Waves: Modeling, Analysis, and Numerics
Radboud University
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Nijmegen, the Netherlands

4TU.AMI

Linear Waves: From Physics to Numerics

Part III

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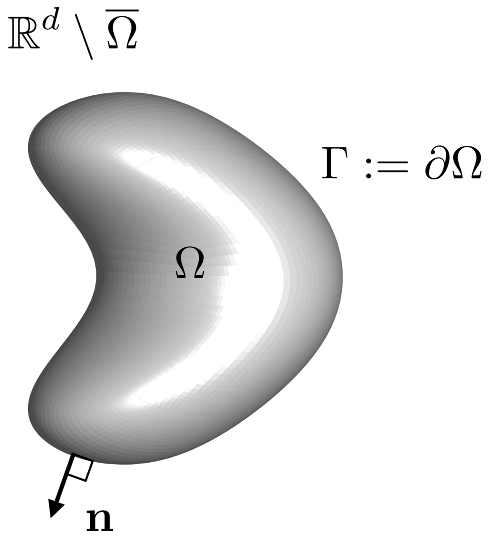
Mathematics of Computational Science
University of Twente

Contents

Scattering Problem Setup

Scattering by Bounded Obstacles



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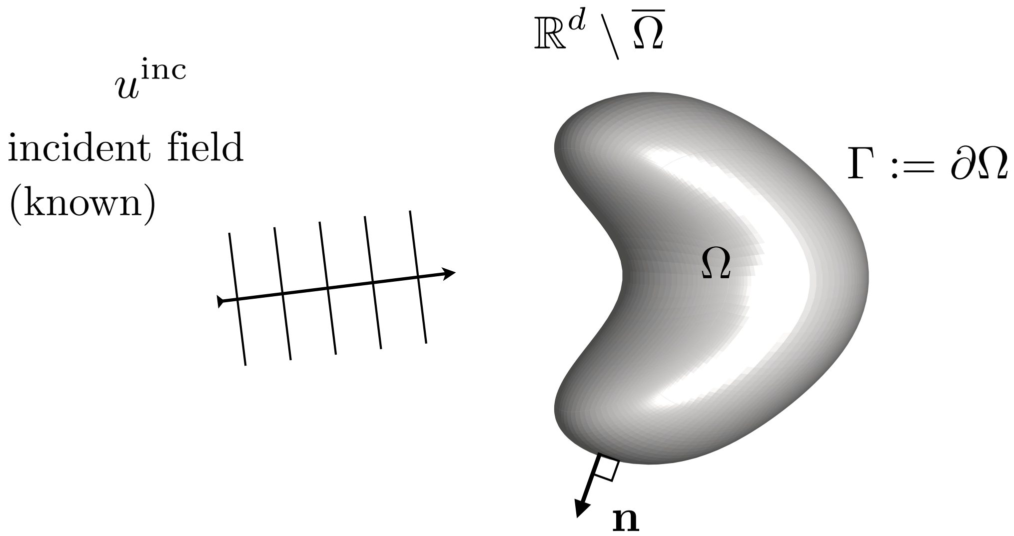

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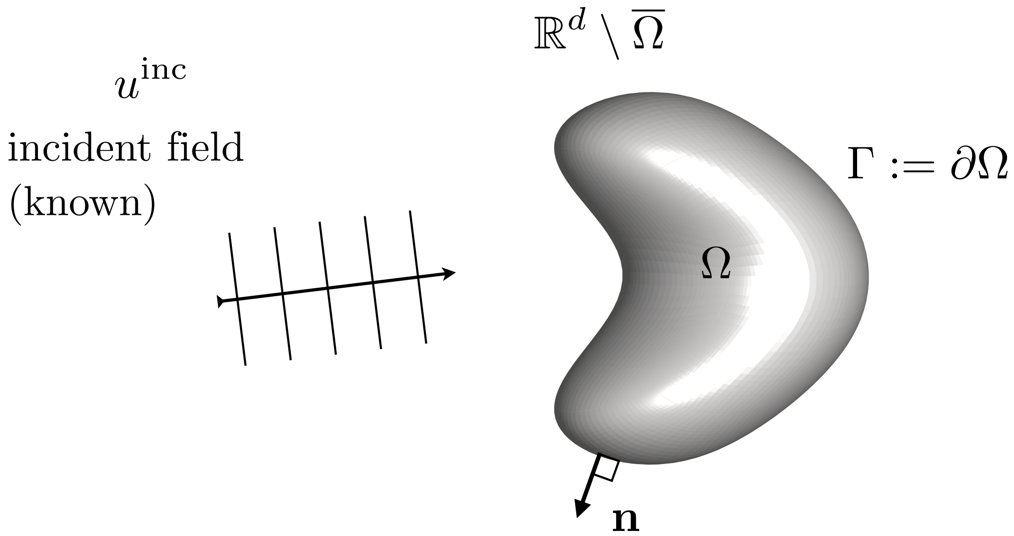

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$$\Delta u^{\text{inc}} + k^2 u^{\text{inc}} = 0 \quad \text{in} \quad D \supset \Gamma$$

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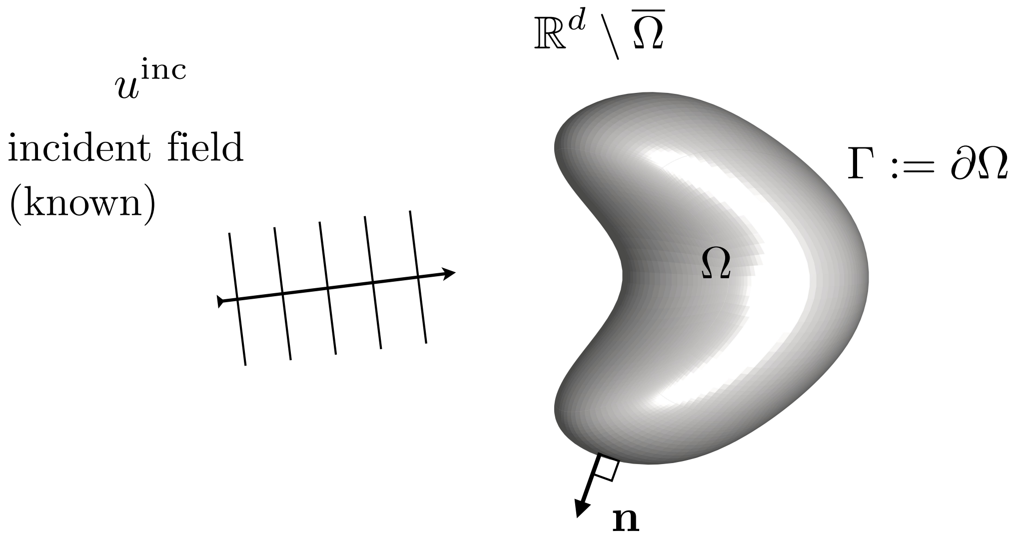

