

Waves: Modeling, Analysis, and Numerics
Radboud University
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4TU.AMI

Linear Waves: From Physics to Numerics

Part III

Carlos Pérez Arancibia (c.a.perezarancibia@utwente.nl)
Mathematics of Computational Science
University of Twente

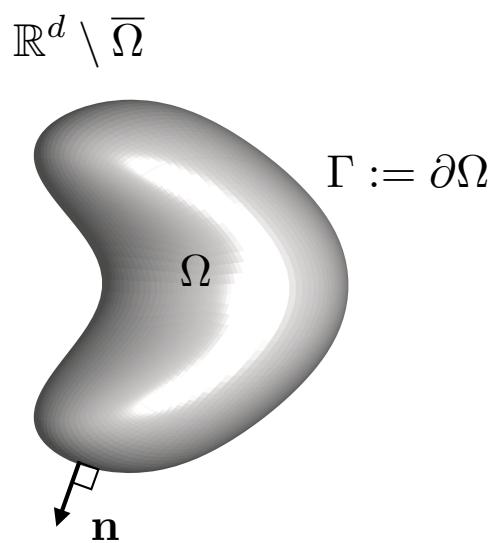


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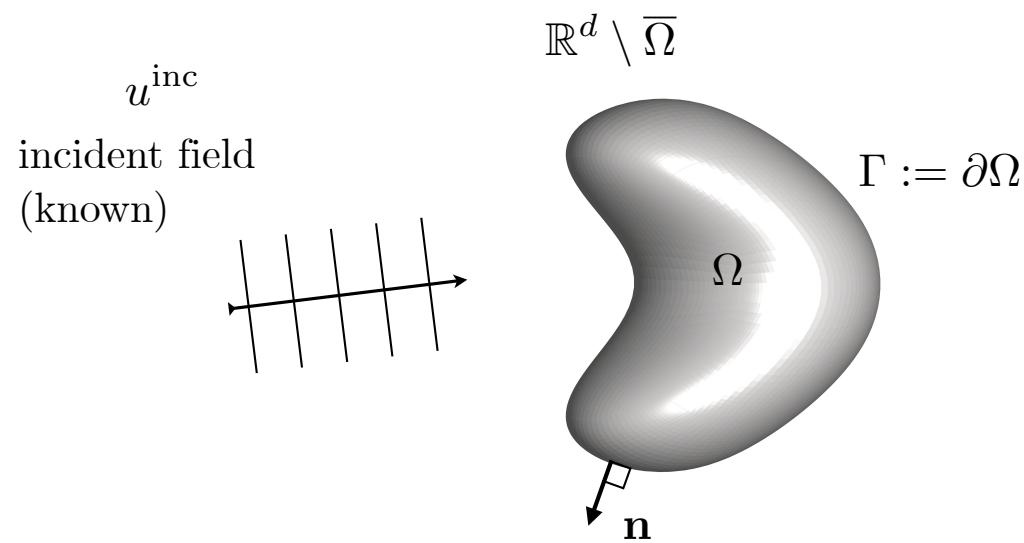
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Scattering Problem Setup

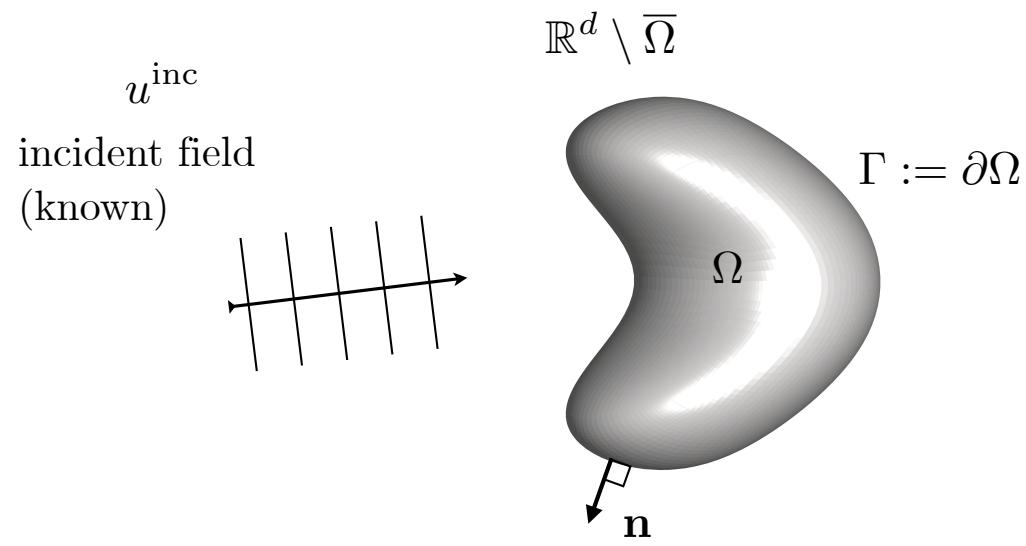
Scattering by Bounded Obstacles



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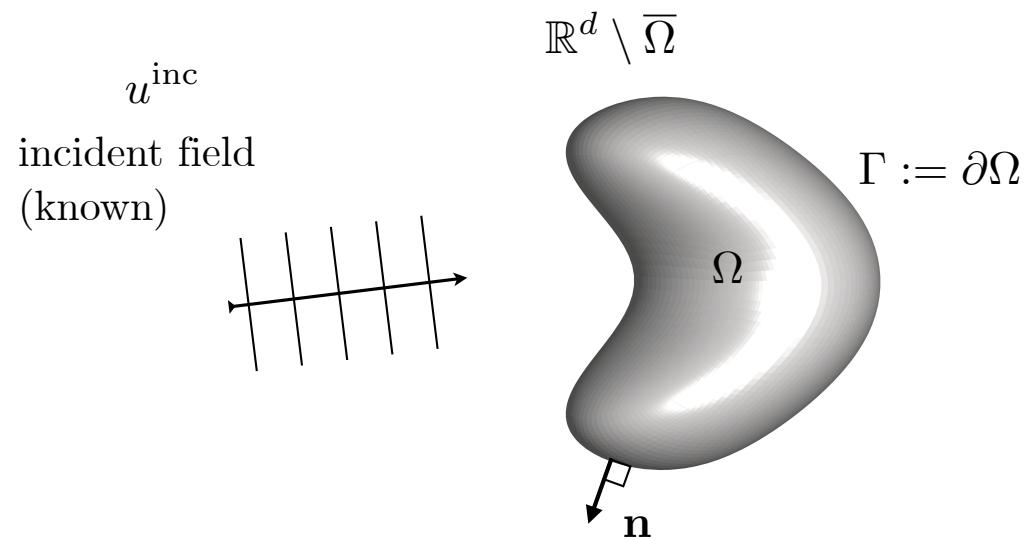
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Helmholtz equation:

$$\Delta u^{\text{inc}} + k^2 u^{\text{inc}} = 0 \quad \text{in } D \supset \Gamma$$

Scattering by Bounded Obstacles

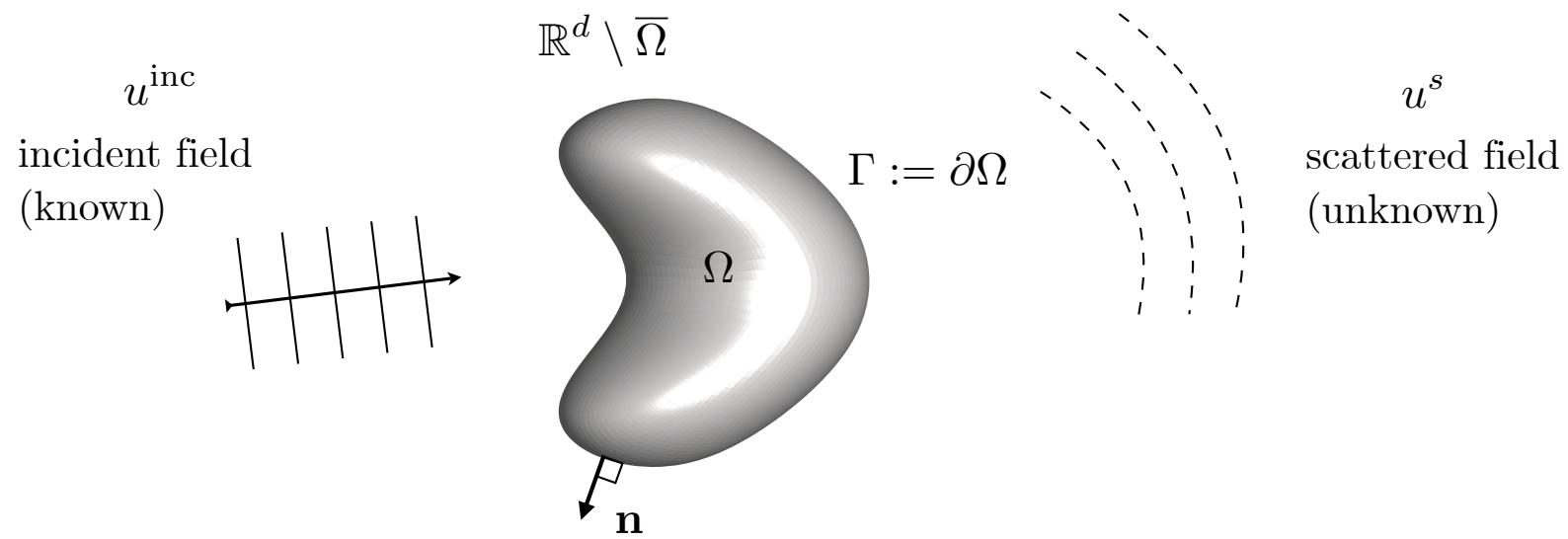


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$$\Delta u^{\text{inc}} + k^2 u^{\text{inc}} = 0 \quad \text{in } D \supset \Gamma$$

Time convention: $e^{-i\omega t}$; angular frequency: $\omega > 0$;
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Scattering by Bounded Obstacles

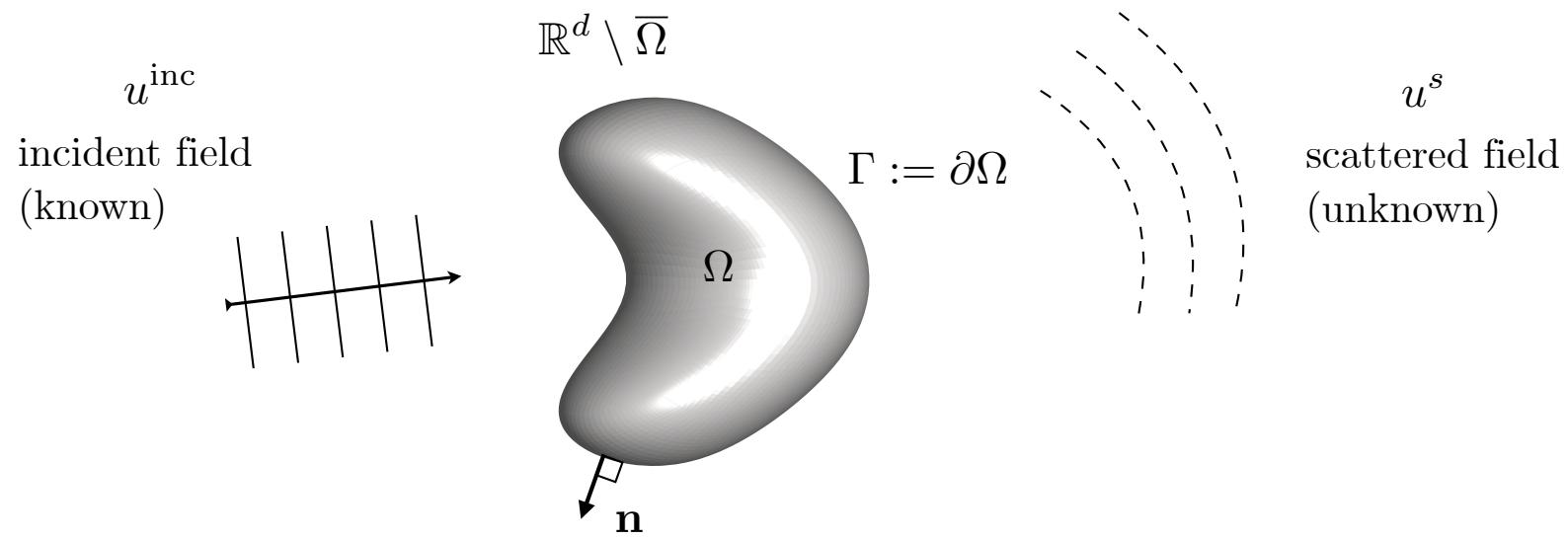


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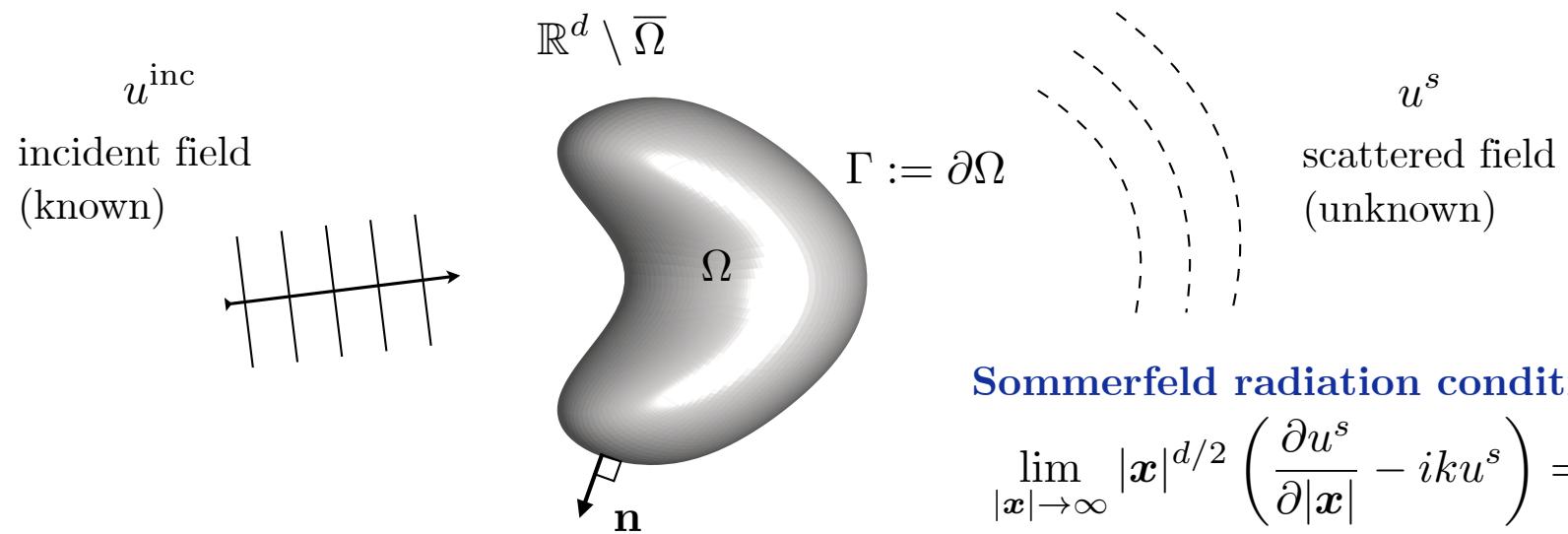
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Scattering by Bounded Obstacles



Sommerfeld radiation condition:

$$\lim_{|\mathbf{x}| \rightarrow \infty} |\mathbf{x}|^{d/2} \left(\frac{\partial u^s}{\partial |\mathbf{x}|} - ik u^s \right) = 0$$

