is radiating and Γ_R is the boundary of the sphere of radius R, then

$$\Re \int_{\Gamma_R} \bar{v} \frac{\partial v}{\partial r} \, ds + R \int_{\Gamma_R} \left(k^2 |v|^2 + \left| \frac{\partial v}{\partial r} \right|^2 - |\nabla_T v|^2 \right) \, ds \le 2kR \, \Im \int_{\Gamma_R} \bar{v} \frac{\partial v}{\partial r} \, ds.$$

Summary

- 1. Discussed wave number explicit lower and upper bounds on the inf-sup constant for the weak formulation in Ω_R^{+a} of the Dirchlet scattering problem.
- 2. Presented results on invertibility of the standard combined singleand double-layer boundary integral equation formulations for this problem, in the case of a Lipschitz domain, including the Brakhage-Werner (1965) formulation $A\varphi = -2\gamma_D u^i$ where $A := I + K - i\eta V$.
- 3. Showed that, if Ω^- is piecewise smooth, Lipschitz and starlike, then $||A^{-1}||_2 \leq C$, with an explicit formula for C as a function of the geometry and η/k .

^aThat part of Ω^+ inside a ball of radius R.

Further Reading on Wave-Number-Explicit Estimates

A hybrid numerical-asymptotic boundary integral method for high-frequency acoustic scattering.

Dominguez, Graham, Smyshlyaev, University of Bath preprint, which builds on ...

Schnelle Summationsverfahren zur numerischen Lösung von Integralgleichungen für Streuprobleme im \mathbb{R}^3 . Giebermann, PhD, Karlsruhe, 1997.

On Generalized Finite Element Methods.

Melenk, PhD, Maryland, 1995.

An elliptic regularity coefficient estimate for a problem arising from a frequncy domain treatment of waves.

Feng & Sheen, Trans. Amer. Math. Soc., 1994.

Sharp regularity coefficient estimates for complex-valued acoustic and

elastic Helmholtz equations.

Cummings and Feng, Math. Models Methods Appl. Sci., 2006.

Wave-number-explicit bounds in time-harmonic scattering. C-W & Monk 2006, preprint.

A well-posed integral equation formulation for 3D rough surface scattering.

C-W, Heinemeyer & Potthast, Proc. R. Soc. Lond. A, 2006.

Existence, uniqueness and variational methods for scattering by unbounded rough surfaces.

C-W & Monk, SIAM J. Math. Anal., 2005.

The mathematics of scattering by unbounded, rough, inhomogeneous layers.

C-W, Monk & Thomas J. Comp. Appl. Math. 2006

For copies of my stuff: www.reading.ac.uk/~sms03snc

Four Open Problems

- 1. Sharp estimates on $||A||_2$ as $k \to \infty$. This is much harder, see the harmonic analysis literature on oscillatory integral operators (Stein, Phong). (A crude bound that $||A||_2 \le \max(||A||_{\infty}, ||A'||_{\infty}) = O(k^{(d-1)/2})$ is straightforward, but it seems, from the circle/sphere, that $||A||_2 = O(k^{1/3})$.)
- 2. Bounds on $||A^{-1}||_2$ and lower bounds on the inf-sup constant for the weak problem in Ω_R^+ when the scatterer is not starlike.
- 3. Any wave-number-explicit bounds in the discrete case.
- 4. Preconditioners/new formulations which remove this k-dependence – and proofs!