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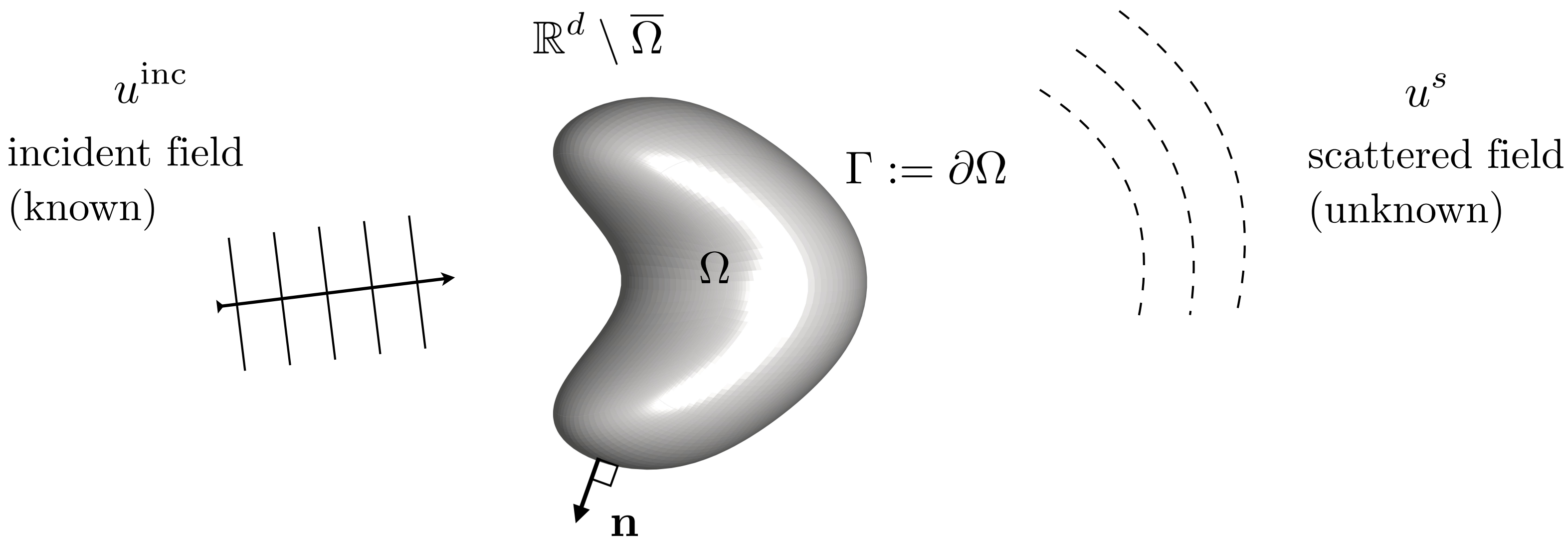

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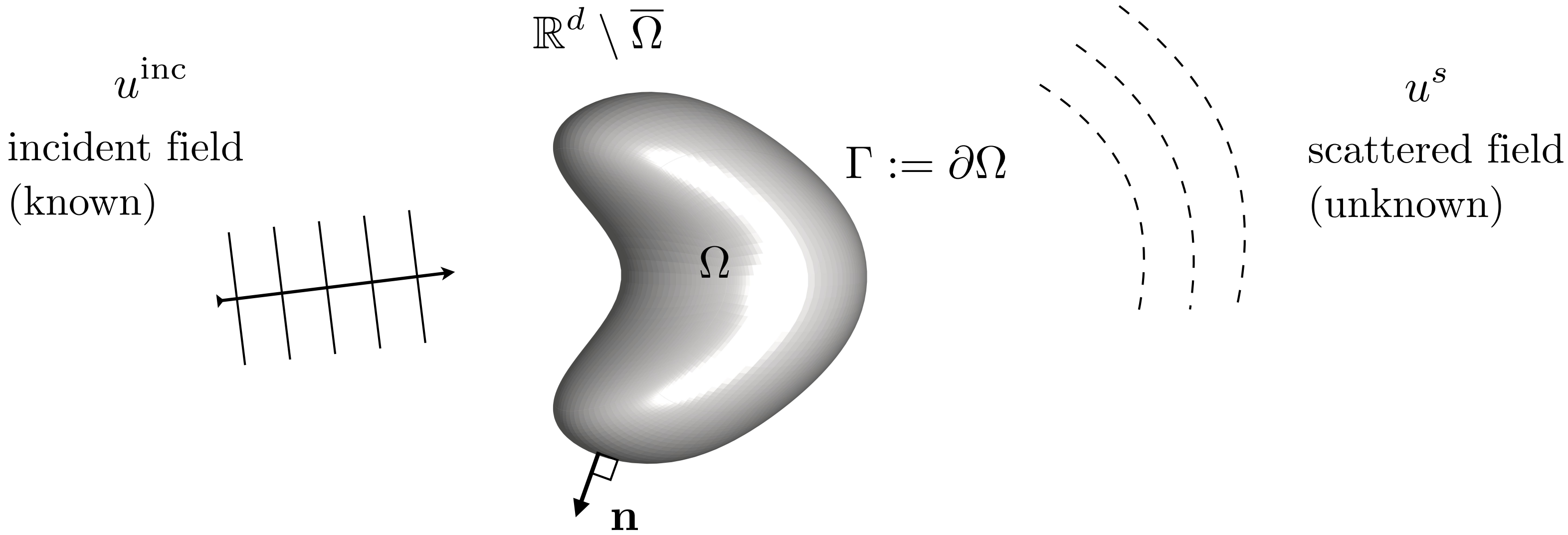

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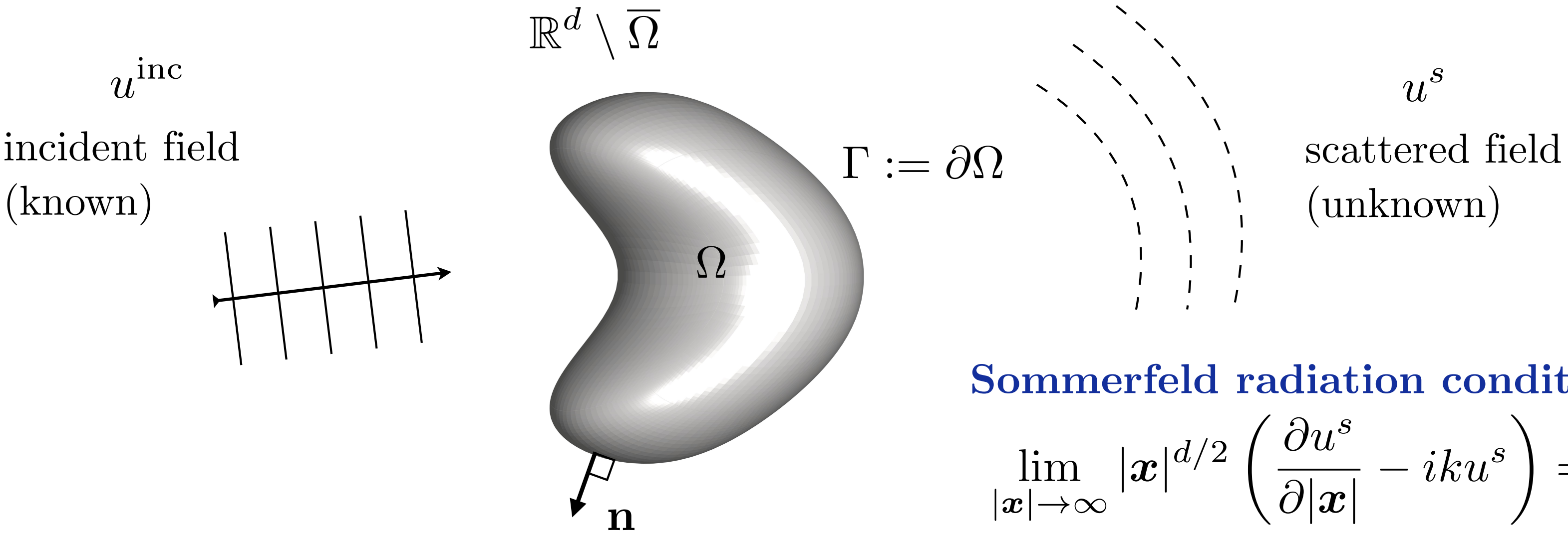