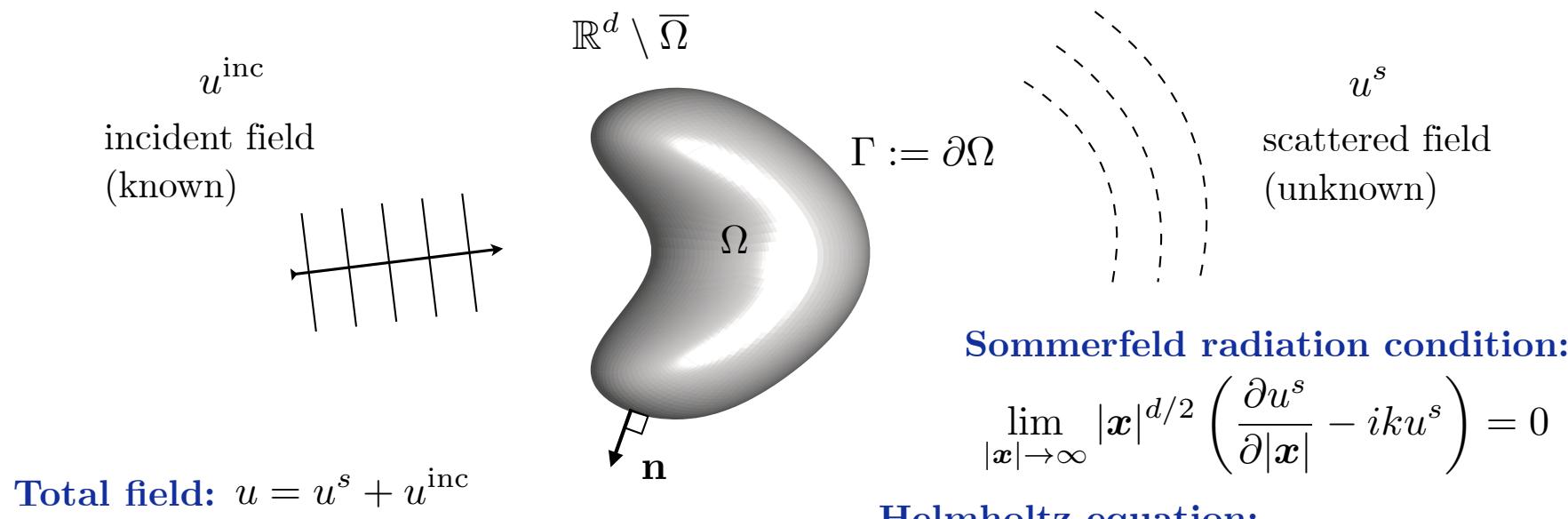
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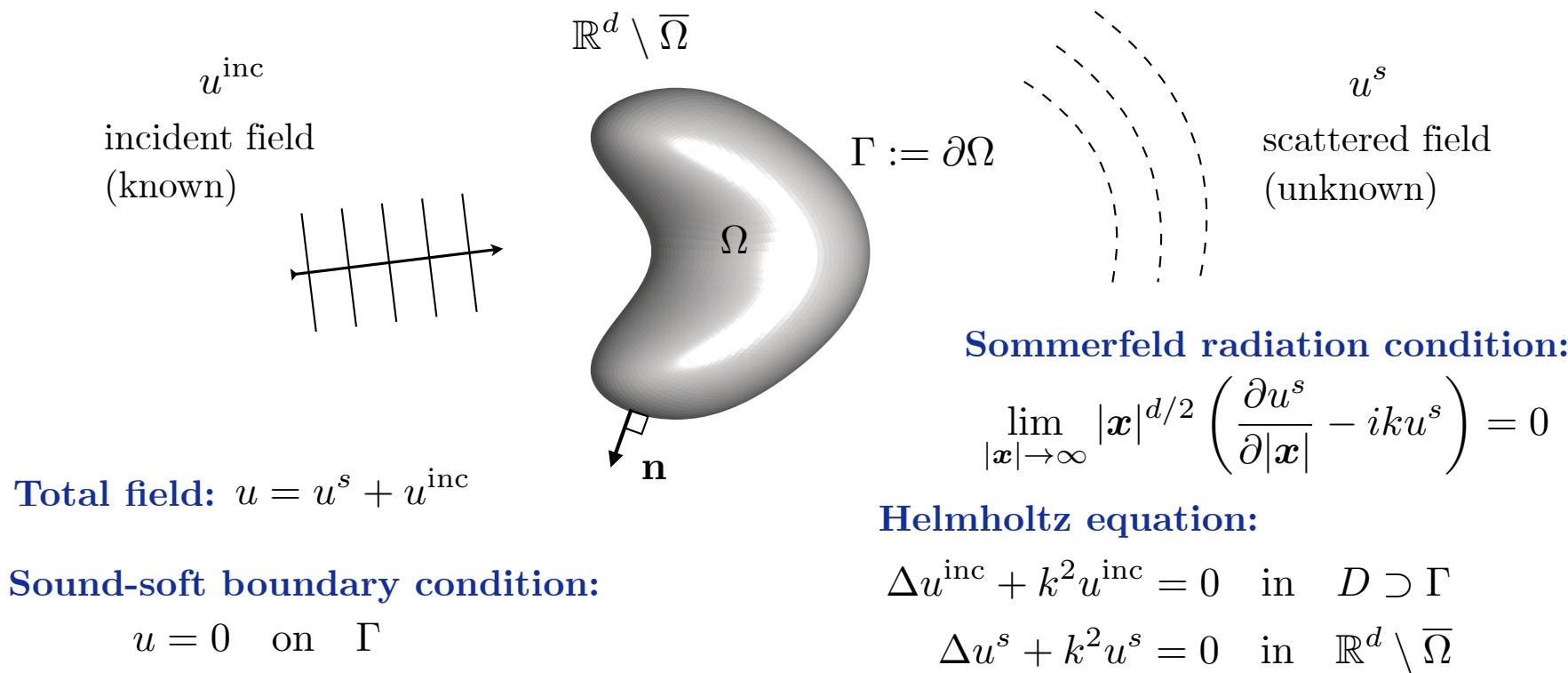
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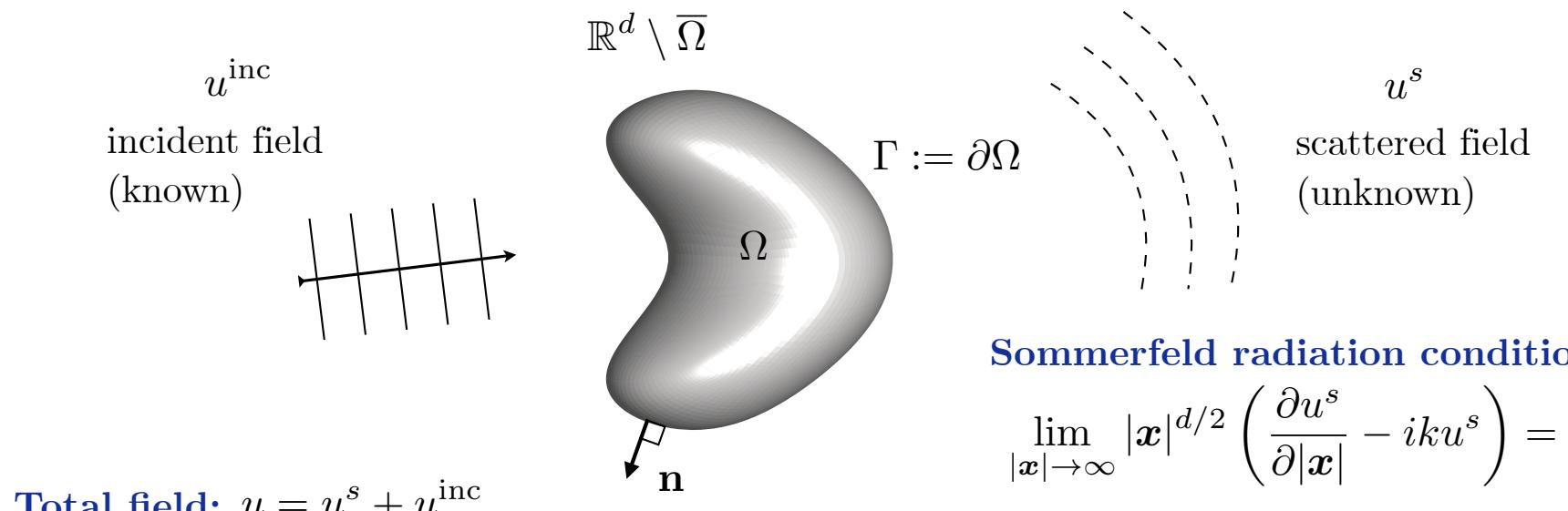
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Scattering by Bounded Obstacles



Sound-soft boundary condition:

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

Boundary condition

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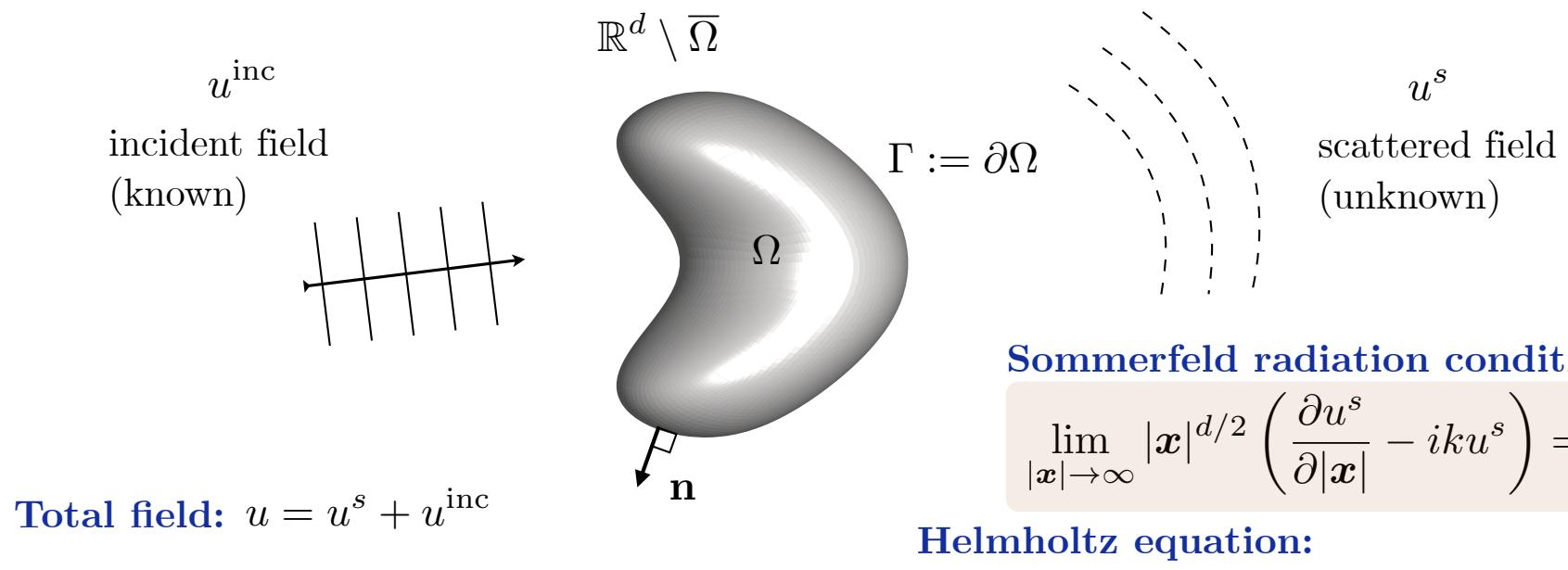
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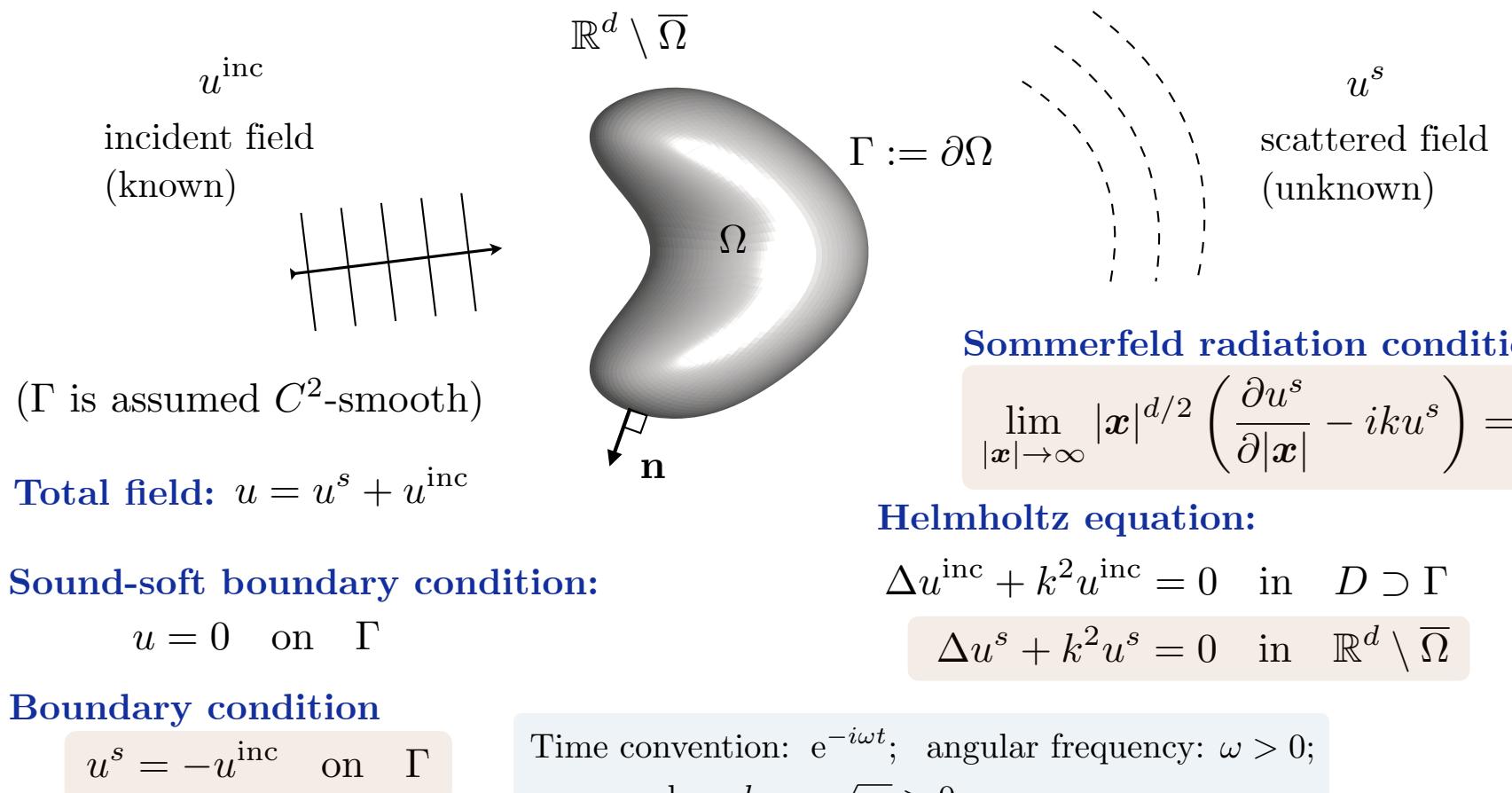
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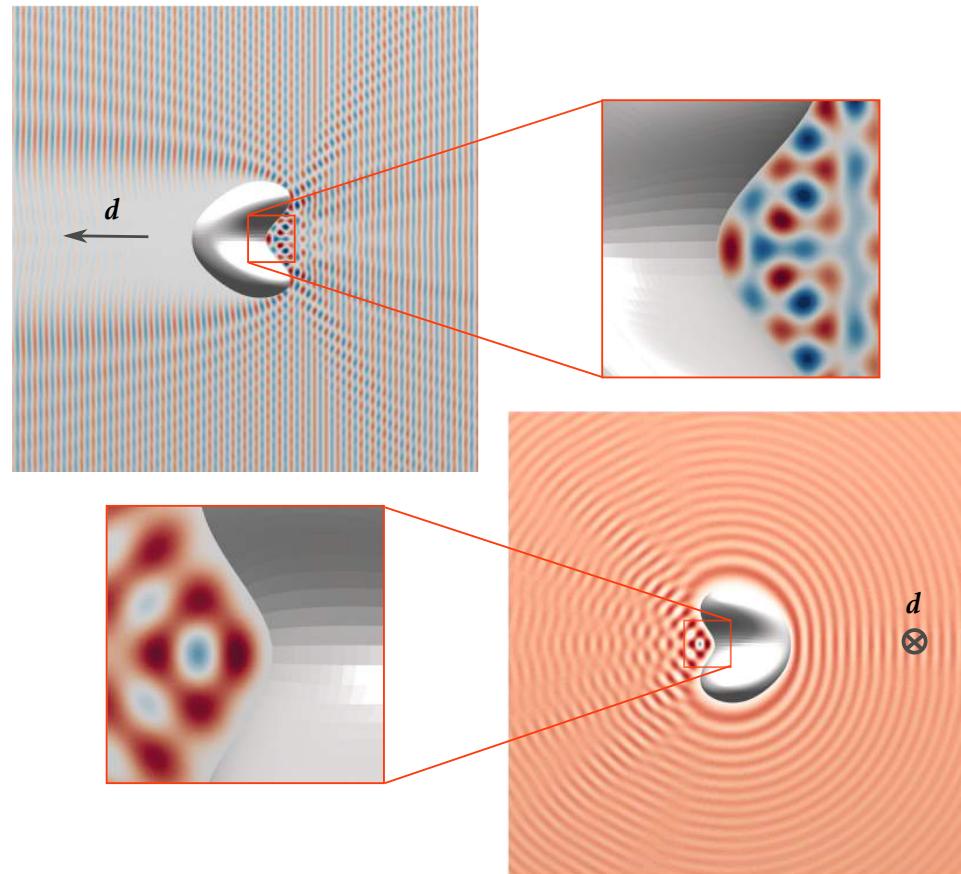
Scattering by Bounded Obstacles



Scattering by Bounded Obstacles

$$u^{\text{inc}}(\mathbf{x}) = e^{ik\mathbf{d} \cdot \mathbf{x}}$$

incident planewave



$$u = u^s + u^{\text{inc}}$$

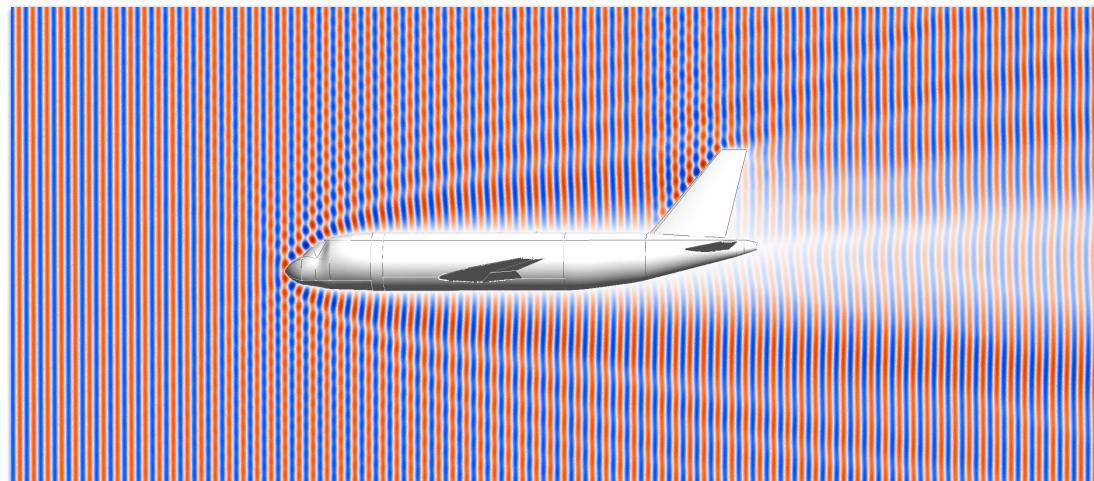
total field satisfies a
boundary condition

P.-A., C., Turc, C., & Faria, L. (2019). Planewave density interpolation methods for 3D Helmholtz boundary integral equations. *SIAM Journal on Scientific Computing*, 41(4), A2088-A2116

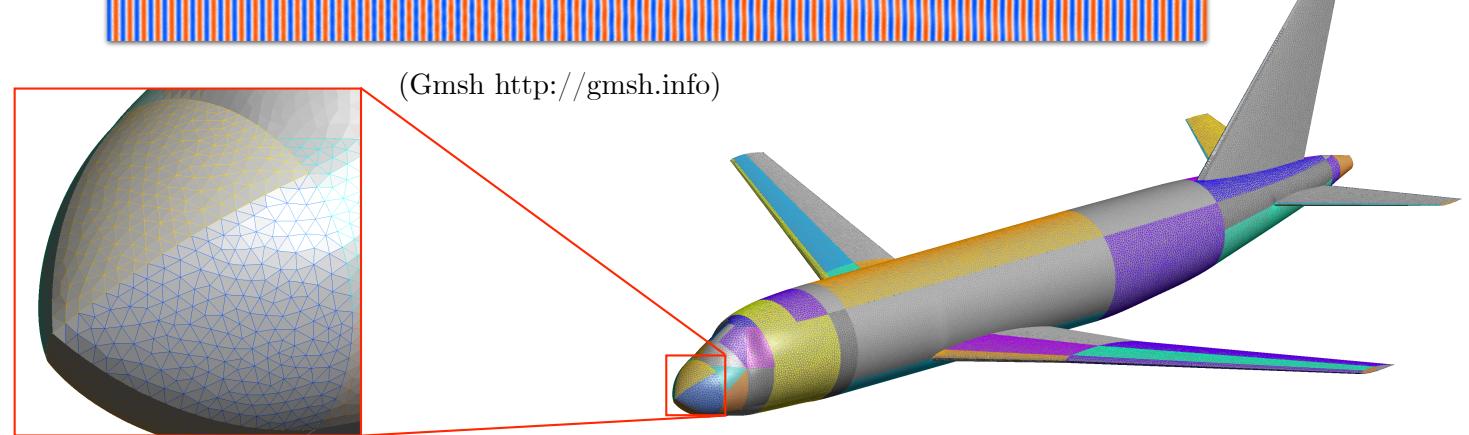
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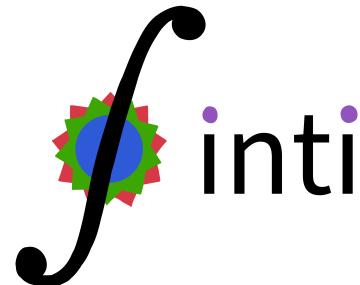


(Gmsh <http://gmsh.info>)



Faria, L., P.-A., C., & Bonnet (2020). General-purpose kernel regularization of boundary integral equations via density interpolation. In preparation.

Scattering by Bounded Obstacles: Inti.jl



[https://github.com/
IntegralEquations/
Inti.jl](https://github.com/IntegralEquations/Inti.jl)

```
Last login: Wed Jun 26 10:15:59 on ttys000
~ % julia
Documentation: https://docs.julialang.org
Type "?" for help, "]?" for Pkg help.
Version 1.10.4 (2024-06-04)
Official https://julialang.org/ release

(@v1.10) pkg> add Inti
  Resolving package versions...
    Updating `~/.julia/environments/v1.10/Project.toml`
[fb74042b] ~ Inti v0.1.0 `https://github.com/IntegralEquations/Inti.jl#main` => v0.1.0
    Updating `~/.julia/environments/v1.10/Manifest.toml`
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julia> using Inti
julia>
```





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Finite-Domain Approximation of Exterior Problems

First-order Absorbing Boundary Condition (ABC)

Problem: To use our preferred numerical methods (e.g., finite elements or finite differences), we need to reduce the computational domain to a **truncated, bounded domain**.

$$\begin{cases} \Delta u^s + k^2 u^s = 0 & \text{in } \mathbb{R}^d \setminus \bar{\Omega} \\ u^s = -u^{\text{inc}} & \text{on } \Gamma \\ \lim_{|\boldsymbol{x}| \rightarrow \infty} |\boldsymbol{x}|^{(d-1)/2} \left(\frac{\partial u^s}{\partial |\boldsymbol{x}|} - iku^s \right) = 0 \end{cases}$$

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The Sommerfeld radiation condition states that

$$\frac{\partial u^s}{\partial r} - iku^s = A, \quad \text{where } |A| = o(r^{-(d-1)/2}) \quad \text{as } r = |\boldsymbol{x}| \rightarrow \infty$$

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On a truncated circular boundary $S_R := \{\boldsymbol{x} \in \mathbb{R}^d : |\boldsymbol{x}| = R\}$, it can be approximated by the Robin (impedance) condition

$$\frac{\partial u^s}{\partial n} - iku^s = 0 \quad \text{on } S_R,$$

which neglects the $o(r^{-(d-1)/2})$ term A on the right-hand side, providing a simple local far-field approximation.

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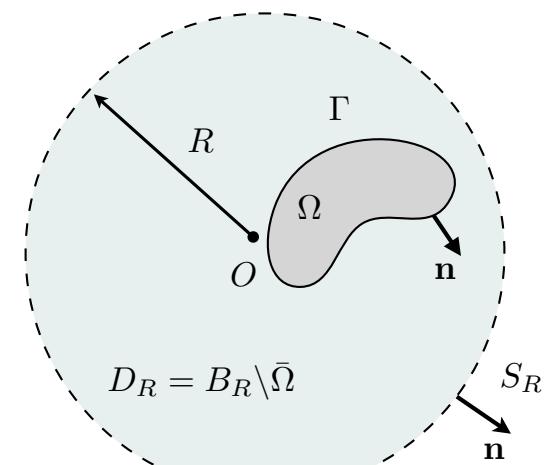
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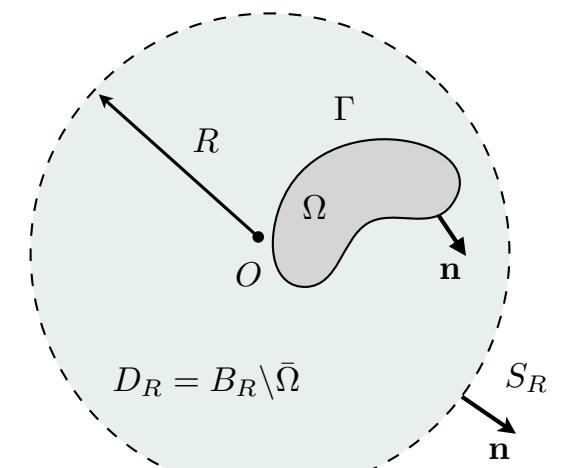
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The problem then reduces to finding $u = u^s + u^{\text{inc}} \in C^2(D_R) \cap C^1(\overline{D_R})$ such that

$$\begin{aligned} \Delta u + k^2 u &= 0 && \text{in } D_R, \\ u &= 0 && \text{on } \Gamma, \\ \frac{\partial u}{\partial n} - iku &= \frac{\partial u^{\text{inc}}}{\partial n} - iku^{\text{inc}} && \text{on } S_R. \end{aligned}$$



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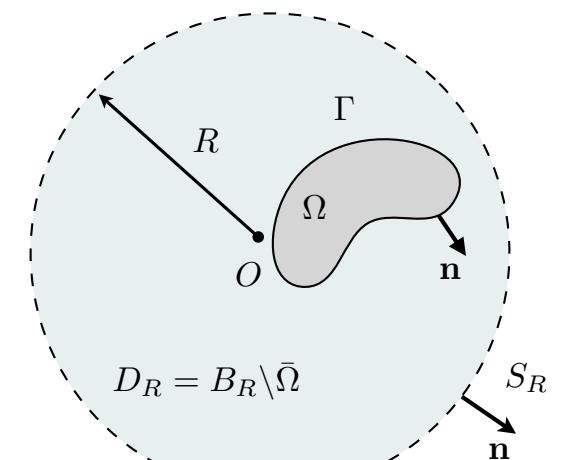
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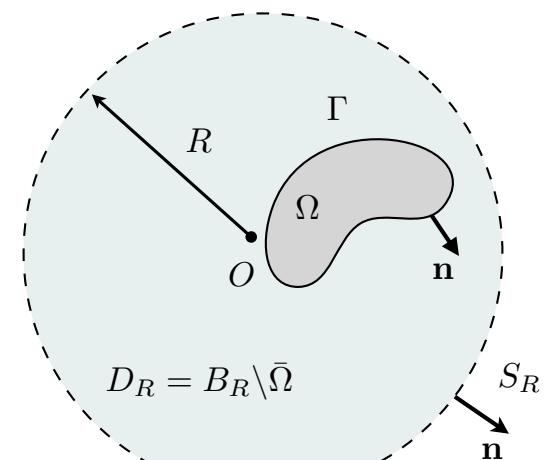
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$$\begin{array}{l} \text{truncated-domain} \\ \text{problem} \\ \text{in the "weak sense"} \end{array} \quad \begin{cases} \Delta u + k^2 u = 0 & \text{in } D_R, \\ u = 0 & \text{on } \Gamma, \\ \frac{\partial u}{\partial n} - iku = \frac{\partial u^{\text{inc}}}{\partial n} - iku^{\text{inc}} & \text{on } S_R. \end{cases}$$



First-order ABC: Variational Formulation

Find $u \in V := H_0^1(D_R) := \{v \in H^1(D_R) : \gamma_0^\Gamma v = 0\}$ such that

$$a(u, v) = F(v) \quad \text{for all } v \in V,$$

where

$$a(u, v) := \int_{D_R} (\nabla u \cdot \nabla \bar{v} - k^2 u \bar{v}) \, d\mathbf{x} - ik \int_{S_R} u \bar{v} \, ds \quad \text{and} \quad F(v) := \int_{S_R} \bar{v} \underbrace{\left\{ \frac{\partial u^{\text{inc}}}{\partial n} - iku^{\text{inc}} \right\}}_{\in L^2(\Gamma)} \, ds.$$

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$a_0 : V \times V \rightarrow \mathbb{C}$ is continuous and coercive. **Lax–Milgram lemma** $\Rightarrow A_0 : V \rightarrow V'$ is invertible

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$a_0 : V \times V \rightarrow \mathbb{C}$ is continuous and coercive. **Lax–Milgram lemma** $\Rightarrow A_0 : V \rightarrow V'$ is invertible

$a_1 : V \times V \rightarrow \mathbb{C}$ defines a compact operator $A_1 : V \rightarrow V'$ ($H_0^1(D_R) \Subset L^2(D_R)$)

First-order ABC: Variational Formulation

Find $u \in V := H_0^1(D_R) := \{v \in H^1(D_R) : \gamma_0^\Gamma v = 0\}$ such that

$$a(u, v) = F(v) \quad \text{for all } v \in V,$$

where

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Is the variational problem well posed?

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$a_0 : V \times V \rightarrow \mathbb{C}$ is continuous and coercive. **Lax–Milgram lemma** $\Rightarrow A_0 : V \rightarrow V'$ is invertible

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$$A_0 u + A_1 u = F \implies \underbrace{u + A_0^{-1} A_1 u}_{\text{compact on } V} = A_0^{-1} F \quad \begin{aligned} &\text{we can apply the \textbf{Fredholm alternative!}} \\ &\text{(uniqueness implies existence)} \end{aligned}$$

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We have then shown that the truncated problem using an approximate radiation condition has a unique solution $u \in H_0^1(D_R)$.

Exact Non-Reflecting Boundary Condition

Problem: Using the radiation condition to truncate the domain is unsatisfactory, as a very large domain D_R is required to avoid spurious reflections from S_R .

$$\begin{cases} \Delta u^s + k^2 u^s = 0 & \text{in } \mathbb{R}^d \setminus \bar{\Omega} \\ u^s = -u^{\text{inc}} & \text{on } \Gamma \\ \lim_{|\boldsymbol{x}| \rightarrow \infty} |\boldsymbol{x}|^{(d-1)/2} \left(\frac{\partial u^s}{\partial |\boldsymbol{x}|} - iku^s \right) = 0 \end{cases}$$

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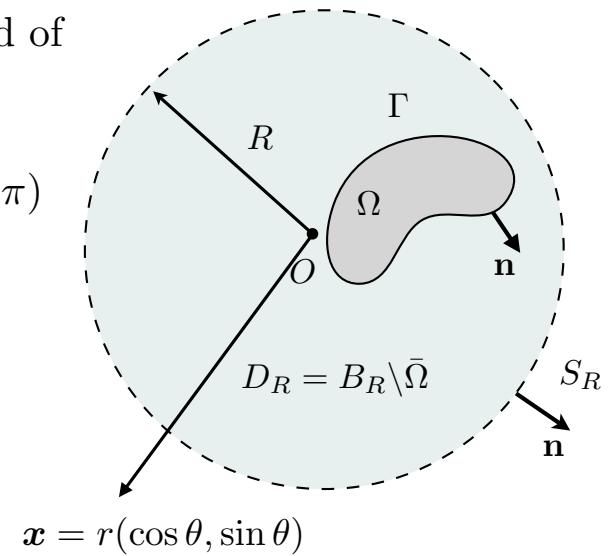
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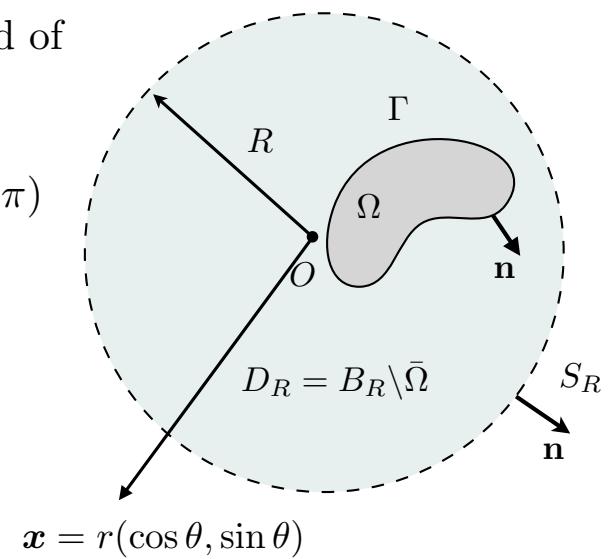
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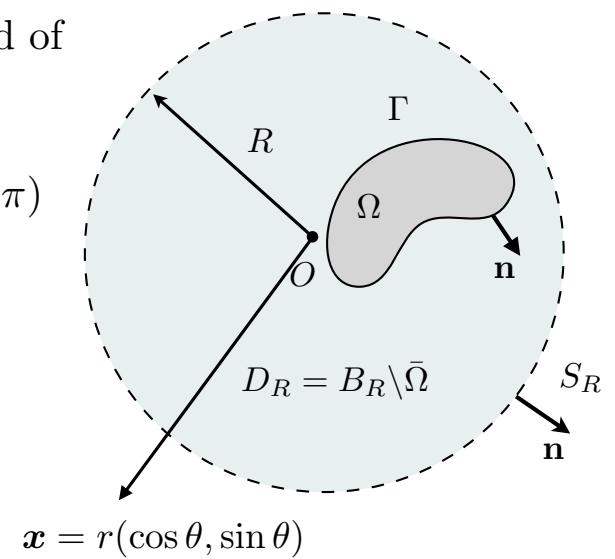
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Imposing the boundary condition:

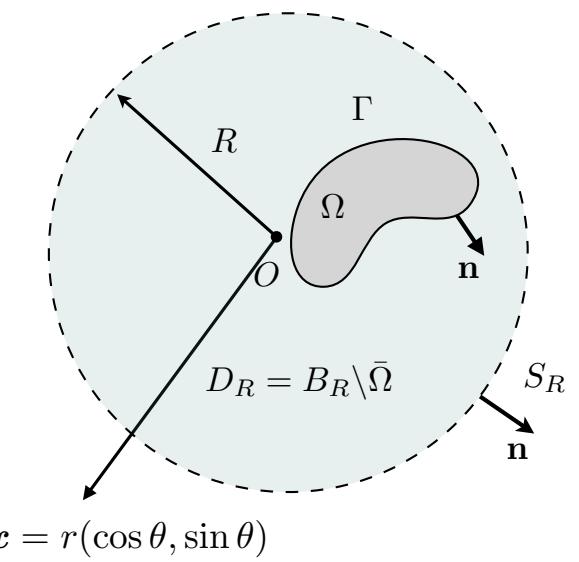
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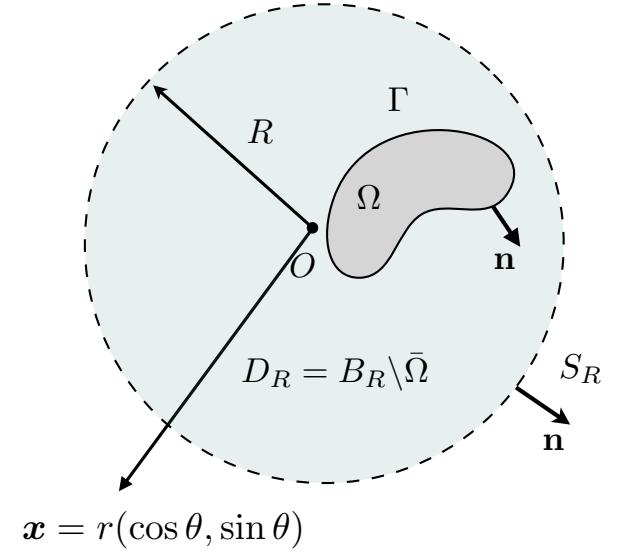


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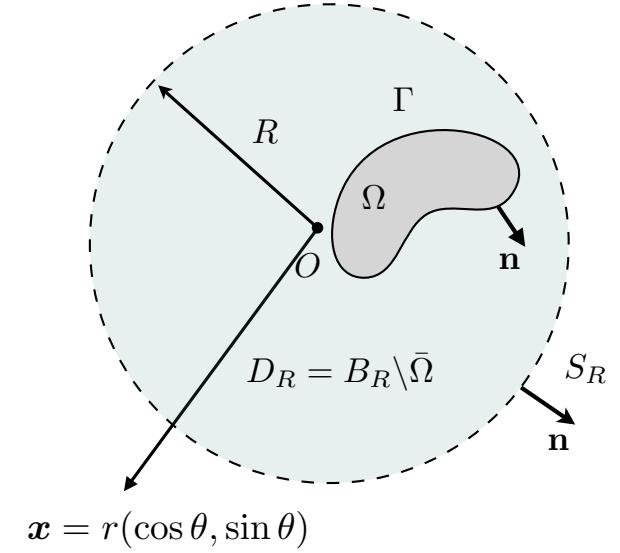
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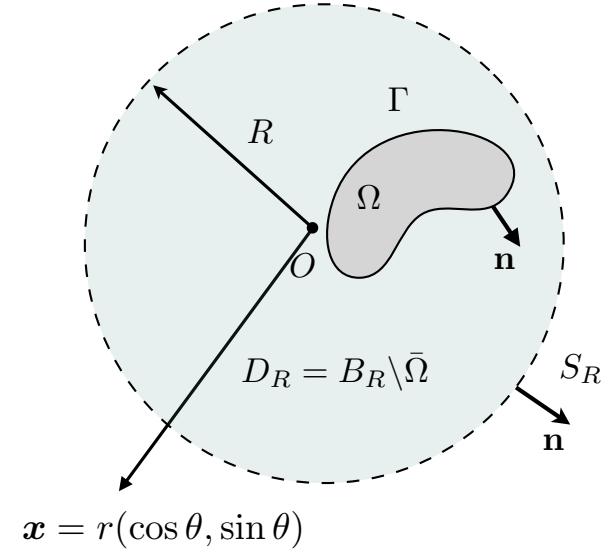
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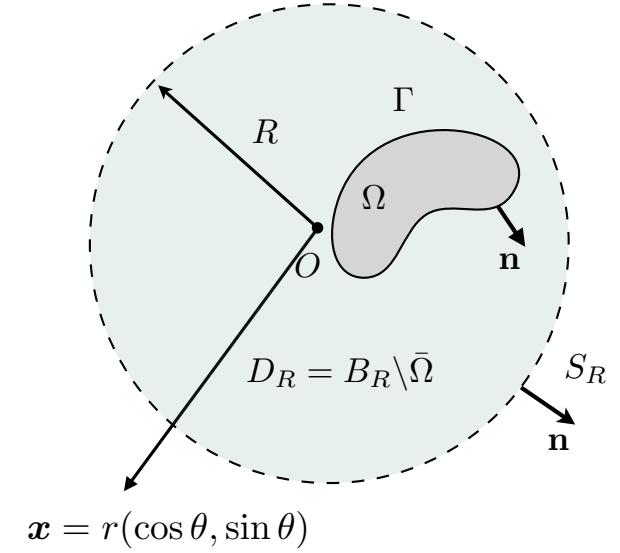
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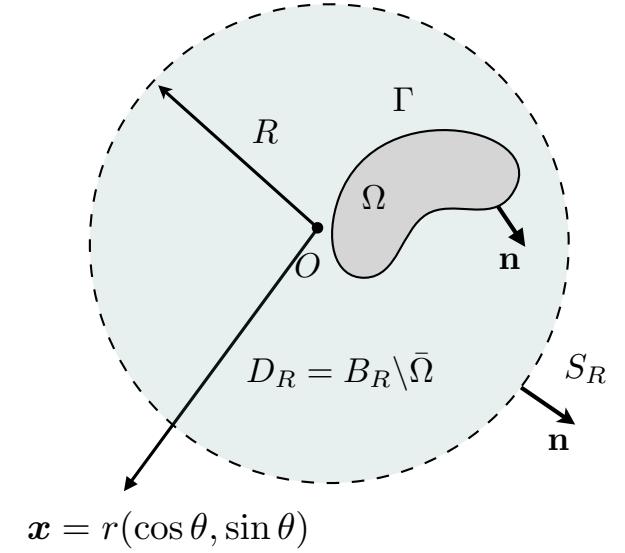
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It can be shown that $\Lambda : H^{1/2}(S_R) \rightarrow H^{-1/2}(S_R)$ is bounded.