Sommerfeld radiation condition:

$$\lim_{|\boldsymbol{x}|\to\infty} |\boldsymbol{x}|^{d/2} \left(\frac{\partial u^s}{\partial |\boldsymbol{x}|} - iku^s \right) = 0$$

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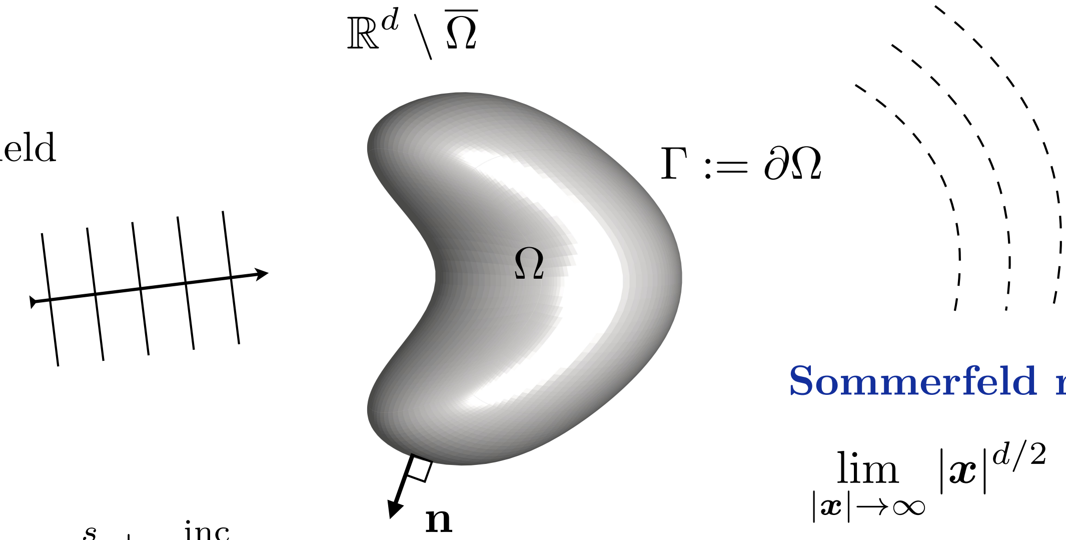

Total field: $u = u^s + u^{\text{inc}}$

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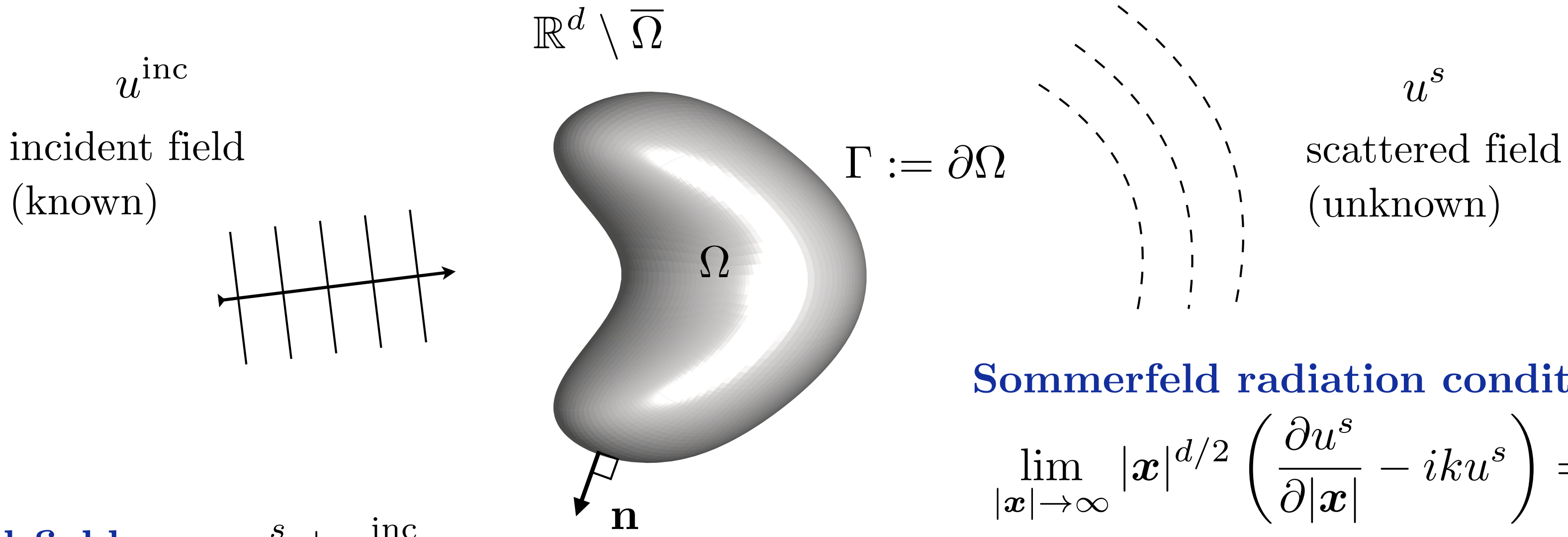

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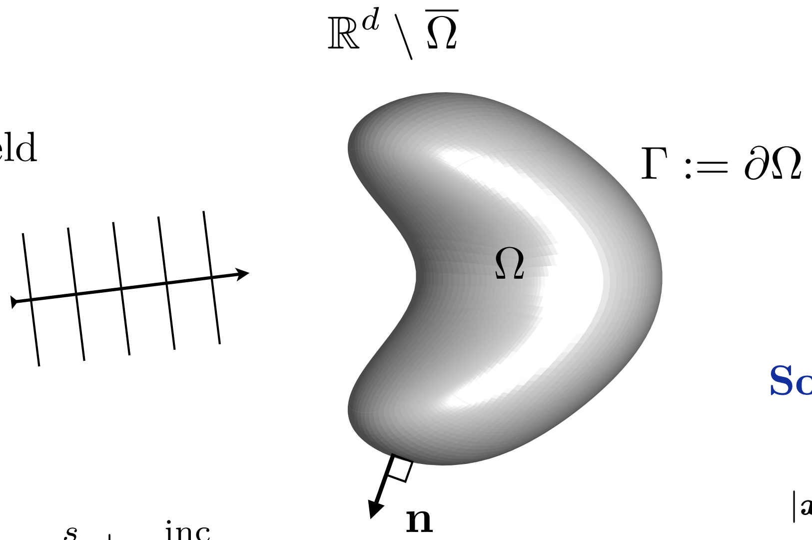
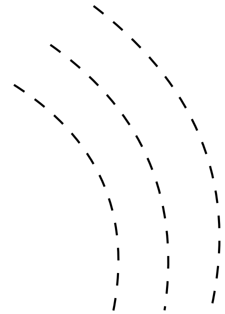
Scattering by Bounded Obstacles

u^{inc}
incident field
(known)





u^s
scattered field
(unknown)