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in general, these integrals should be interpreted as duality pairings

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$$\left. \begin{array}{l} \Delta u + k^2 u = 0 \quad \text{in } D_R \\ u = 0 \quad \text{on } \Gamma \\ \frac{\partial u}{\partial n} - \Lambda[\gamma_0^{S_R} u] = \underbrace{\frac{\partial u^{\text{inc}}}{\partial n} - \Lambda[\gamma_0^{S_R} u^{\text{inc}}]}_{f \in H^{-1/2}(S_R)} \quad \text{on } S_R \end{array} \right\} \iff \left\{ \begin{array}{l} \Delta u^s + k^2 u^s = 0 \quad \text{in } \mathbb{R}^d \setminus \overline{\Omega} \\ u^s = -u^{\text{inc}} \quad \text{on } \Gamma \\ \lim_{|\boldsymbol{x}| \rightarrow \infty} |\boldsymbol{x}|^{(d-1)/2} \left(\frac{\partial u^s}{\partial |\boldsymbol{x}|} - iku^s \right) = 0 \end{array} \right.$$

Variational formulation: Find $u \in H_0^1(D_R)$ such that

$$a(u, v) = F(v) \quad \text{for all } v \in H_0^1(D_R)$$

$$\text{where: } a(u, v) = - \int_{D_R} \{ \nabla u \cdot \nabla \bar{v} - k^2 u \bar{v} \} \, d\boldsymbol{x} + \int_{S_R} \Lambda[\gamma_0^{S_R} u] \bar{v} \, ds \quad \text{and} \quad F(v) = - \int_{S_R} f \bar{v} \, ds.$$

Exact Non-Reflecting Boundary Condition

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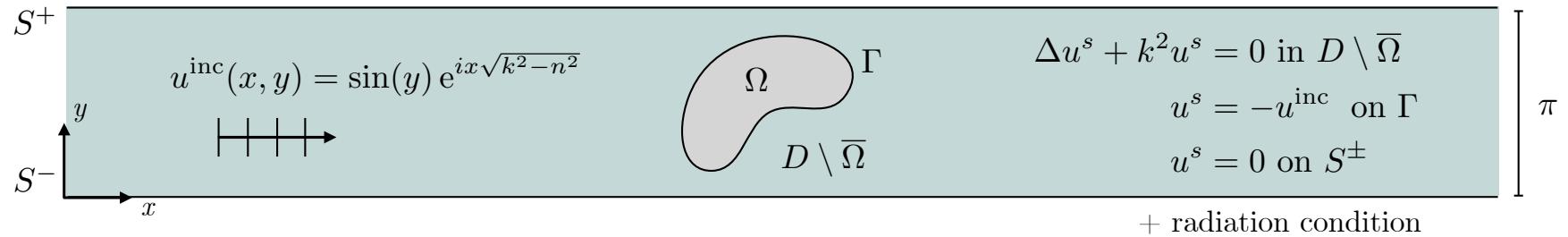
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this problem can be directly solved using standard (Lagrange) finite elements!

DtN Map for Waveguides

$$\begin{array}{c} S^+ \\ \text{---} \\ \begin{array}{c} u^{\text{inc}}(x, y) = \sin(y) e^{ix\sqrt{k^2 - n^2}} \\ | \quad | \quad | \quad | \end{array} \\ \begin{array}{c} y \\ \uparrow \\ S^- \end{array} \end{array} \quad \begin{array}{c} \Omega \\ D \setminus \bar{\Omega} \\ \Gamma \end{array} \quad \begin{array}{l} \Delta u^s + k^2 u^s = 0 \text{ in } D \setminus \bar{\Omega} \\ u^s = -u^{\text{inc}} \text{ on } \Gamma \\ u^s = 0 \text{ on } S^\pm \end{array} \quad \begin{array}{c} \pi \\ | \\ + \text{ radiation condition} \end{array}$$

DtN Map for Waveguides

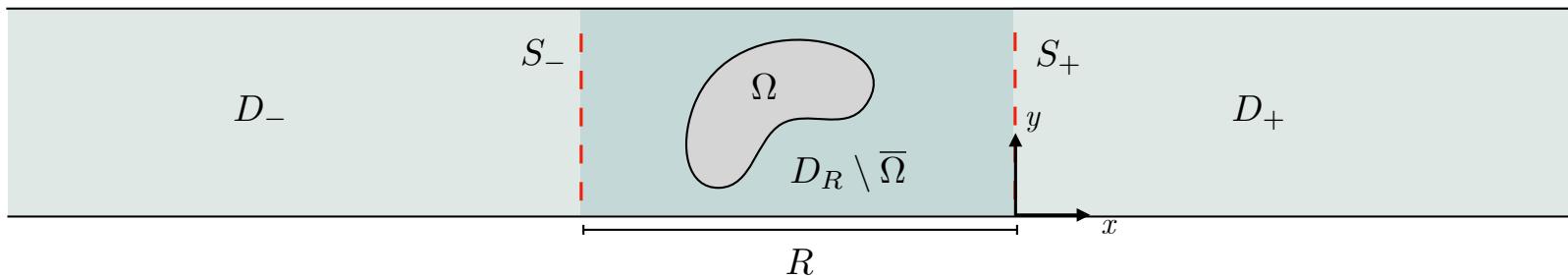


How can the DtN map be constructed in this situation?

DtN Map for Waveguides

$u^{\text{inc}}(x, y) = \sin(y) e^{ix\sqrt{k^2 - n^2}}$ Γ $\Delta u^s + k^2 u^s = 0 \text{ in } D \setminus \bar{\Omega}$
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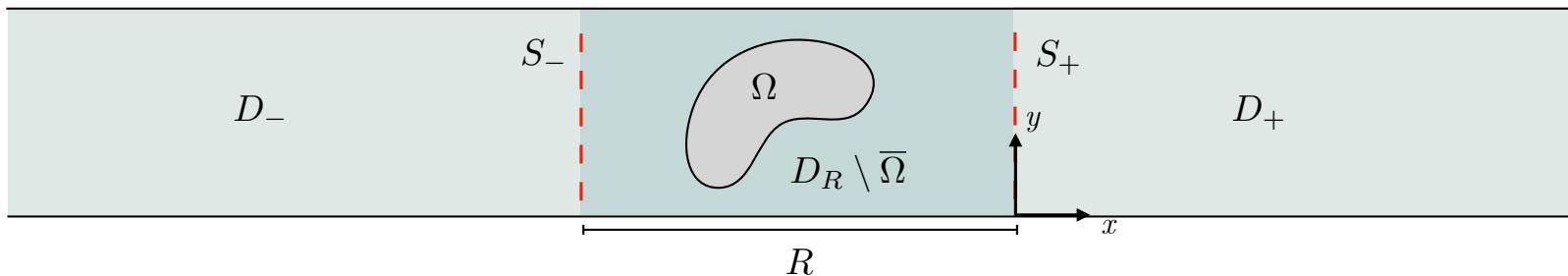
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DtN Map for Waveguides

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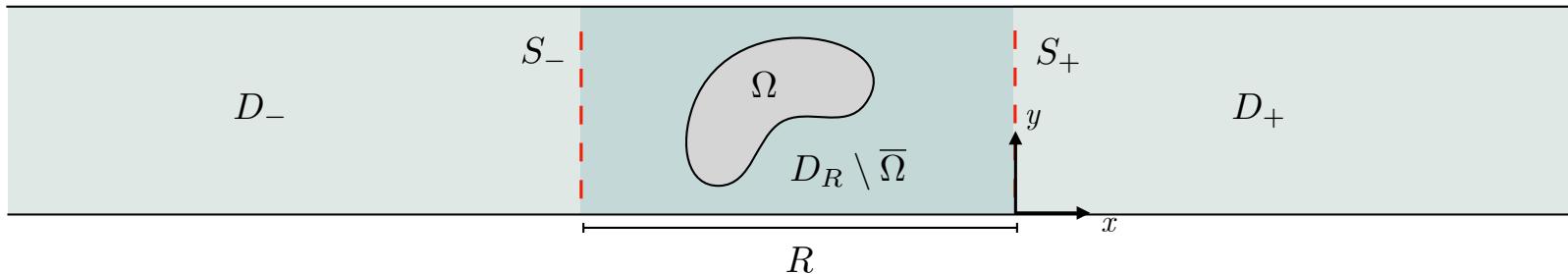


Assuming $u^s = f$ on S_+ , the solution in D_+ is given by: $u_+(x, y) = \frac{2}{\pi} \sum_{n=0}^{\infty} \sin(ny) e^{ix\sqrt{k^2 - n^2}} \int_0^\pi f(t) \sin(nt) dt.$

DtN Map for Waveguides

$\Delta u^s + k^2 u^s = 0$ in $D \setminus \bar{\Omega}$
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How can the DtN map be constructed in this situation?



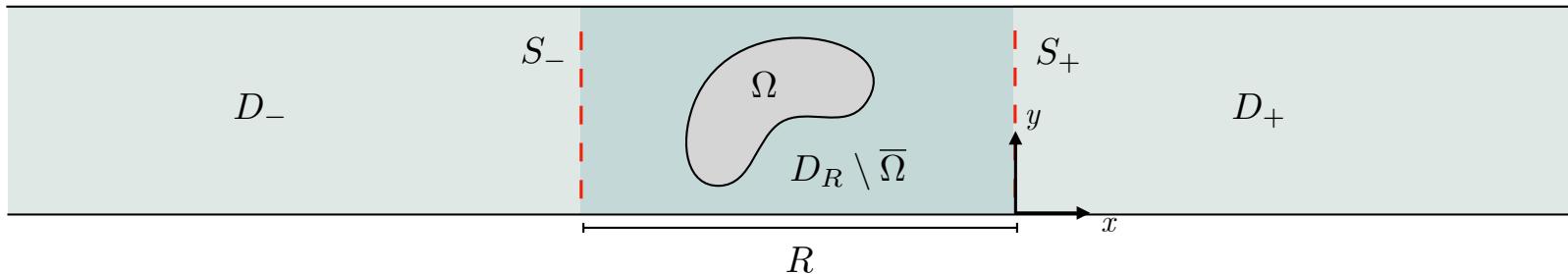
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$$\left. \frac{\partial u^s}{\partial x} \right|_{S_+} = \Lambda_+ [\gamma_0^{S_+} u^s](y) := \frac{2i}{\pi} \sum_{n=0}^{\infty} \sqrt{k^2 - n^2} \sin(ny) \int_0^\pi u^s(0, t) \sin(n\pi t) dt, \quad \Lambda_+ : \widetilde{H}^{1/2}(S_+) \rightarrow H^{-1/2}(S_+)$$

DtN Map for Waveguides

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How can the DtN map be constructed in this situation?



Assuming $u^s = f$ on S_- , the solution in D_- is given by: $u_-(x, y) = \frac{2}{\pi} \sum_{n=0}^{\infty} \sin(ny) e^{-ix\sqrt{k^2 - n^2}} \int_0^\pi f(t) \sin(nt) dt.$

$$-\frac{\partial u^s}{\partial x} \Big|_{S_-} = \Lambda_- [\gamma_0^{S_-} u^s](y) := \frac{2i}{\pi} \sum_{n=0}^{\infty} \sqrt{k^2 - n^2} \sin(ny) \int_0^\pi u(-R, t) \sin(n\pi t) dt, \quad \Lambda_- : \tilde{H}^{1/2}(S_-) \rightarrow H^{-1/2}(S_-)$$

DtN Map for Waveguides

S^+
 y
 x
 $u^{\text{inc}}(x, y) = \sin(y) e^{ix\sqrt{k^2 - n^2}}$
 Γ
 $D \setminus \bar{\Omega}$
 $\Delta u^s + k^2 u^s = 0 \text{ in } D \setminus \bar{\Omega}$
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 π
+ radiation condition

Truncated waveguide problem:

S_R^+
 $D_R \setminus \bar{\Omega}$
 Ω
 $D_R \setminus \bar{\Omega}$
 S_-
 S_+
 S_R^-

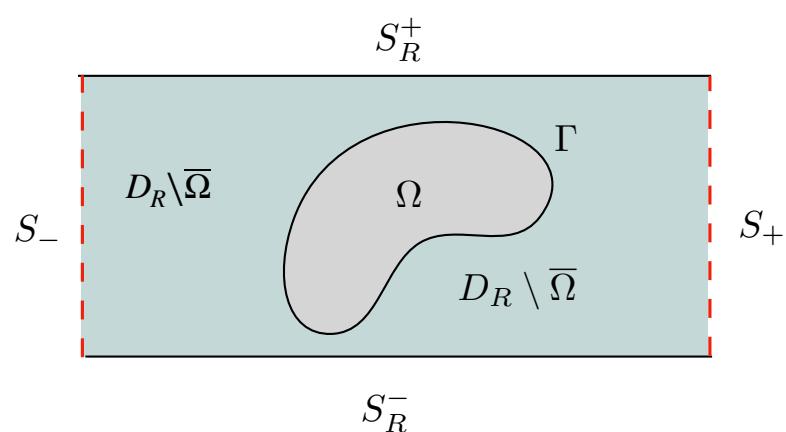
\Updownarrow

$\left\{ \begin{array}{ll} \Delta u^s + k^2 u = 0 & \text{in } D_R \setminus \bar{\Omega}, \\ u^s = 0 & \text{on } S_R^\pm, \\ u^s = -u^{\text{inc}} & \text{on } \Gamma, \\ \frac{\partial u^s}{\partial n} = \Lambda_\pm [\gamma_0^{S_\pm} u^s] & \text{on } S_\pm. \end{array} \right.$

DtN Map for Waveguides

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 π
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Truncated waveguide problem:



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Perfectly Matched Layers (PMLs)

Problem: We seek a domain truncation method that allows more geometric flexibility than the approach based on the DtN map.

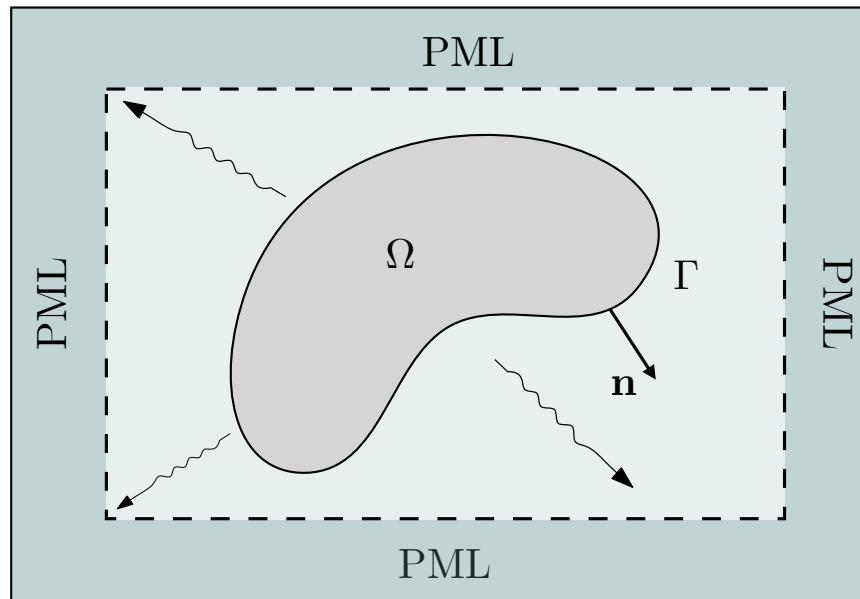
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Perfectly Matched Layers (PMLs)

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Idea: Embed the domain of interest Ω within a **wave-absorbing** box.

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Perfectly Matched Layers (PMLs)

Let us consider the Green's function in \mathbb{R} : $\{E'' + k^2 E = -\delta_0\} + \text{R.C.} \implies E(x) = \begin{cases} \frac{i}{2k} e^{ikx}, & x > 0 \\ \frac{i}{2k} e^{-ikx}, & x < 0 \end{cases}$

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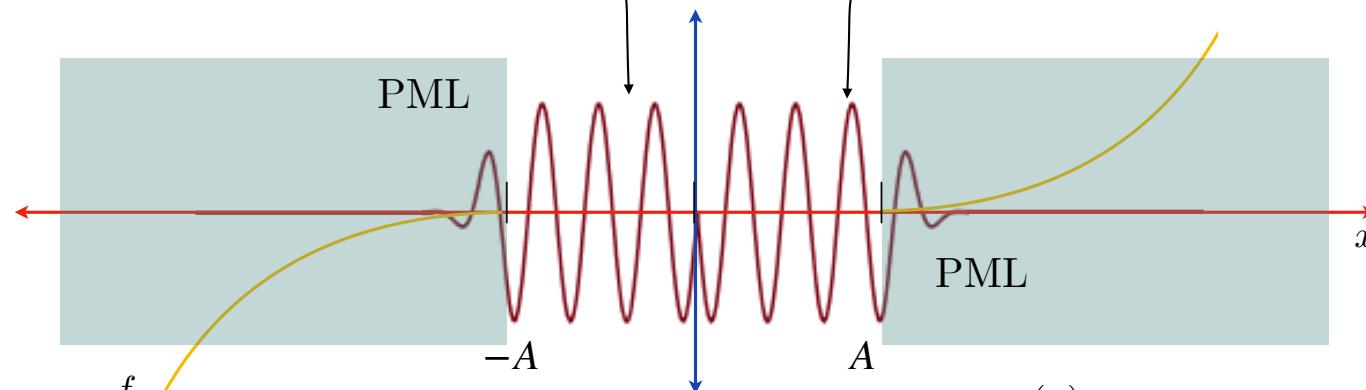
Apply the coordinate transformation $\tilde{x}(x) = x + i f(x)$ with: $f(x) = \begin{cases} (x - A)^2, & x > A \\ -(x + A)^2, & x < -A \\ 0, & |x| \leq A \end{cases}$

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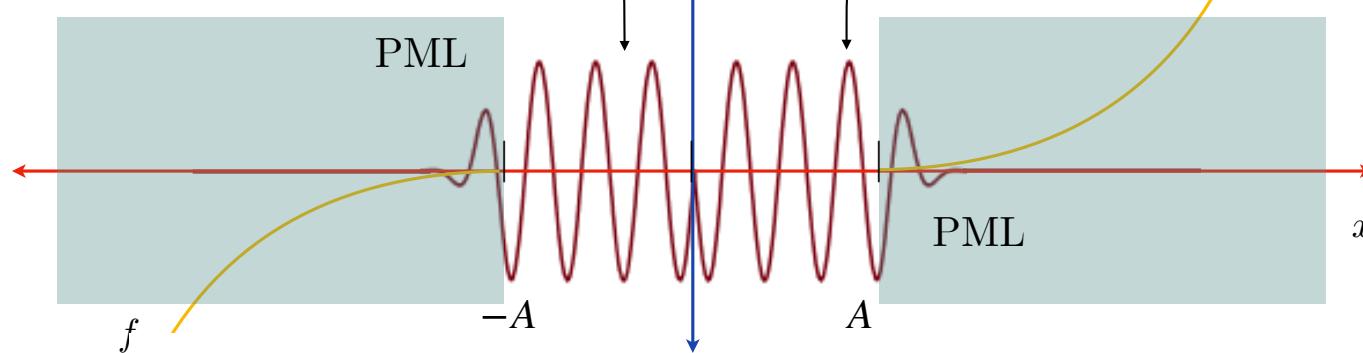
$$(E \circ \tilde{x})(x) = \frac{i}{2k} e^{-ikx} e^{-k(x-A)^2} \text{ for } x < -A$$



$$f'(x) = \frac{\sigma(x)}{k}, \quad \text{where } \sigma > 0 \text{ inside the PML}$$

Perfectly Matched Layers (PMLs)