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Boundary condition

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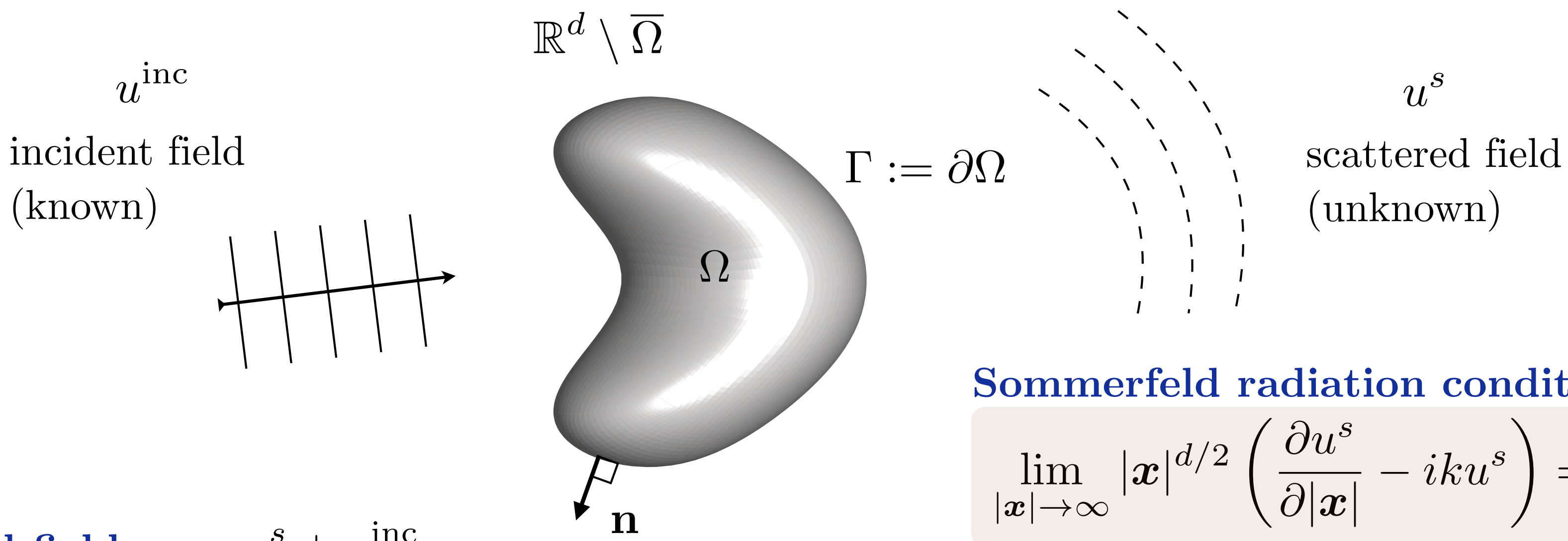

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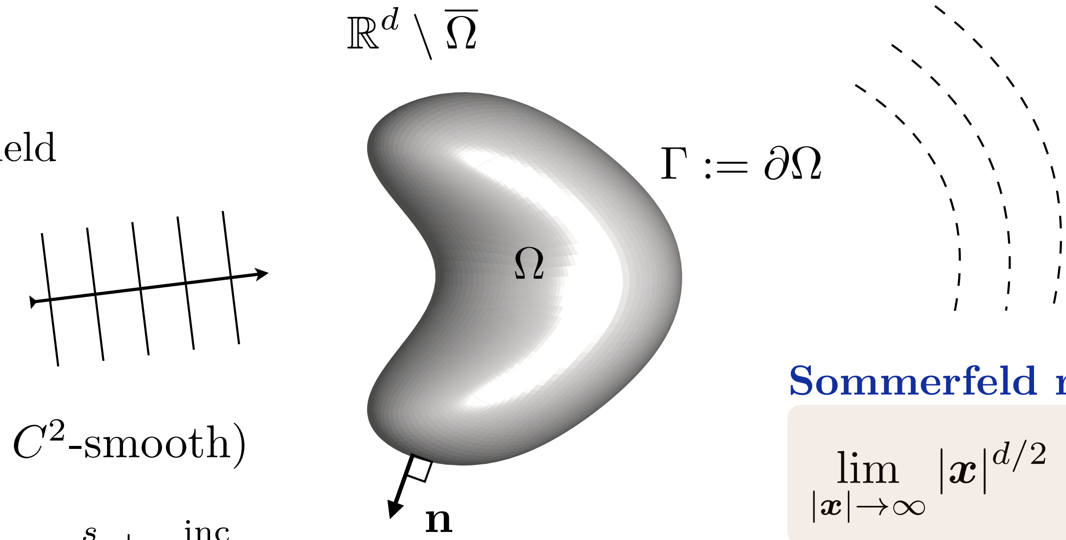

u^s
scattered field
(unknown)

(Γ is assumed C^2-smooth)

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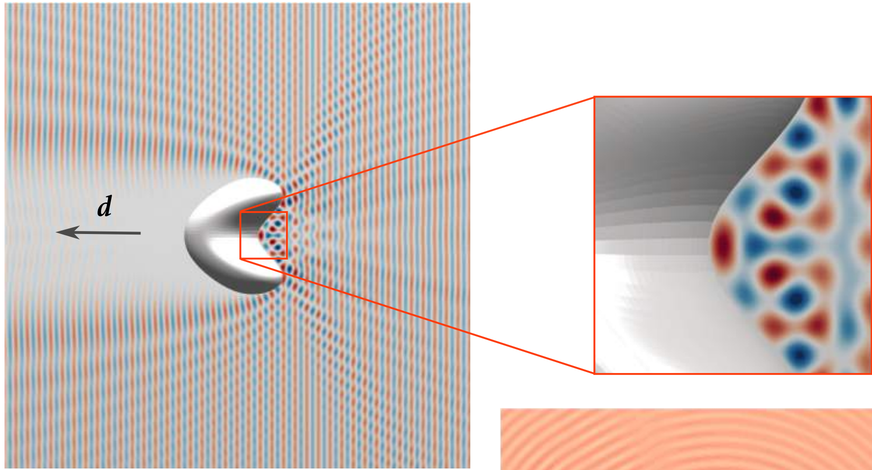
Scattering by Bounded Obstacles

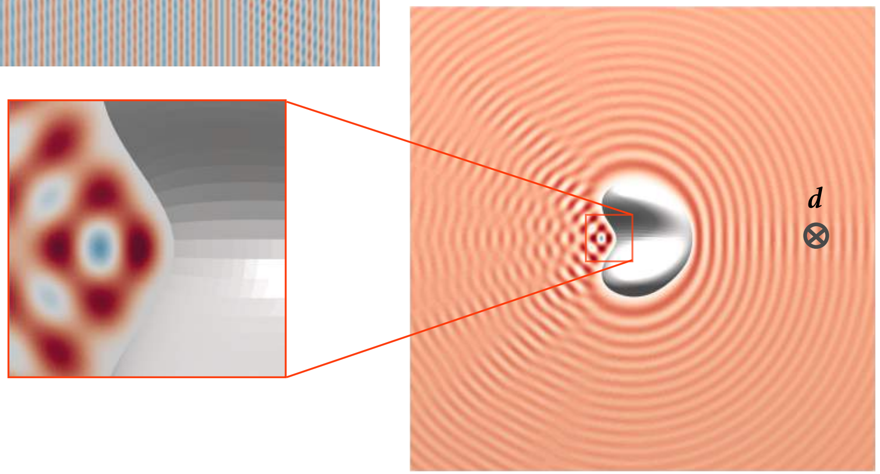
$$u^{\text{inc}}(\boldsymbol{x}) = \mathrm{e}^{ik\boldsymbol{d}\cdot\boldsymbol{x}}$$

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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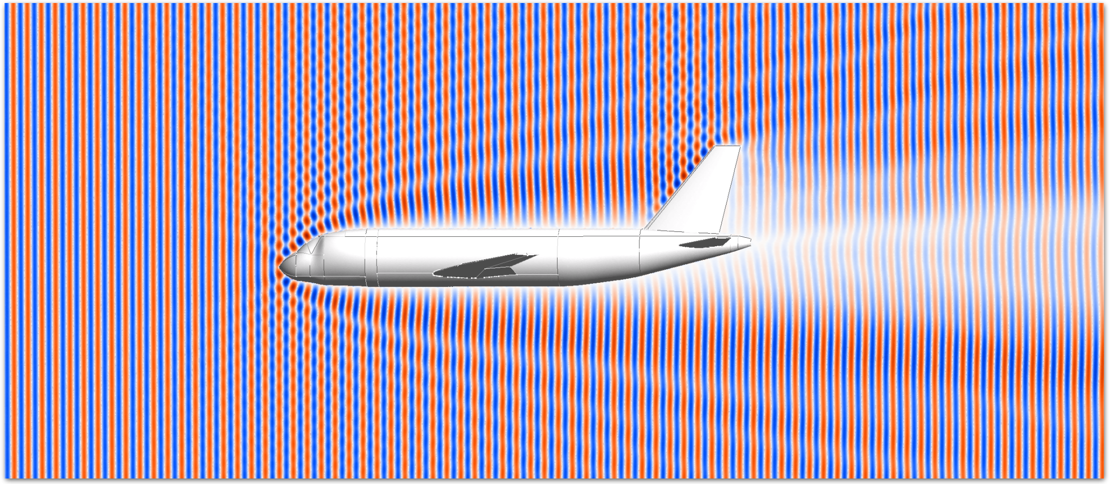
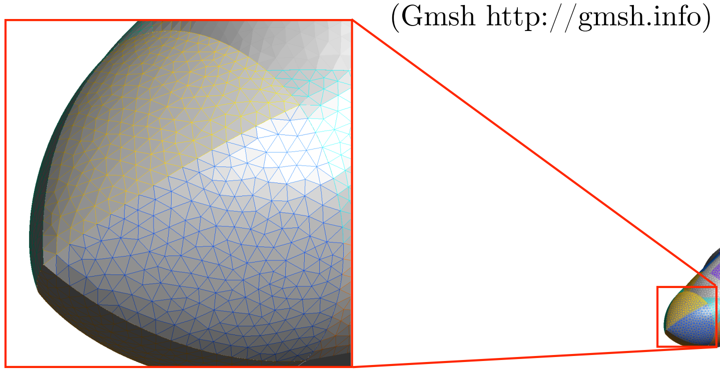
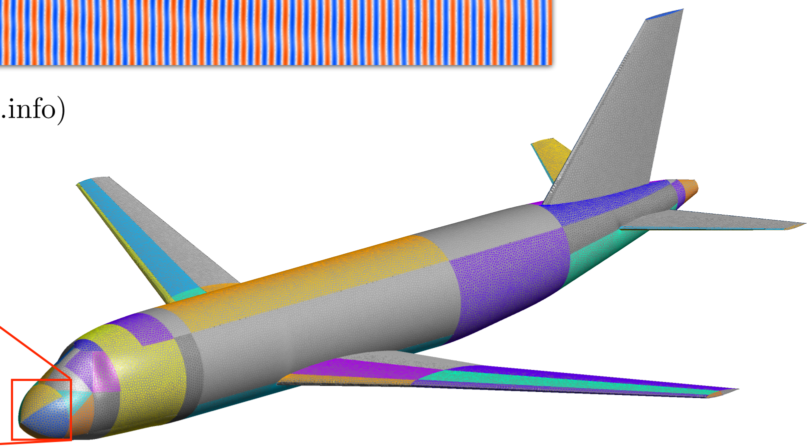


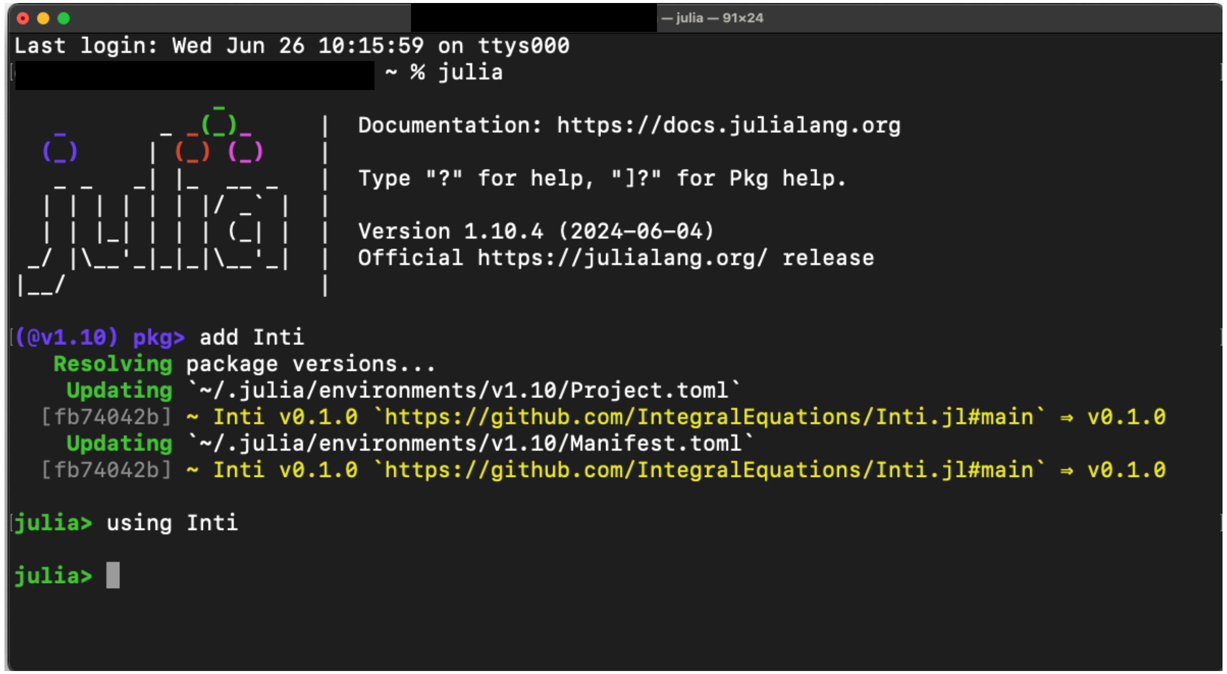
(Gmsh http://gmsh.info)





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

+

Gmsh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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**.