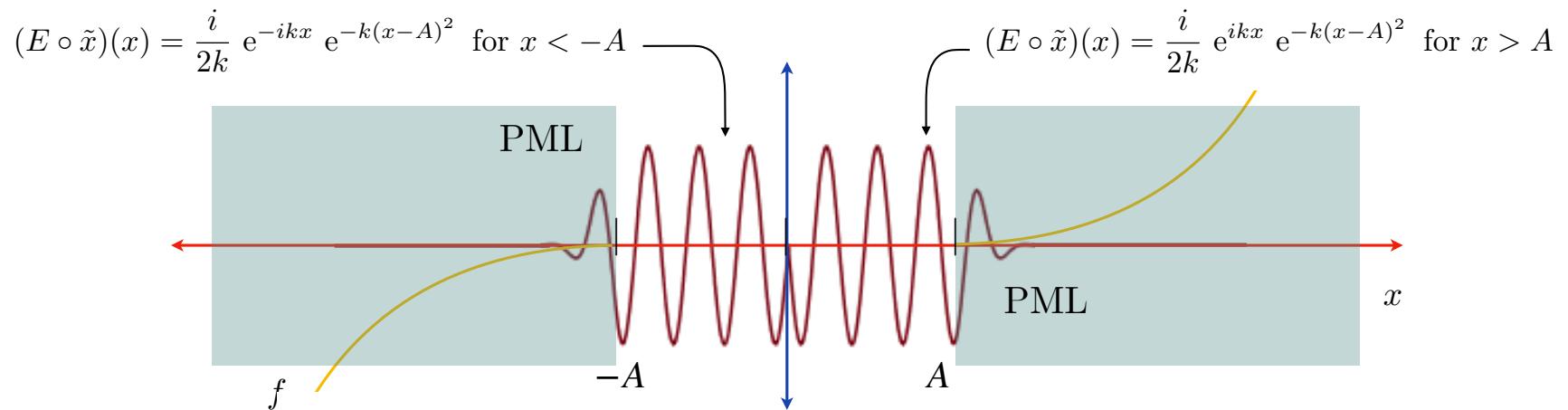
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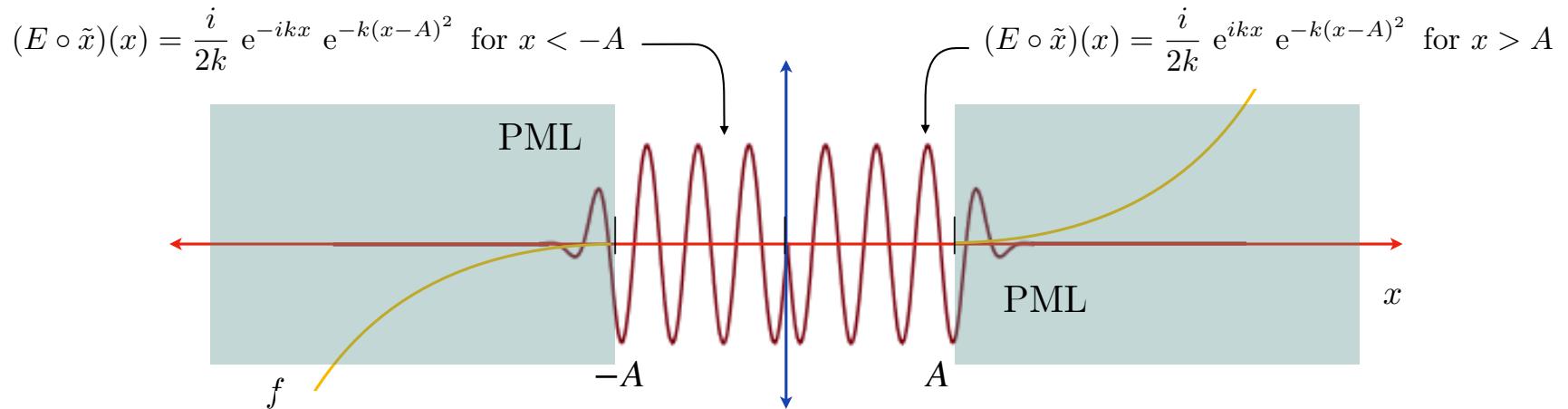
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Perfectly Matched Layers (PMLs)



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- It coincides with E on the interval $(-A, A)$;
- It decays exponentially in the PML region, $|x| > A$.
- Since $\tilde{E}' = E'\tilde{x}'$, $\tilde{E}'' = E''\tilde{x}' + E'\tilde{x}'' = E''\tilde{x}' + \tilde{E}'\frac{\tilde{x}''}{\tilde{x}'}$ and $E'' + k^2E = -\delta_0$, we have that \tilde{E} satisfies

$$\frac{1}{1 + i\frac{\sigma(x)}{k}} \frac{d}{dx} \left(\frac{1}{1 + i\frac{\sigma(x)}{k}} \frac{d\tilde{E}}{dx} \right) + k^2 \tilde{E} = -\delta_0 \quad (\tilde{x}' = 1 + i\frac{\sigma}{k})$$

Perfectly Matched Layers (PMLs)

Idea: Instead of seeking the solution in the “real” domain, we consider its analytic extension \tilde{u} given by the coordinate transformation $\tilde{x} = x + if(x)$, $\tilde{y} = y + if(y)$, which decays exponentially inside the PML:

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whose solution provides an accurate **approximation** of the exact analytic extension.

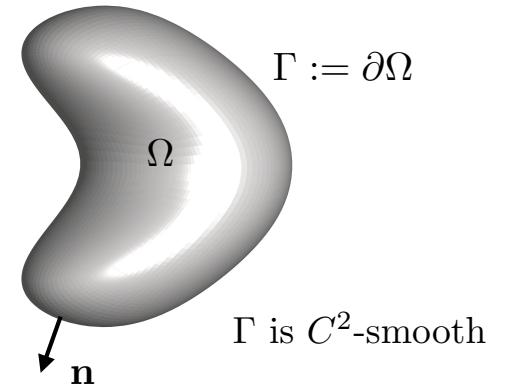
Boundary Integral Equation Methods

Combined Field Integral Equation (CFIE)

Consider once again for problem of scattering:

$$\begin{cases} \Delta u^s + k^2 u^s = 0 & \text{in } \mathbb{R}^d \setminus \overline{\Omega} \\ u^s = -u^{\text{inc}} & \text{on } \Gamma \\ \lim_{|\boldsymbol{x}| \rightarrow \infty} |\boldsymbol{x}|^{(d-1)/2} \left(\frac{\partial u^s}{\partial |\boldsymbol{x}|} - iku^s \right) = 0 \end{cases}$$

$$\mathbb{R}^d \setminus \overline{\Omega}$$

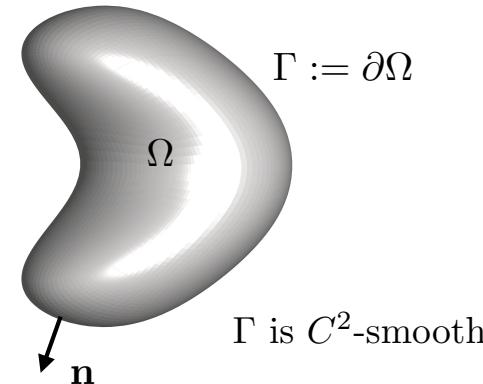


Combined Field Integral Equation (CFIE)

Consider once again for problem of scattering:

$$\begin{cases} \Delta u^s + k^2 u^s = 0 & \text{in } \mathbb{R}^d \setminus \overline{\Omega} \\ u^s = -u^{\text{inc}} & \text{on } \Gamma \\ \lim_{|\boldsymbol{x}| \rightarrow \infty} |\boldsymbol{x}|^{(d-1)/2} \left(\frac{\partial u^s}{\partial |\boldsymbol{x}|} - iku^s \right) = 0 \end{cases}$$

$$\mathbb{R}^d \setminus \overline{\Omega}$$



We seek the solution given by the **combined-field potential**:

$$u(\boldsymbol{x}) = (\mathcal{D} - i\eta\mathcal{S})\varphi(\boldsymbol{x}), \quad \boldsymbol{x} \in \mathbb{R}^d \setminus \overline{\Omega}, \quad \eta > 0$$

$$(\mathcal{S}\varphi)(\boldsymbol{x}) := \int_{\Gamma} G(\boldsymbol{x}, \boldsymbol{y})\varphi(\boldsymbol{y})ds(\boldsymbol{y}) \quad \text{and} \quad (\mathcal{D}\varphi)(\boldsymbol{x}) := \int_{\Gamma} \frac{\partial G(\boldsymbol{x}, \boldsymbol{y})}{\partial \mathbf{n}(\boldsymbol{y})}\varphi(\boldsymbol{y})ds(\boldsymbol{y})$$

$$G(\boldsymbol{x}, \boldsymbol{y}) := \begin{cases} \frac{i}{4} H_0^{(1)}(k|\boldsymbol{x} - \boldsymbol{y}|) & \text{if } d = 2, \\ \frac{e^{ik|\boldsymbol{x} - \boldsymbol{y}|}}{4\pi|\boldsymbol{x} - \boldsymbol{y}|} & \text{if } d = 3. \end{cases}$$

Combined Field Integral Equation (CFIE)

Imposing the boundary condition on Γ and making use of the jump relations for the double-layer potential, we obtain:

$$\text{CFIE: } \left(\frac{I}{2} + K - i\eta S \right) \varphi = -u^{\text{inc}} \quad \text{on } \Gamma$$

which is a **Fredholm equation of the second kind**, where both operators:

$$(S\varphi)(\mathbf{x}) = \int_{\Gamma} G(\mathbf{x}, \mathbf{y}) \varphi(\mathbf{y}) ds(\mathbf{y}) \quad \text{and} \quad (K\varphi)(\mathbf{x}) = \int_{\Gamma} \frac{\partial G(\mathbf{x}, \mathbf{y})}{\partial n(\mathbf{y})} \varphi(\mathbf{y}) ds(\mathbf{y}), \quad \mathbf{x} \in \Gamma$$

are **compact** on $C(\Gamma)$ (and also on $H^{1/2}(\Gamma)$), since

$$G(\mathbf{x}, \mathbf{y}) = \begin{cases} O(\log |\mathbf{x} - \mathbf{y}|) & \text{if } d = 2 \\ O(|\mathbf{x} - \mathbf{y}|^{-1}) & \text{if } d = 3 \end{cases} \quad \text{and} \quad \frac{\partial G(\mathbf{x}, \mathbf{y})}{\partial n(\mathbf{y})} = \begin{cases} O(|\mathbf{x} - \mathbf{y}|^2 \log |\mathbf{x} - \mathbf{y}|) & \text{if } d = 2 \\ O(|\mathbf{x} - \mathbf{y}|^{-1}) & \text{if } d = 3 \end{cases}$$

as $\Gamma \ni \mathbf{y} \rightarrow \mathbf{x} \in \Gamma$ (they are weakly singular).

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Can we numerically solve this BIE?

Boundary Element Method (BEM)

Suppose we wish to solve:

$$\varphi(\mathbf{x}) + \int_{\Gamma} L(\mathbf{x}, \mathbf{y}) \varphi(\mathbf{y}) \, ds(\mathbf{y}) = f(\mathbf{x}), \quad \mathbf{x} \in \Gamma,$$

where $L(\mathbf{x}, \mathbf{y}) := 2 \left\{ \frac{\partial G(\mathbf{x}, \mathbf{y})}{\partial n(\mathbf{y})} - i\eta G(\mathbf{x}, \mathbf{y}) \right\}$ and $f(\mathbf{x}) := -2u^{\text{inc}}(\mathbf{x})$

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(i) **Variational formulation:** Find $\varphi \in H^{1/2}(\Gamma)$ such that

$$\int_{\Gamma} \psi(\mathbf{x}) \left\{ \varphi(\mathbf{x}) + \int_{\Gamma} L(\mathbf{x}, \mathbf{y}) \varphi(\mathbf{y}) \, ds(\mathbf{y}) \right\} \, ds(\mathbf{x}) = \int_{\Gamma} \psi(\mathbf{x}) f(\mathbf{x}) \, ds, \quad \forall \psi \in H^{1/2}(\Gamma)$$

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(ii) **Galerkin method:** Find $\varphi_h \in V_h \subset H^{1/2}(\Gamma)$ ($\dim V_h = N < \infty$)

$$\int_{\Gamma} \psi_h(\mathbf{x}) \left\{ \varphi_h(\mathbf{x}) + \int_{\Gamma} L(\mathbf{x}, \mathbf{y}) \varphi_h(\mathbf{y}) \, ds(\mathbf{y}) \right\} \, ds(\mathbf{x}) = \int_{\Gamma} \psi_h(\mathbf{x}) f(\mathbf{x}) \, ds, \quad \forall \psi_h \in V_h$$

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(iii) **Linear system assembly:** Substituting $\varphi_h(\mathbf{x}) = \sum_{j=1}^N c_j v_j(\mathbf{x})$, with $V_h = \text{span}\{v_1, \dots, v_N\}$,

$$\sum_{j=1}^N c_j \int_{\Gamma_h} v_i(\mathbf{x}) \left\{ v_j(\mathbf{x}) + \int_{\Gamma_h} L(\mathbf{x}, \mathbf{y}) v_j(\mathbf{y}) \, ds(\mathbf{y}) \right\} \, ds(\mathbf{x}) = \int_{\Gamma_h} v_i(\mathbf{x}) f(\mathbf{x}) \, ds$$

where the test functions are chosen as $\psi(\mathbf{x}) = v_i(\mathbf{x})$, $i = 1, \dots, N$.

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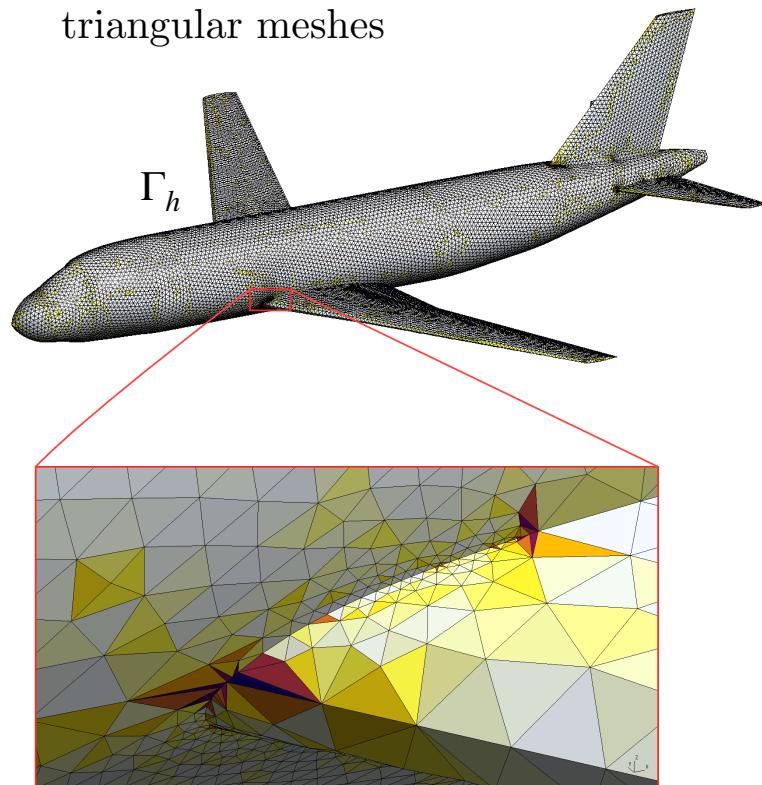
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**double surface integral
with a singular kernel!**

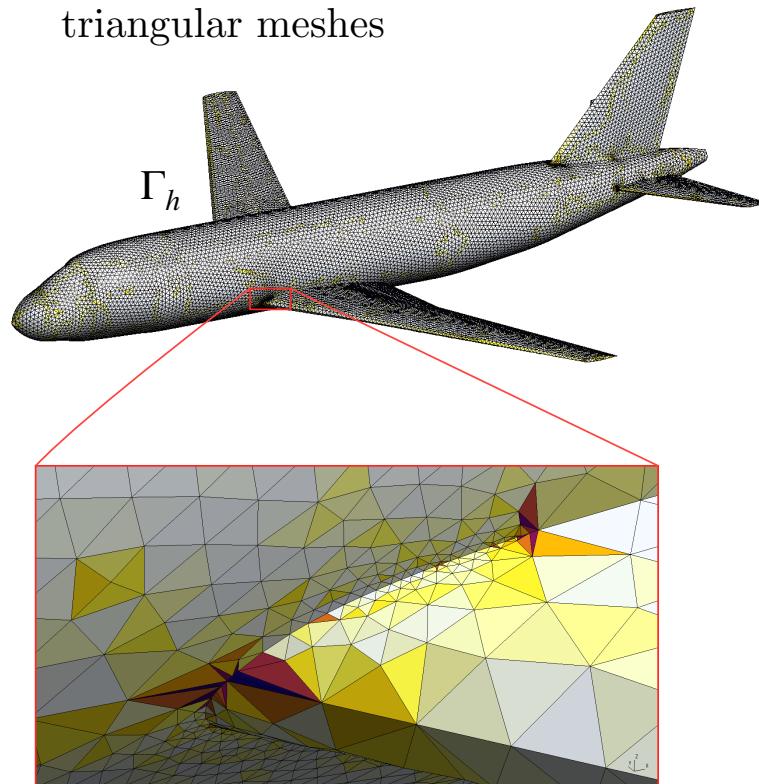
Boundary Element Method (BEM)

In the BEM, surfaces are most commonly represented by triangular meshes



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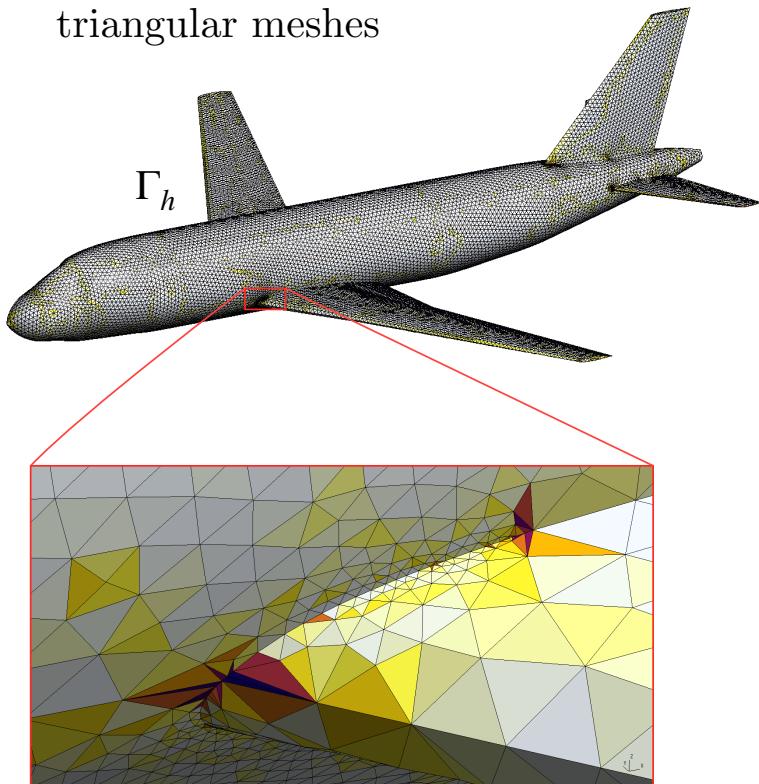
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To compute $A \in \mathbb{C}^{N \times N}$, it is necessary to evaluate weakly singular kernel integrals over triangles