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

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The Sommerfeld radiation condition states that

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

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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

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

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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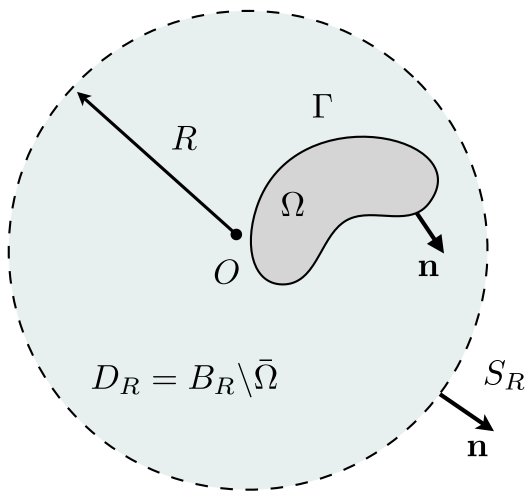

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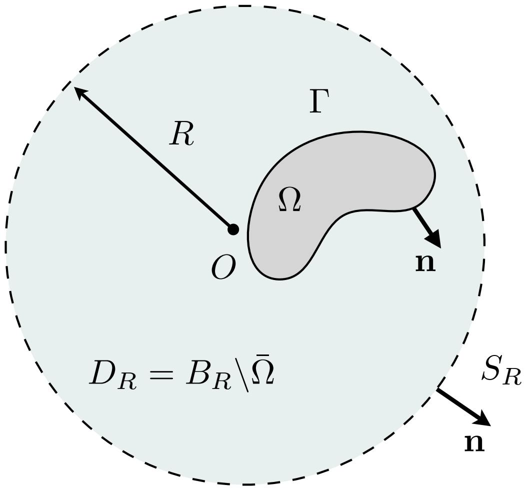

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truncated-domain problem

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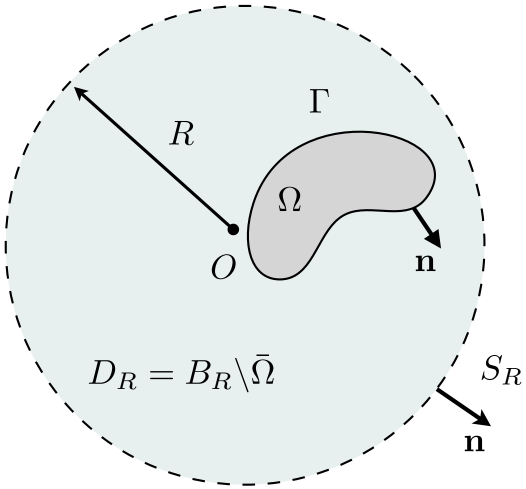

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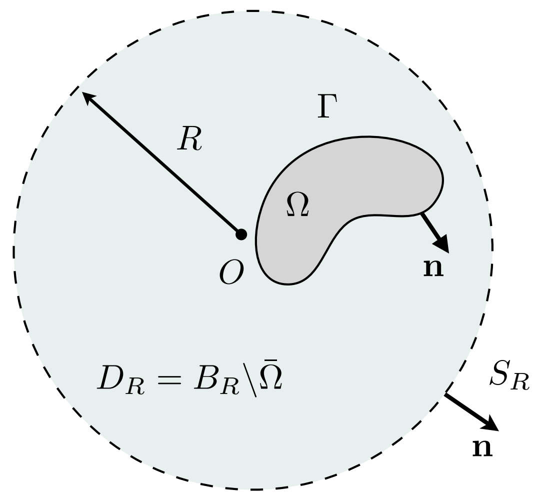
The problem then reduces to finding $u = u^s + u^{\text{inc}} \in H^1_{\text{loc}}(D_R)$ such that

truncated-domain problem

in the "weak sense"

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



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

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

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Is the variational problem well posed?

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Is the variational problem well posed?

$$a(u,v) = \int_\Omega \nabla u \cdot \nabla \overline{v} \, \mathrm{d}\boldsymbol{x} - ik \int_{S_R} u \overline{v} \, \mathrm{d}s - k^2 \int_\Omega u \overline{v} \, \mathrm{d}\boldsymbol{x}$$

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

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we can apply the **Fredholm alternative**!
(uniqueness implies existence)

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Suppose there exists $0 \neq w \in H_0^1(D_R)$ such that

$$a(w, v) = 0 \qquad \forall v \in H_0^1(D_R).$$

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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.

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

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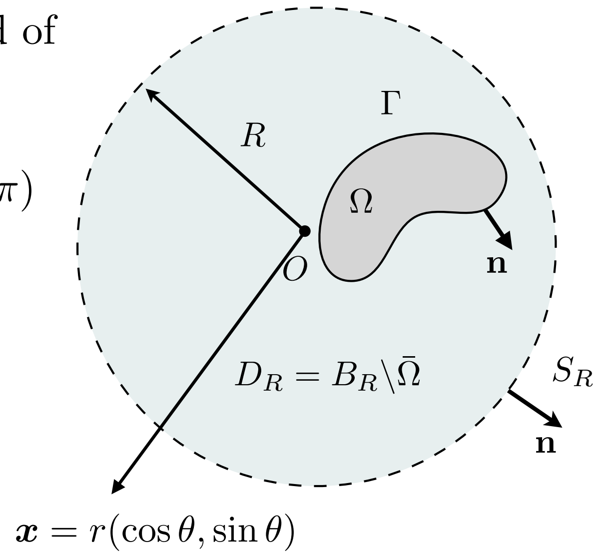

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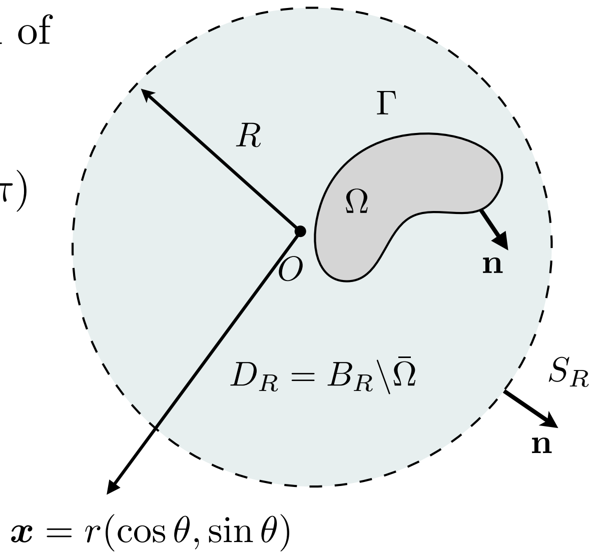

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Imposing the boundary condition:

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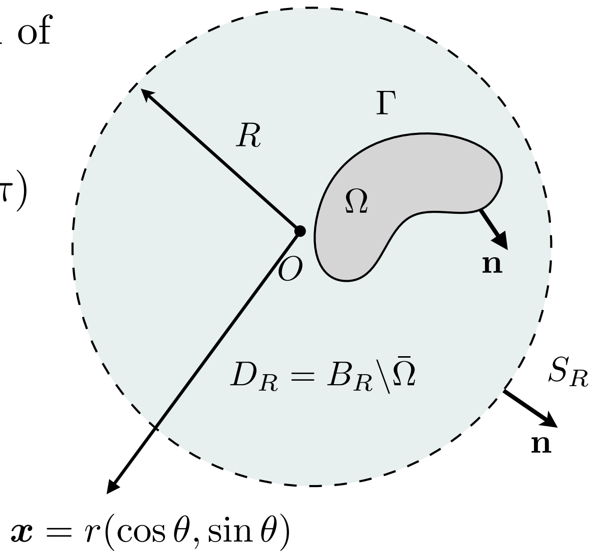

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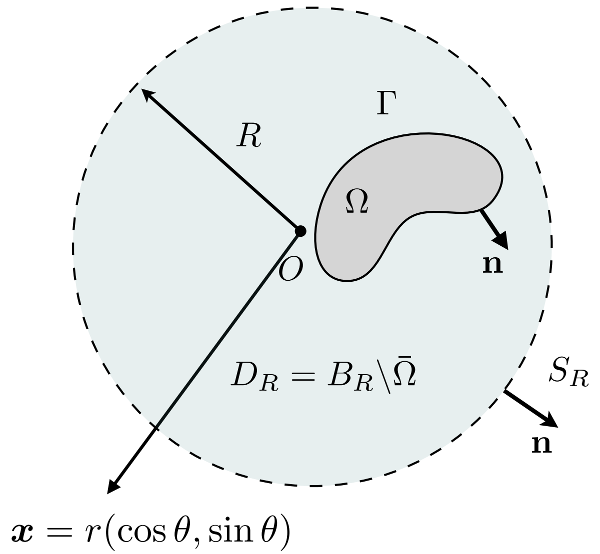

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Applying the normal derivative on S_R :

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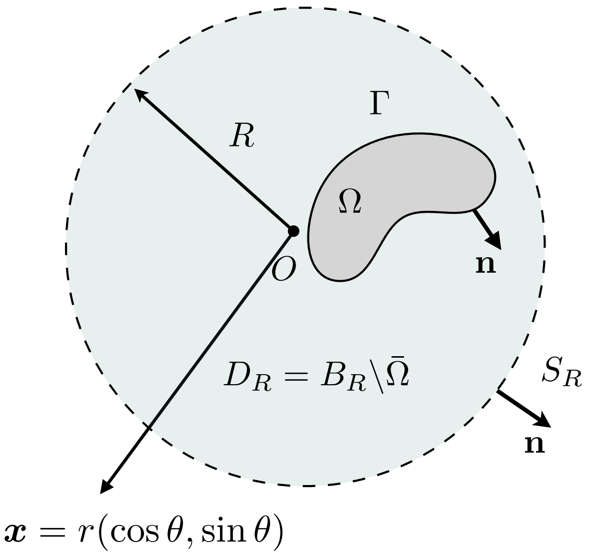

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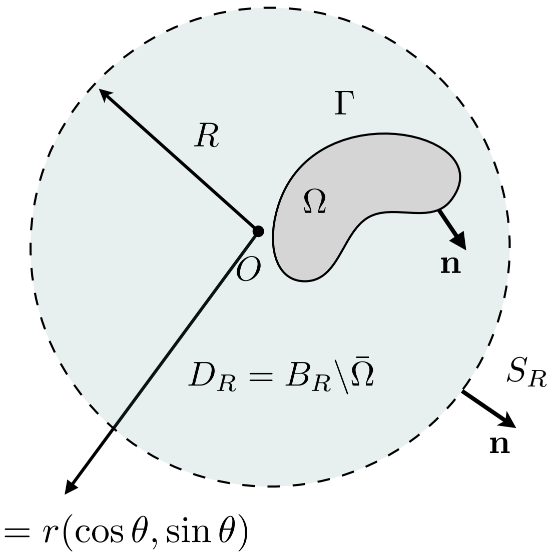

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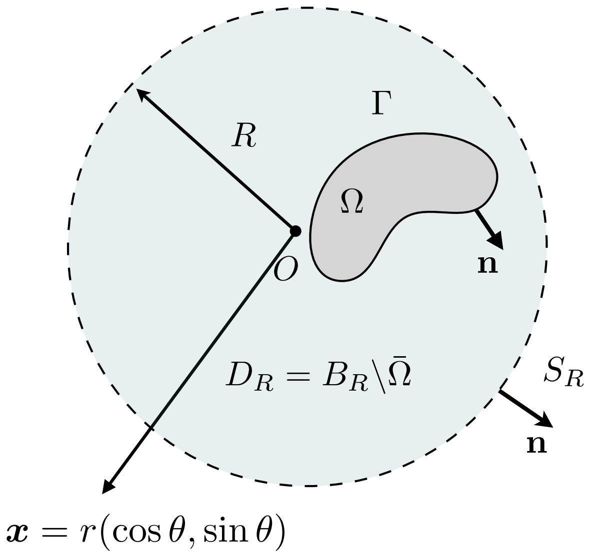

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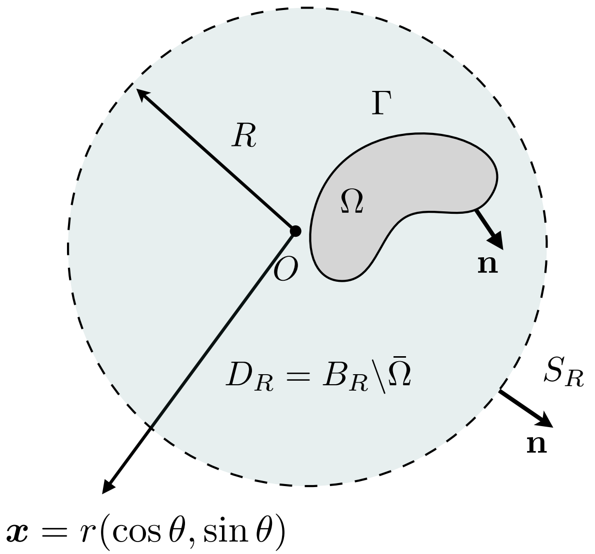

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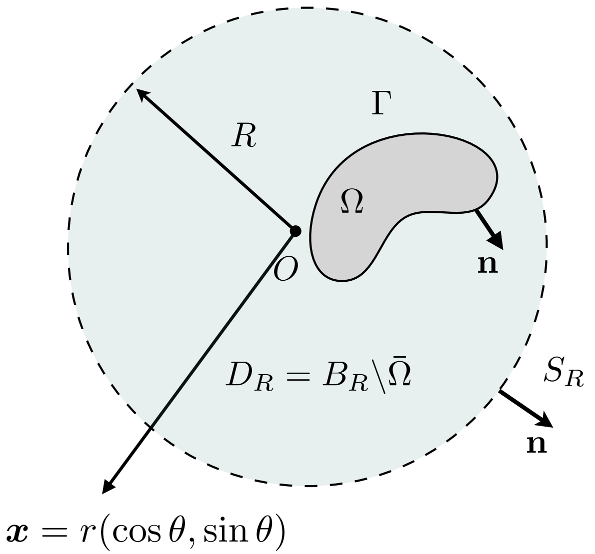
It can be shown that $\Lambda : H^{1/2}(S_R) \to H^{-1/2}(S_R)$ is bounded.