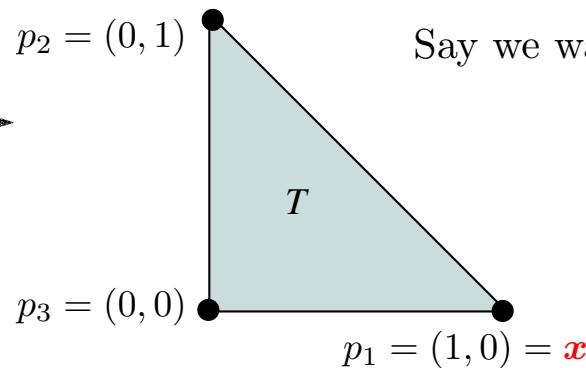
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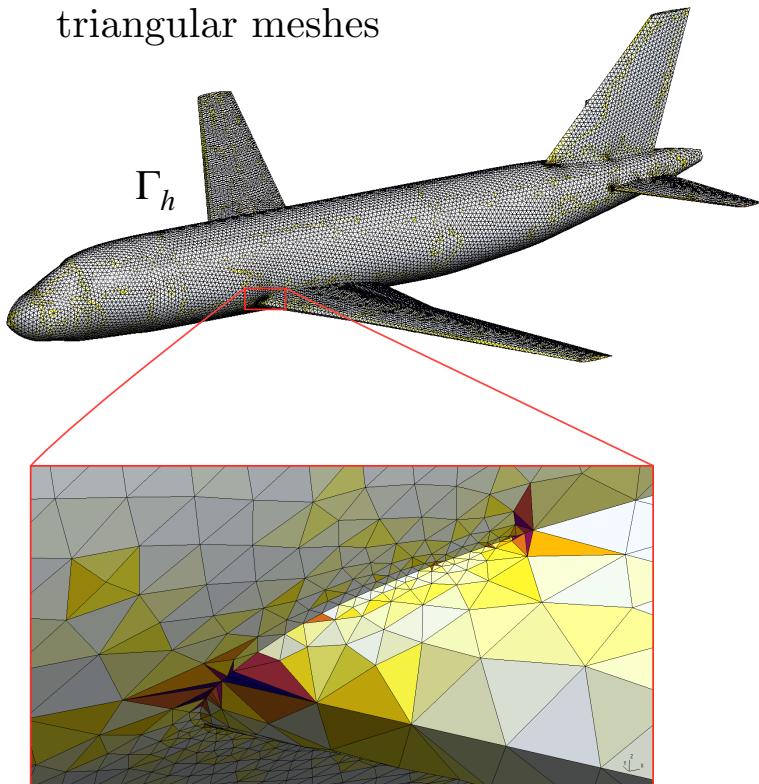
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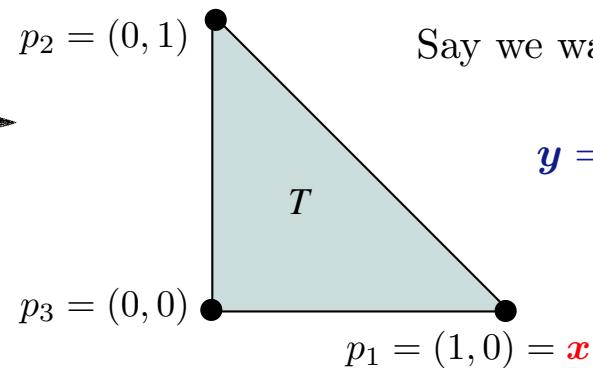
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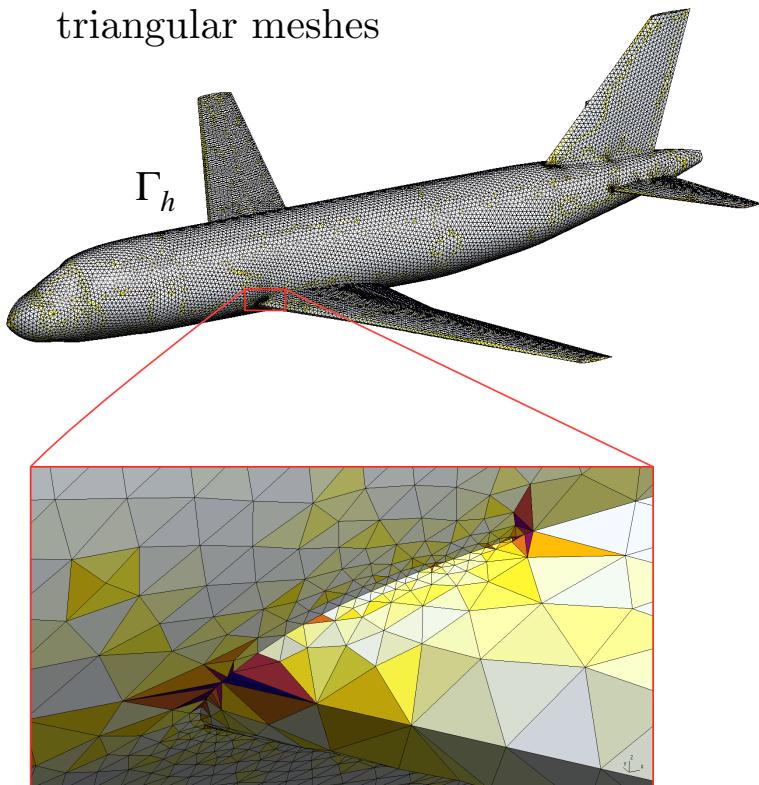


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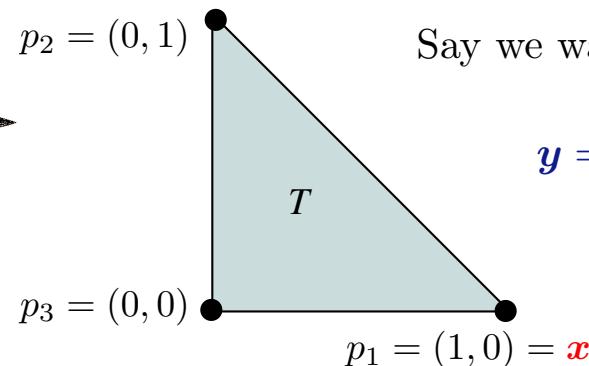
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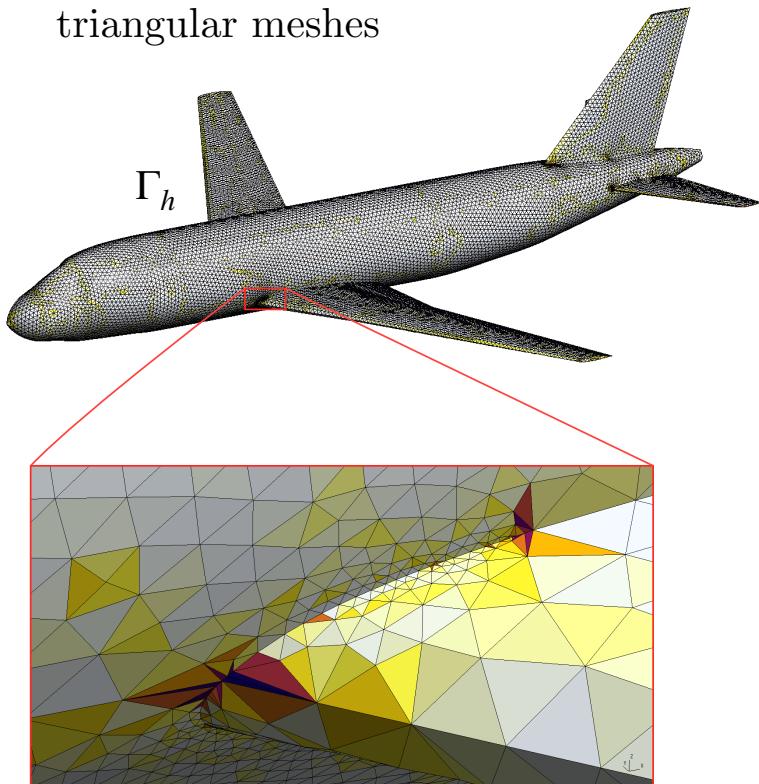
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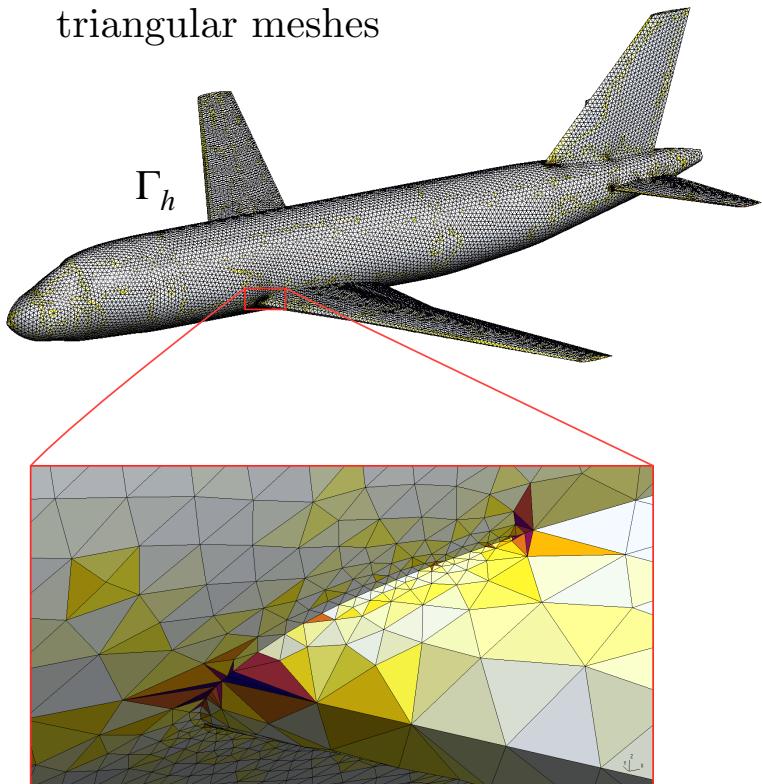
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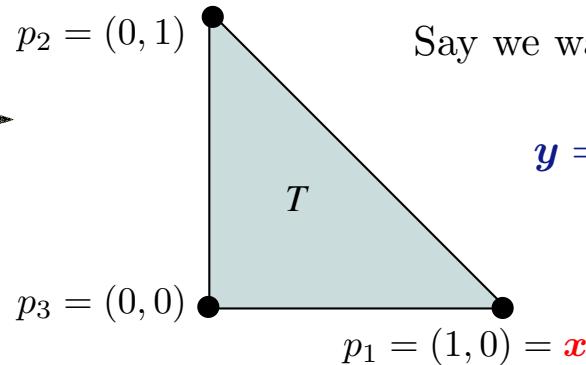
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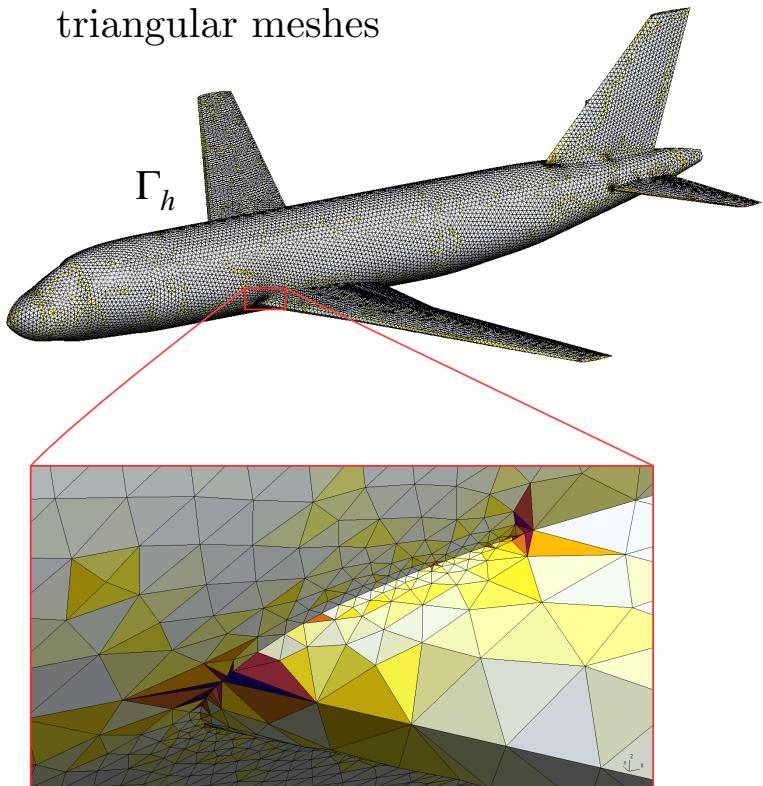
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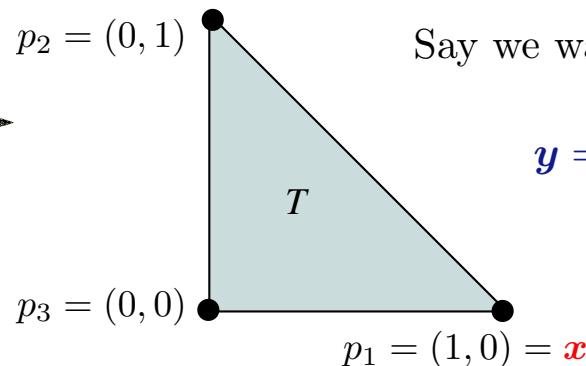
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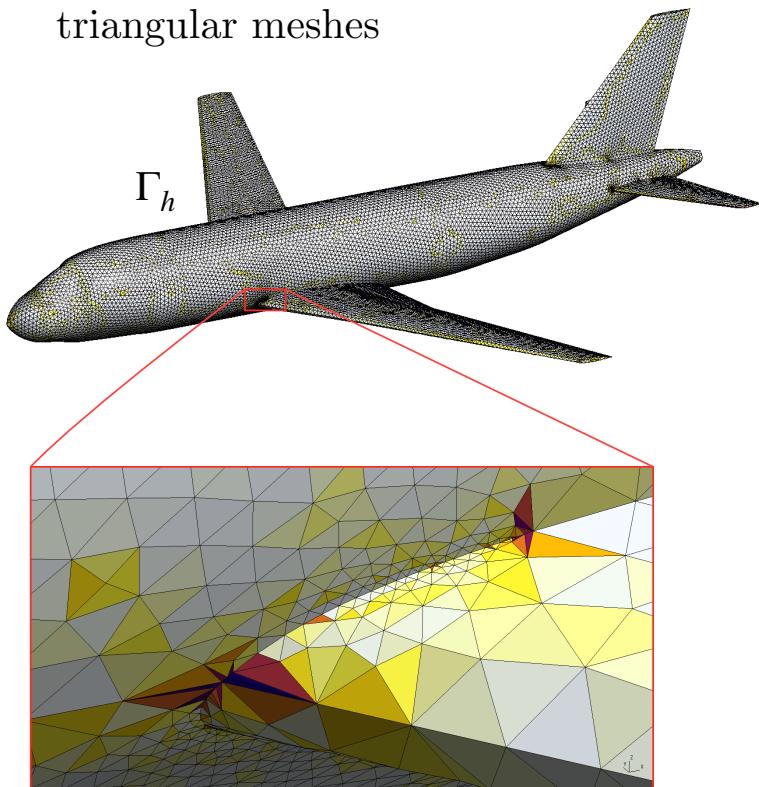
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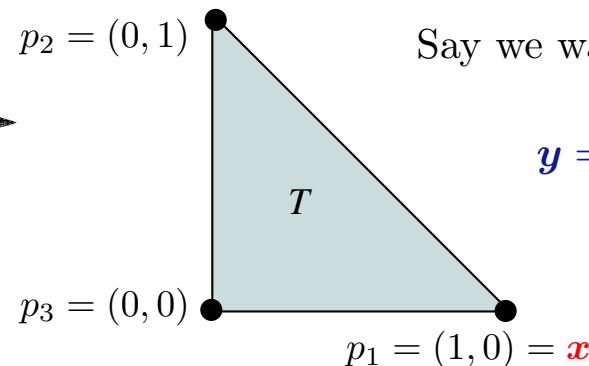
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**smooth
integrand!**

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(i) **Parametrize the surface:** Letting $\Gamma = \{\mathbf{x}(t) = (x(t), y(t)), t \in [0, 2\pi]\}$, the BIE can be recast as:

$$\tilde{\varphi}(t) + \int_0^{2\pi} \tilde{L}(t, \tau) \tilde{\varphi}(\tau) \, d\tau = \tilde{f}(t), \quad t \in [0, 2\pi],$$

where $\tilde{\varphi}(t) := \varphi(\mathbf{x}(t))$, $\tilde{L}(t, \tau) := L(\mathbf{x}(t), \mathbf{x}(\tau)) |\mathbf{x}'(\tau)|$, and $\tilde{f}(t) = f(\mathbf{x}(t))$.

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(ii) **Apply singular quadrature rule:** Approximate the integral operator as

$$\int_0^{2\pi} \tilde{L}(t, \tau) \tilde{\varphi}(\tau) \, d\tau \approx \sum_{j=1}^N L_j^{(N)}(t) \varphi_j, \quad t \in [0, 2\pi],$$

where $\varphi_j = \tilde{\varphi}(\mathbf{x}(t_j))$, and $\{t_j\}_{j=1}^N$ are the quadrature nodes.

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(iii) **Collocation:** By substituting the approximate integral operator into the BIE and evaluating the equation at the quadrature/collocation points, we obtain:

$$\varphi_i + \sum_{j=1}^N L_j^{(N)}(t_i) \varphi_j = \tilde{f}(t_i), \quad i = 1, \dots, N.$$

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(iv) **Linear system assembly:** The resulting system of equations can be written as

$$(\mathbf{E} + \mathbf{A}) \mathbf{x} = \mathbf{b}, \quad \text{where}$$

$$(\mathbf{E})_{i,j} = \delta_{i,j} \quad (\mathbf{A})_{i,j} = L_j^{(N)}(t_i) \quad (\mathbf{b})_i = \tilde{f}(t_i) \quad (\mathbf{x})_j = \varphi_j \approx \tilde{\varphi}(t_j) = \varphi(\mathbf{x}(t_j))$$

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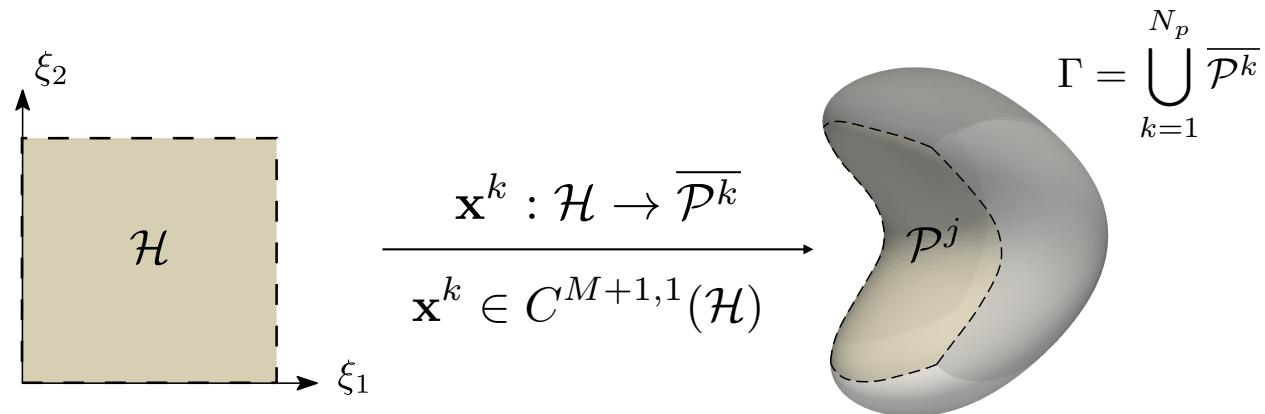
Nyström Method: Surface Representation

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- Parametrizing the surface via disjoint smooth coordinate charts (patches):



$$\mathbf{x}^k(\boldsymbol{\xi}) := (\mathbf{x}_1^k(\xi_1, \xi_2), \mathbf{x}_2^k(\xi_1, \xi_2), \mathbf{x}_3^k(\xi_1, \xi_2)), \quad k = 1, \dots, N_p, \quad (\boldsymbol{\xi} = (\xi_1, \xi_2))$$

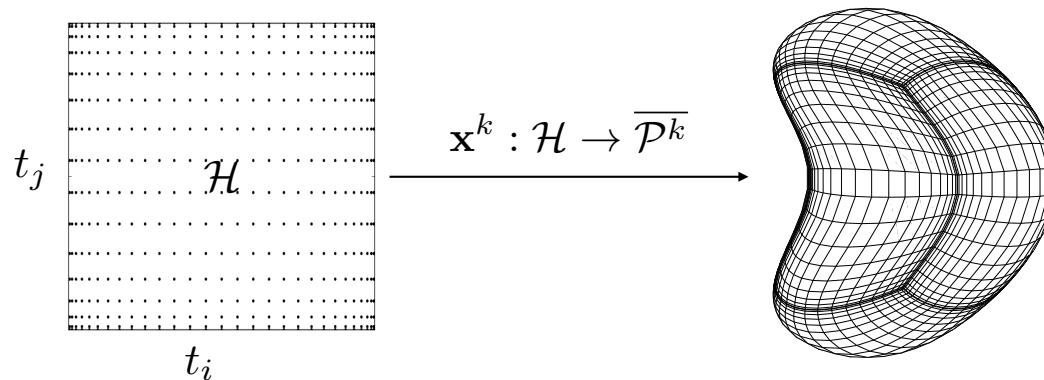
Nyström Method: High-Order Quadratures

- Integrating over each patch using **Fejér's first quadrature rule**:

$$S[\varphi](\mathbf{x}) = \sum_{k=1}^{N_p} \int_{\mathcal{H}} F_k(\mathbf{x}, \mathbf{x}^k(\xi)) |\partial_1 \mathbf{x}^k(\xi) \wedge \partial_2 \mathbf{x}^k(\xi)| d\xi = \int_{\mathcal{H}} f(\mathbf{x}, \boldsymbol{\xi}) d\boldsymbol{\xi} \approx \sum_{i=1}^N \sum_{j=1}^N f(t_i, t_j) \omega_i \omega_j$$

Quadrature nodes: $(t_i, t_j) \in \mathcal{H} = [-1, 1] \times [-1, 1]$, $i, j = 1, \dots, N$

$$t_j := \cos(\vartheta_j), \quad \vartheta_j := \frac{(2j-1)\pi}{2N}, \quad j = 1, \dots, N$$



For smooth (analytic) integrands, this rule exhibits **spectral accuracy**, i.e. the error decays faster than any algebraic rate as $N \rightarrow \infty$.

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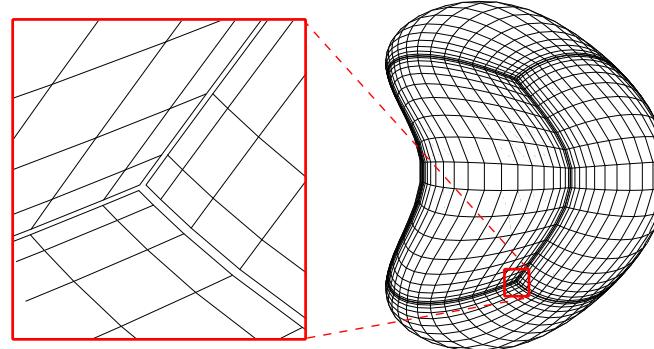
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- Derivatives with respect to the surface parametrization (i.e. along the coordinate directions of the chart) can also be computed efficiently using the FFT:

$$\partial^\alpha f(t_i, t_j) \approx (-1)^{\alpha_1 + \alpha_2} \sin(\vartheta_i)^{-\alpha_1} \sin(\vartheta_j)^{-\alpha_2} (D_{\text{FFT}}^\alpha F)_{i,j} \quad (f : \mathcal{H} \rightarrow \mathbb{C})$$

where $F(\vartheta, \vartheta') = f(\cos \vartheta, \cos \vartheta')$ is a smooth periodic function.

Linear System Solution and Fast BIE Methods

To obtain the numerical solution of the boundary integral equation

$$\left(\frac{I}{2} + K - i\eta S \right) \varphi = -u^{\text{inc}} \quad \text{on } \Gamma,$$

we must solve a linear system of the form

$$(\mathbf{E} + \mathbf{A}) \mathbf{x} = \mathbf{b}, \quad \mathbf{E}, \mathbf{A} \in \mathbb{C}^{N \times N}, \quad \mathbf{b} \in \mathbb{C}^N,$$

where the matrix \mathbf{E} arises from the discretization of the identity operator I , and the matrix \mathbf{A} from the discretization of the **compact operator** $K - i\eta S$.

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- In practice, at least 5 nodes/elements per wavelength $\lambda = 2\pi/k$ are typically required. For high-frequency problems ($k \gg 1$), the matrix $\mathbf{E} + \mathbf{A}$ may become too large to fit in memory!

GMRES (Generalized Minimal Residual Method)

- Iterative solver for linear systems $\mathbf{M}\mathbf{x} = \mathbf{b}$, particularly suitable for **non-symmetric matrices**.
- Constructs approximations \mathbf{x}_m by minimizing the residual $\|\mathbf{b} - \mathbf{M}\mathbf{x}_m\|$ over the Krylov subspace

$$\mathcal{K}_m(\mathbf{M}, \mathbf{r}_0) = \text{span}\{\mathbf{r}_0, \mathbf{M}\mathbf{r}_0, \dots, \mathbf{M}^{m-1}\mathbf{r}_0\}.$$

Only the action of \mathbf{M} as a linear mapping (i.e., matrix-vector products) is required, rather than explicit access to all entries of \mathbf{M} .

- Uses Arnoldi iteration to build an orthonormal basis of the Krylov subspace.
- Effective for dense BIE matrices, especially when combined with preconditioning. Memory grows with iterations; restarted GMRES (GMRES(m)) is sometimes used.
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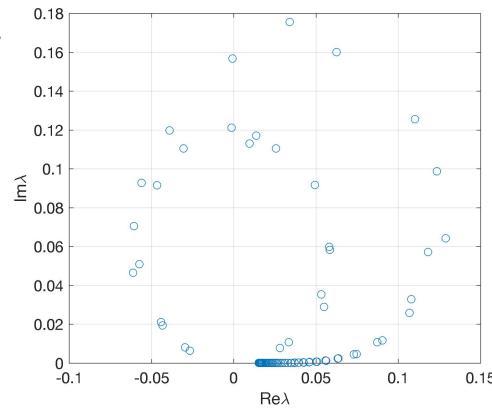
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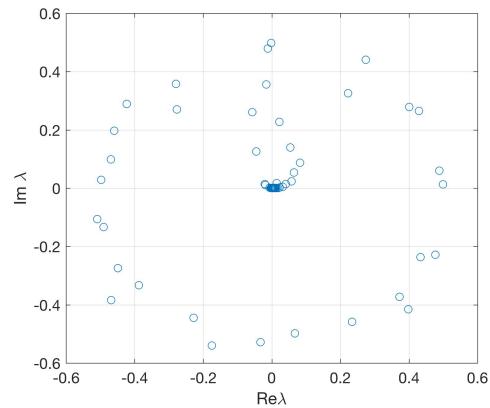
Linear System Solution and Fast BIE Methods

- Since K and S are compact, their spectra cluster near zero, so the spectrum of A (discretizing $K - i\eta S$) is also near zero.

spectrum of
discretized
operator S

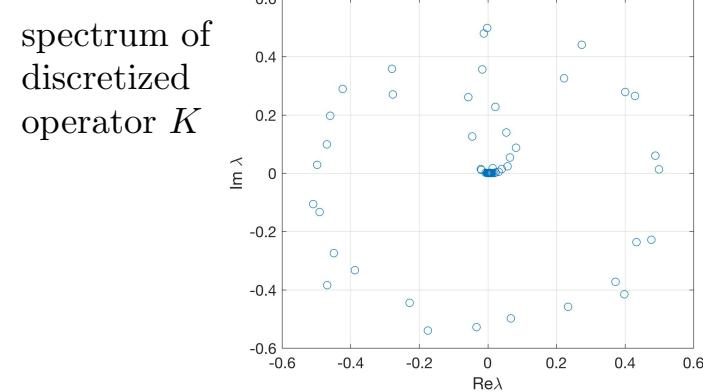
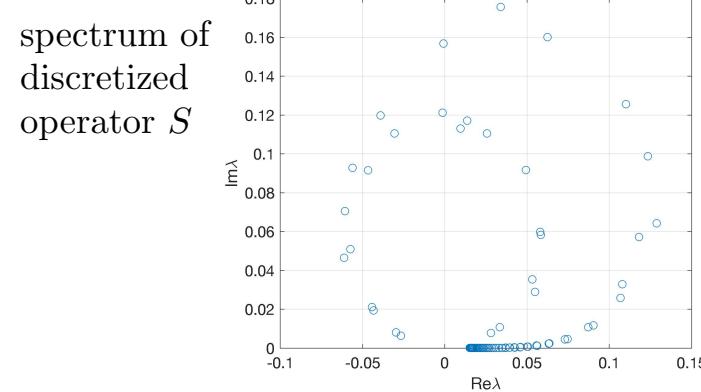


spectrum of
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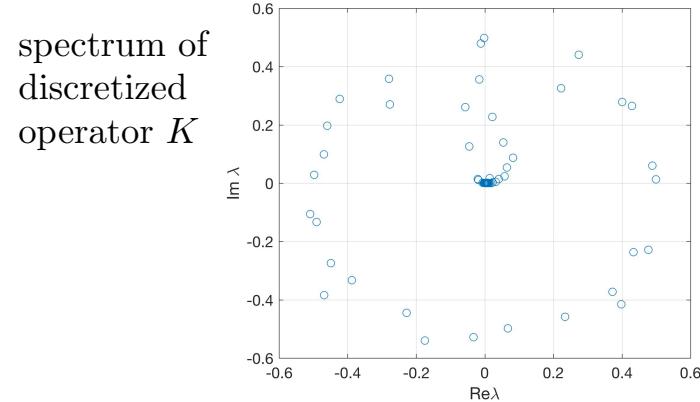
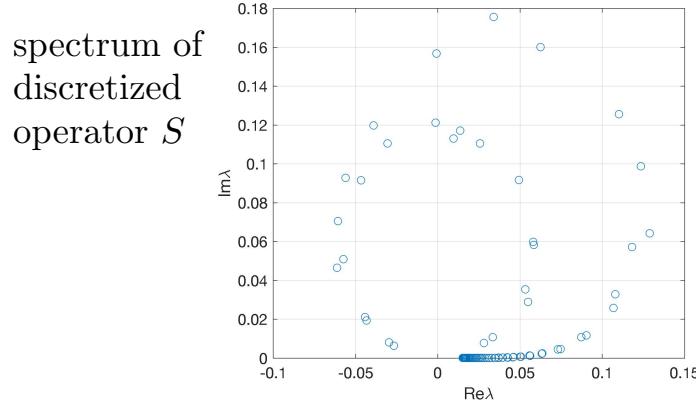
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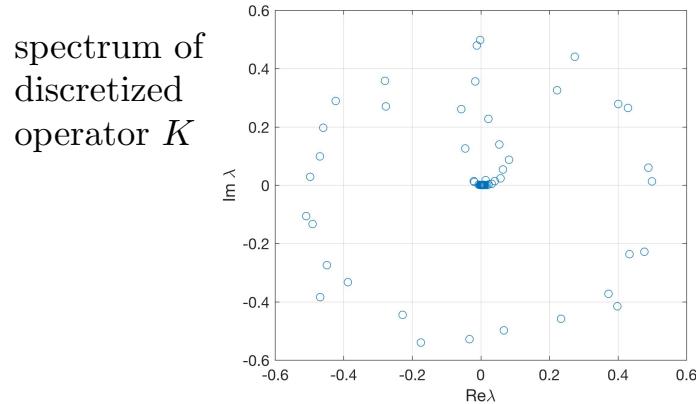
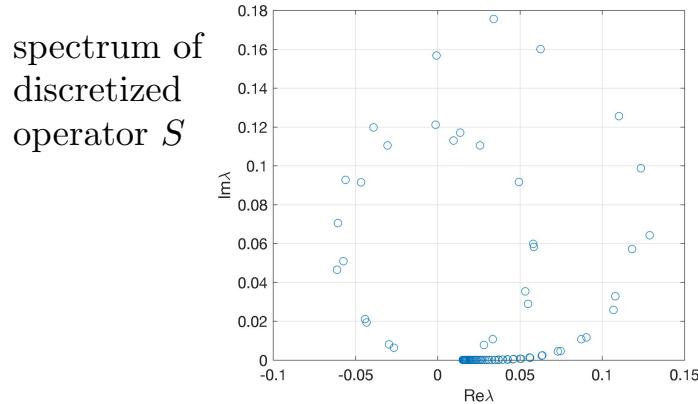
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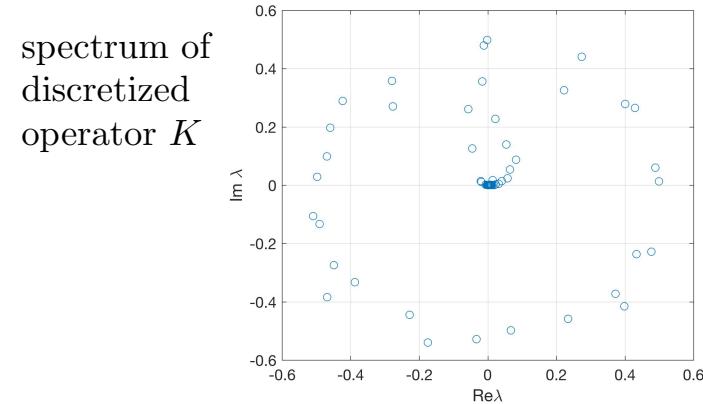
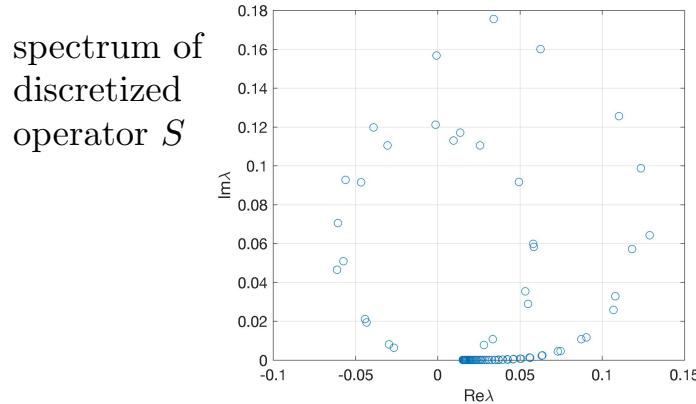
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can we do even better?

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Linear System Solution and Fast BIE Methods

- Matrix-vector products can be accelerated using the Fast Multipole Method (FMM) or other fast algorithms such as \mathcal{H} -matrices and hierarchical low-rank approximations.
- With these methods, the computational cost of a **dense matrix-vector product is reduced from $O(N^2)$ to $O(N \log N)$ or even $O(N)$ operations**, enabling the solution of the linear system and the underlying integral equation efficiently.

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from SIAM News, Volume 33, Number 4

The Best of the 20th Century: Editors Name Top 10 Algorithms

By Barry A. Cipra

Algo is the Greek word for "path." Algo in Latin, to be cold. Neither is the root for algorithm, which stems instead from al-Khwarizmi, the name of the ninth-century Arab scholar whose book of *solver* was translated into today's high school algebra textbooks. Al-Khwarizmi shared the importance of methodical procedures for solving problems. Were he around today, he'd be a computer scientist, not a mathematician.

Some of the very best algorithms of the computer age are highlighted in the January/February 2000 issue of *Computing in Science & Engineering*, a joint publication of the American Institute of Physics and the IEEE Computer Society. Guest editors Jack Dongarra and Cleve Moler have selected 10 algorithms that have had the greatest impact on science and engineering.

"We chose them because they have had a major influence on the development of computing and practice of science and engineering in the 20th century," Dongarra says. "They are the top 10 algorithms of the century."

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When it comes to picking the algorithmic best, there seems to be no best algorithm. Without exception, the 10 algorithms have had a significant impact on science and engineering with the algorithms being used as first-order approximations.

Without exception, the 10 algorithms have had a significant impact on science and engineering with the algorithms being used as first-order approximations. Most algorithms take shape over time, with many contributors.

1946: John von Neumann, Stan Ulam, and Nick Metropolis, all at the Los Alamos Scientific Laboratory, cook up the Metropolis algorithm, also known as the Monte Carlo method.

The Metropolis algorithm uses random approaches to numerical problems with manageable numbers of degrees of freedom and to continuous distributions.

In terms of wide spread use, George Forsythe's 1950 paper on the simplex method for linear programming is a close second.

1947: George Dantzig, at the RAND Corporation, creates the simplex method for linear programming.

In terms of elegance, David Krylov's 1950 paper on iterative methods for solving systems of linear equations with boundary and other constraints. (Of course, the real "problem" of systems of linear equations are often nonlinear; the use of iterative methods to solve them is a separate issue.) Krylov's paper is considered one of the most elegant ways of arriving at optimal answers. Although originally designed for exponential delays, the method is highly efficient—which itself is something to brag about since the nature of computation is not.

1950: Magnus Hestenes, Eduard Stiefel, and Cornelius Lanczos, all from the Institute for Numerical Analysis at a National Bureau of Standards, initiate the development of conjugate gradient methods.

Of course, that is a huge $n \times n$ matrix, so the algorithm is not $A^{-1} b$. The calculation of A^{-1} is the problem. The conjugate gradient method is much faster, but still not fast enough. The conjugate gradient method is still slow, but it is much faster than the direct method of Krylov subspaces.

1953: John von Neumann, Stan Ulam, and Nicholas Metropolis, all at the Los Alamos Scientific Laboratory, create the form $K_{ij} = B_{ij} - B_{ii}$ to B_{jj} in a simple matrix B that's "closely" \sim to A —the heat map of Krylov subspaces.

1954: Russian mathematician Nikolai Krylov. Krylov subspaces are spanned by powers of a matrix applied to an initial "residual." The conjugate gradient method is a variation of this idea. The conjugate gradient method is much faster than the direct method of Krylov subspaces.

1956: Cleve Moler and John Steward, both at the University of Colorado, publish an even newer method, known as the conjugate gradient method, for systems that are both symmetric and positive definite. In the last 50 years, numerous researchers have refined and extended these algorithms. The conjugate gradient techniques for solving linear systems became widely known through OLESEN and Bi-CGSTAB (GARNES and Bi-CGSTAB) presented in *SIAM Journal on Scientific and Statistical Computing*, in 1986 and (1992, respectively).

1957: Arnold Householder of Oak Ridge National Laboratory formalizes the decompositional approach to matrix computations.

The ability to factor matrix into triangular, diagonal, and other forms has had to be taken for granted. This is the decompositional approach. It is the basis for many of the most popular software packages, including MATLAB, and it facilitates the analysis of rounding errors—one of the big bugaboos of numerical linear algebra. (In 1961, James Wilkinson of the National Physical Laboratory in London published a seminal paper in the *Journal of the Institute of Mathematics and its Applications* titled "Error Analysis of Direct Methods of Matrix Inversion," based on the LU decomposition of a matrix as a product of lower and upper triangular factors.)

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The ability to factor matrix into triangular, diagonal, and other forms has had to be taken for granted. This is the decompositional approach. It is the basis for many of the most popular software packages, including MATLAB, and it facilitates the analysis of rounding errors—one of the big bugaboos of numerical linear algebra. (In 1961, James Wilkinson of the National Physical Laboratory in London published a seminal paper in the *Journal of the Institute of Mathematics and its Applications* titled "Error Analysis of Direct Methods of Matrix Inversion," based on the LU decomposition of a matrix as a product of lower and upper triangular factors.)

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The Backus team creates a language at IBM that is single most important event in the history of computer programming. Finally, scientists

all from the Institute for Numerical Analysis.

Krylov subspace iteration methods

g equations of the form $Ax = b$. The c
: answer $x = b/A$ is not so easy to com
ative methods—such as solving equation

arch Center and John Tukey of Princeton University developed the fast Fourier transform.

the fast multipole algorithm. tions: the fact that accurate calc n a galaxy, or atoms in a protein] either costs $\mathcal{O}(N^2)$ or $\mathcal{O}(N^3)$.

(and others) could tell the computer what they wanted it to do, without having to decipher the interleaved code machine code. Although this was a modest computer capability of many years ago, it was because of such basic programming instructions – the early computer was nonetheless capable of surprisingly sophisticated computation. As Buckley himself recalls in a recent history of Fortran I, II, and III, published in 1998 in the *IEEE Annals of the History of Computing*, the compiler “produced code of such efficiency that its output would startle the programmers who studied it.”

1970) [4]. Francis's QR algorithm, however, does not make use of complex numbers. Eigenvalues and eigenvectors are most important parameters associated with matrices – and they can be the trickiest to compute. It is relatively easy to transform a square matrix into a matrix that's "almost" upper triangular, meaning one with a single extra set of non-zero entries just below the main diagonal. But chopping away those few nonzeros is not enough. The QR algorithm is just as ticked. Based on the QR decomposition, which writes A as the product of an orthogonal matrix Q and an upper-triangular matrix R, this approach iteratively changes A, QR, or $A = QR$ until there are no more 1s and 0s left, and then it backs out by multiplying Q and R back together. For accelerating convergence to upper triangular form. By the mid-1960s, the QR algorithm was once-formidable eigenvalue problems into routine calculations.

1963. *Tony House of Elliott Brothers, Ltd., London*, presents **Quicksort**. Putting things in numerical or alphabetical order is mind-numbingly mundane. The intellectual challenge lies in devising ways of doing so quickly. House's algorithm uses the old-age recursive strategy of divide and conquer to solve the problem: Pick one element as a "pivot," separate the rest into piles of "big" and "small" elements (as compared with the pivot), and then repeat the process on each pile until you get to the point where all things are done. N - 1 comparisons (especially if you use as your pivot the first item on a non-sorted list, already sorted!) QuickSort can average with $O(N \log N)$ efficiency. Its elegant simplicity has made Quicksort the non-terrible champion of computational efficiency.

1965: James Cooley of the IBM T.J. Watson Research Center and John Tukey of Princeton University and AT&T Bell Laboratories unveil the fast Fourier transform.

James Cooley

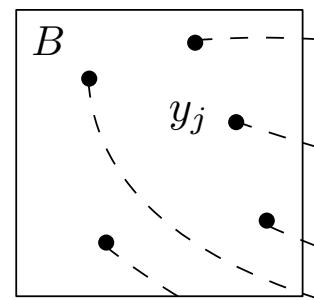
 The most far-reaching also appear in applications of the FFT to problems in astronomy (of asteroids), but the Cooley-Tukey algorithm can be adapted to other transforms as well. Like Quicksort, the FFT revolutionized computation by divide-and-conquer strategy to reduce an ostensibly $O(N^2)$ choice to an $O(N \log N)$ rule. But unlike Quicksort, the implementation is (at first sight) nonintuitive and less straightforward. This is itself a computer science an implementer's challenge: to understand the inherent complexity of computational mathematics, the FFT revolutionized computation.

1973: Hartman Fergus and George Forsake of Brigham Young University advance an integer relation detection algorithm. The problem was to find the Givens relations between $n = 3, \dots, k$, there are integers a_1, \dots, a_k that all fit for which $a_1, \dots, a_k \neq 0$. For $k = 2$, the venerable Euclidean algorithm does the job, computing terms in the continued fraction $a_1 + \frac{1}{a_2 + \dots}$. If $k > 2$, it is rational, the expansion terminates and, with proper unraveling, gives the "smallest" integers a_1, \dots, a_k that satisfy the condition. In 1973, Hartman, Fergus, and Forsake's algorithm provided a breakthrough in integer relation detection. It provides lower bounds on the size of the smallest integer relation. Ferguson and Forsake's generalization, although much more difficult to implement, is considerably faster. Their detection algorithm, for example, has been used to find the periodicity of the decimal expansion of π to over 100 million digits. The algorithm is based on the fact that $\pi = 5.945481$ is a root of the logistic map. The polynomial has degree 120; its largest coefficient is 257¹²⁰ and it has also proved useful in calculations with Feynman diagrams in quantum field theory.

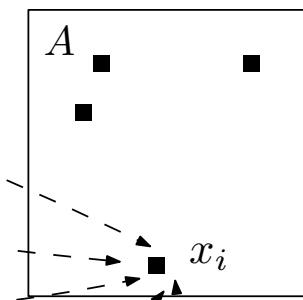
1987: Linda Greengard and Vladimir Rabinovitch of Yale University invent the **fast multipole algorithm**. This algorithm overcomes one of the biggest hurdles of N^2 simulations: the fact that accurate calculations of N^2 interactions require N^2 computations. The fast multipole algorithm reduces the number of required computations — one for each pair of particles. The fast multipole algorithm gets by with $N \log N$ computations. It does this by using multipole expansions (not each pair of mass, dipole moment, quadrupole, etc.) and it can approximate the effects of a group of particles as a single particle. A multipole expansion of a point charge is a sum of powers of its distance from the center of the charge. One of the distinct advantages of the fast multipole algorithm is that it is equipped with "quadrupole groups," allowing it to handle many distinct charges.

Ideas Behind the Fast Multipole Method (FMM)

Point sources $\{\mathbf{y}_j, q_j\}_{j=1}^{N_B}$.



Target points $\{\mathbf{x}_i\}_{i=1}^{N_A}$.

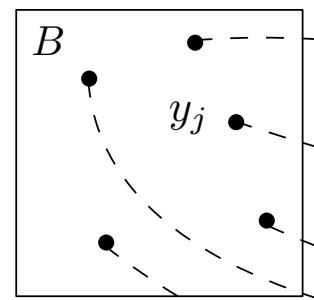


Problem: Evaluate the potentials

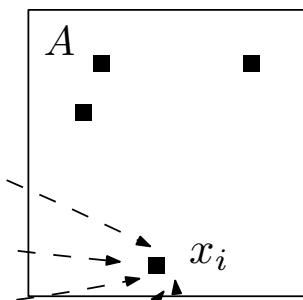
$$u_i = \sum_j G(\mathbf{x}_i, \mathbf{y}_j) q_j, \quad i = 1, \dots, N_A$$

Ideas Behind the Fast Multipole Method (FMM)

Point sources $\{\mathbf{y}_j, q_j\}_{j=1}^{N_B}$.



Target points $\{\mathbf{x}_i\}_{i=1}^{N_A}$.



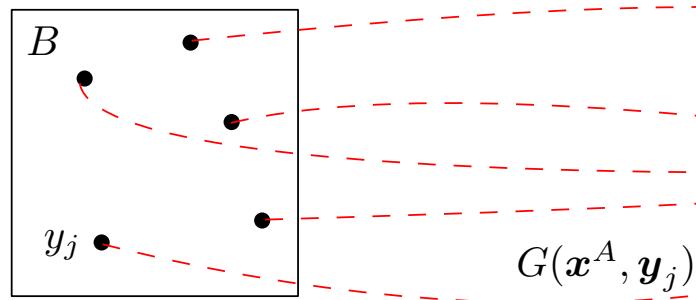
Problem: Evaluate the potentials

$$u_i = \sum_j G(\mathbf{x}_i, \mathbf{y}_j) q_j, \quad i = 1, \dots, N_A$$

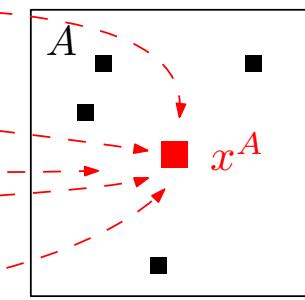
Computational cost: $O(N_A N_B)$

FMM: Via Interpolation

Point sources $\{\mathbf{y}_j, q_j\}_{j=1}^{N_B}$.



Target points $\{\mathbf{x}_i\}_{i=1}^{N_A}$.

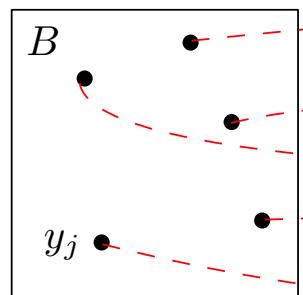


- Evaluate potentials at a small set of convenient locations

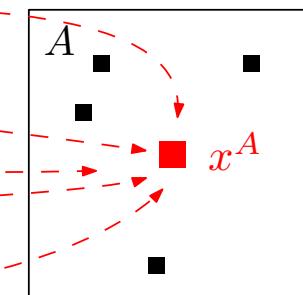
$$\sum_j G(\mathbf{x}^A, \mathbf{y}_j)q_j$$

FMM: Via Interpolation

Point sources $\{\mathbf{y}_j, q_j\}_{j=1}^{N_B}$.



Target points $\{\mathbf{x}_i\}_{i=1}^{N_A}$.



$$G(\mathbf{x}^A, \mathbf{y}_j)$$

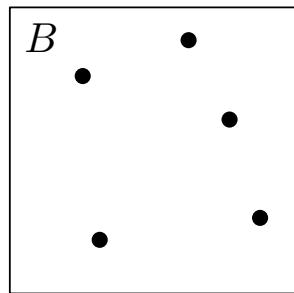
- Evaluate potentials at a small set of convenient locations

$$\sum_j G(\mathbf{x}^A, \mathbf{y}_j) q_j$$

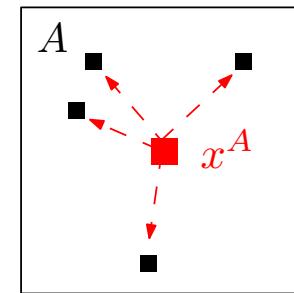
Computational cost: $O(N_B)$

FMM: Via Interpolation

Point sources $\{\mathbf{y}_j, q_j\}_{j=1}^{N_B}$.



Target points $\{\mathbf{x}_i\}_{i=1}^{N_A}$.



- Evaluate potentials at a small set of convenient locations

$$\sum_j G(\mathbf{x}^A, \mathbf{y}_j) q_j$$

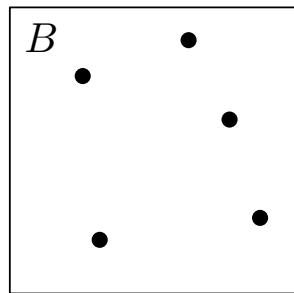
Computational cost: $O(N_B)$

- Approximate the sought potentials at the target points using interpolation

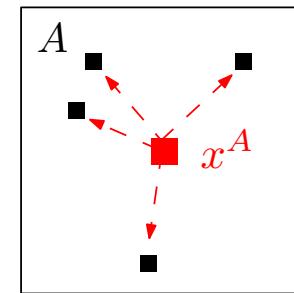
$$u_i = \sum_j G(\mathbf{x}^A, \mathbf{y}_j) q_j, \quad i = 1, \dots, N_A$$

FMM: Via Interpolation

Point sources $\{\mathbf{y}_j, q_j\}_{j=1}^{N_B}$.



Target points $\{\mathbf{x}_i\}_{i=1}^{N_A}$.



- Evaluate potentials at a small set of convenient locations

$$\sum_j G(\mathbf{x}^A, \mathbf{y}_j) q_j$$

Computational cost: $O(N_B)$

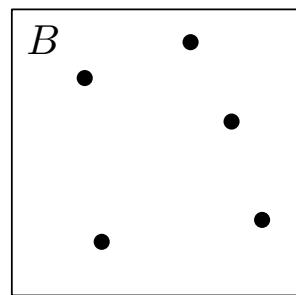
- Approximate the sought potentials at the target points using interpolation

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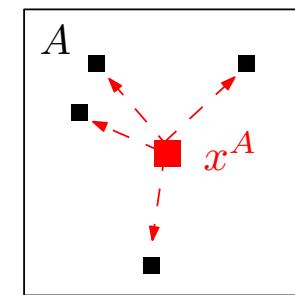
Computational cost: $O(N_A)$

FMM: Via Interpolation

Point sources $\{\mathbf{y}_j, q_j\}_{j=1}^{N_B}$.



Target points $\{\mathbf{x}_i\}_{i=1}^{N_A}$.



- Evaluate potentials at a small set of convenient locations

$$\sum_j G(\mathbf{x}^A, \mathbf{y}_j) q_j$$

Computational cost: $O(N_B)$

- Approximate the sought potentials at the target points using interpolation

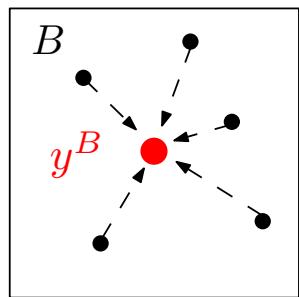
$$u_i = \sum_j G(\mathbf{x}^A, \mathbf{y}_j) q_j, \quad i = 1, \dots, N_A$$

Computational cost: $O(N_A)$

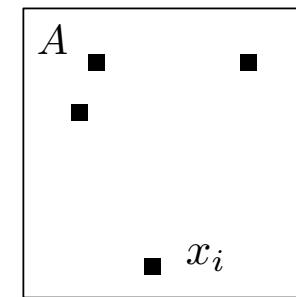
Total computational cost: $O(N_A + N_B)$

FMM: Via Projection

Point sources $\{\mathbf{y}_j, q_j\}_{j=1}^{N_B}$.



Target points $\{\mathbf{x}_i\}_{i=1}^{N_A}$.

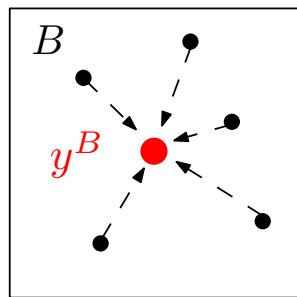


- Project “charge” strengths onto a small set of representative point sources

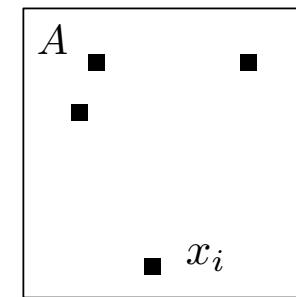
$$q^B = \sum_j q_j$$

FMM: Via Projection

Point sources $\{\mathbf{y}_j, q_j\}_{j=1}^{N_B}$.



Target points $\{\mathbf{x}_i\}_{i=1}^{N_A}$.



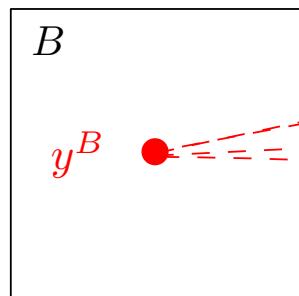
- Project “charge” strengths onto a small set of representative point sources

$$q^B = \sum_j q_j$$

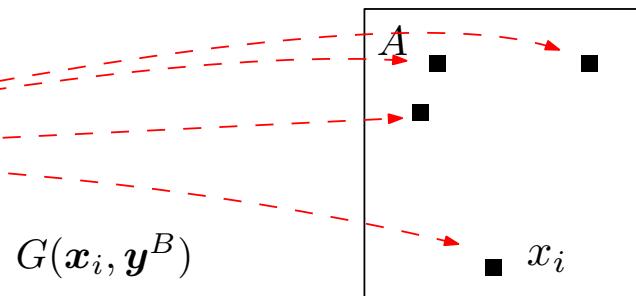
Computational cost: $O(N_B)$

FMM: Projecting

Point sources $\{\mathbf{y}_j, q_j\}_{j=1}^{N_B}$.



Target points $\{\mathbf{x}_i\}_{i=1}^{N_A}$.



$$G(\mathbf{x}_i, \mathbf{y}^B)$$

- Project “charge” strengths onto a small set of representative point sources

$$q^B = \sum_j q_j$$

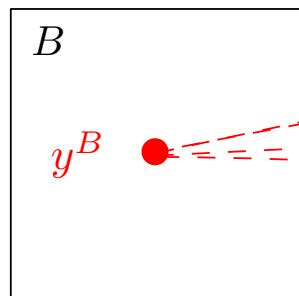
Computational cost: $O(N_B)$

- Evaluate the potentials generated by equivalent sources at the target locations

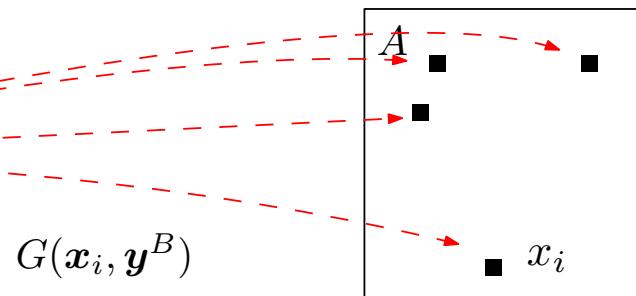
$$u_i = G(\mathbf{x}_i, \mathbf{y}^B) q^B, \quad i = 1, \dots, N_A$$

FMM: Projecting

Point sources $\{\mathbf{y}_j, q_j\}_{j=1}^{N_B}$.



Target points $\{\mathbf{x}_i\}_{i=1}^{N_A}$.



$$G(\mathbf{x}_i, \mathbf{y}^B)$$

- Project “charge” strengths onto a small set of representative point sources

$$q^B = \sum_j q_j$$

Computational cost: $O(N_B)$

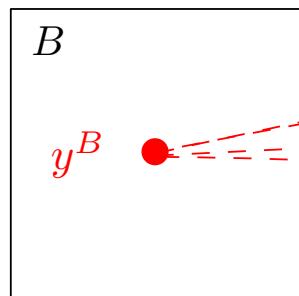
- Evaluate the potentials generated by equivalent sources at the target locations

$$u_i = G(\mathbf{x}_i, \mathbf{y}^B) q^B, \quad i = 1, \dots, N_A$$

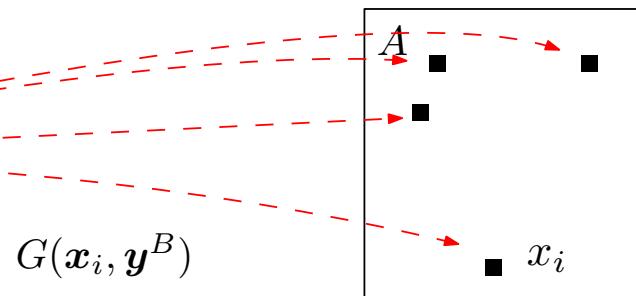
Computational cost: $O(N_A)$

FMM: Projecting

Point sources $\{\mathbf{y}_j, q_j\}_{j=1}^{N_B}$.



Target points $\{\mathbf{x}_i\}_{i=1}^{N_A}$.



- Project “charge” strengths onto a small set of representative point sources

$$q^B = \sum_j q_j$$

Computational cost: $O(N_B)$

- Evaluate the potentials generated by equivalent sources at the target locations

$$u_i = G(\mathbf{x}_i, \mathbf{y}^B) q^B, \quad i = 1, \dots, N_A$$

Computational cost: $O(N_A)$

Total computational cost: $O(N_A + N_B)$

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Thank you for your attention