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in general, these integrals should be interpreted as duality pairings

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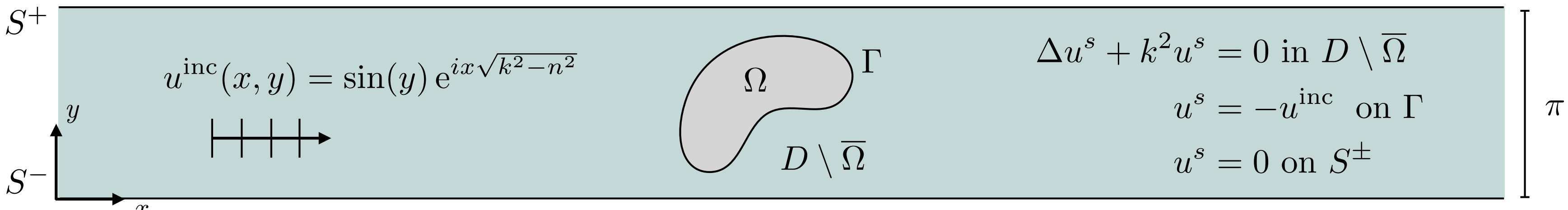
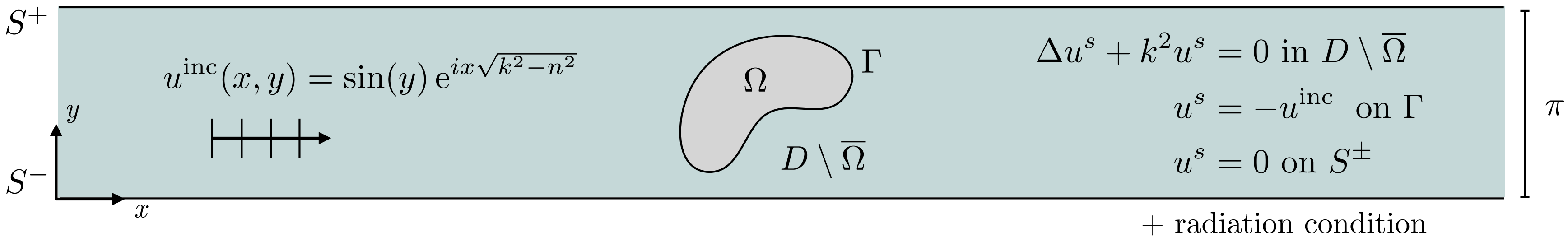
this problem can be directly solved using standard (Lagrange) finite elements!

DtN Map for Waveguides



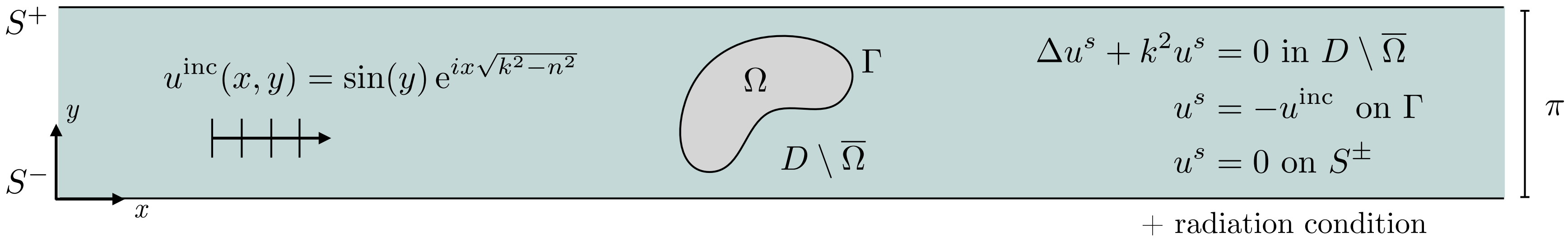
+ radiation condition

DtN Map for Waveguides



How can the DtN map be constructed in this situation?

DtN Map for Waveguides



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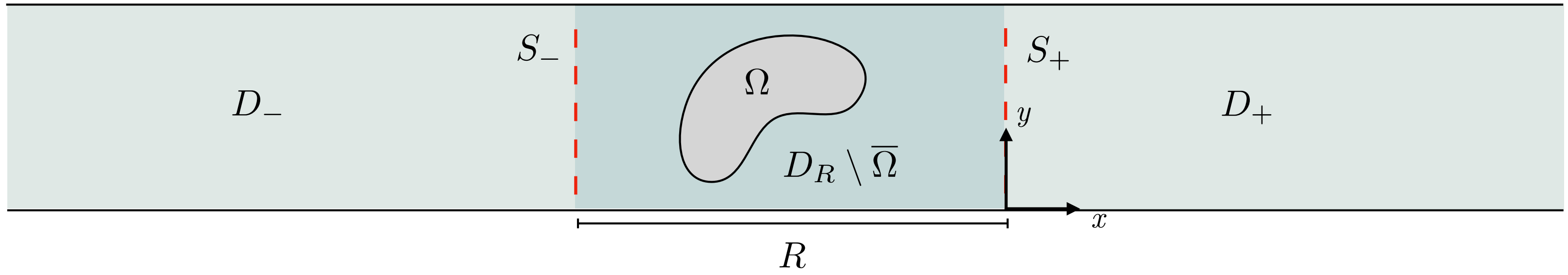

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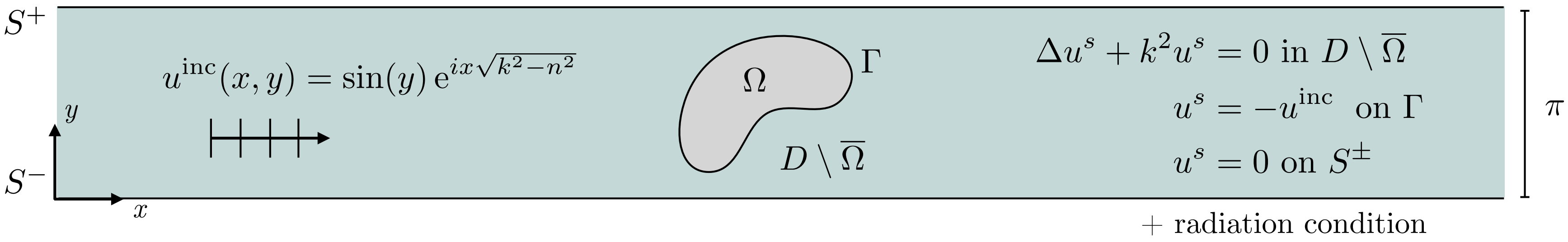

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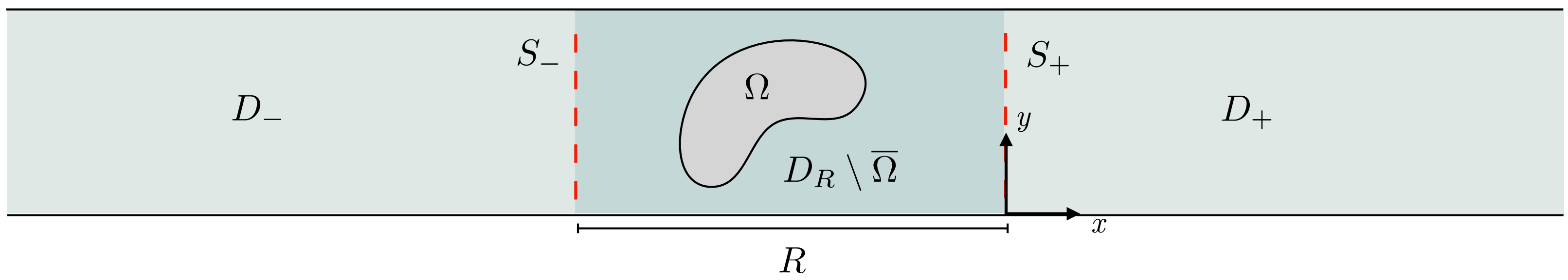

Assuming $u^s = f$ on S_+, the solution in D_+ is given by: $u_+(x,y) = \dfrac{2}{\pi}\displaystyle\sum_{n=0}^{\infty} \sin(ny)\,\mathrm{e}^{ix\sqrt{k^2-n^2}} \int_0^{\pi} f(t)\,\sin(nt)\,\mathrm{d}t.$

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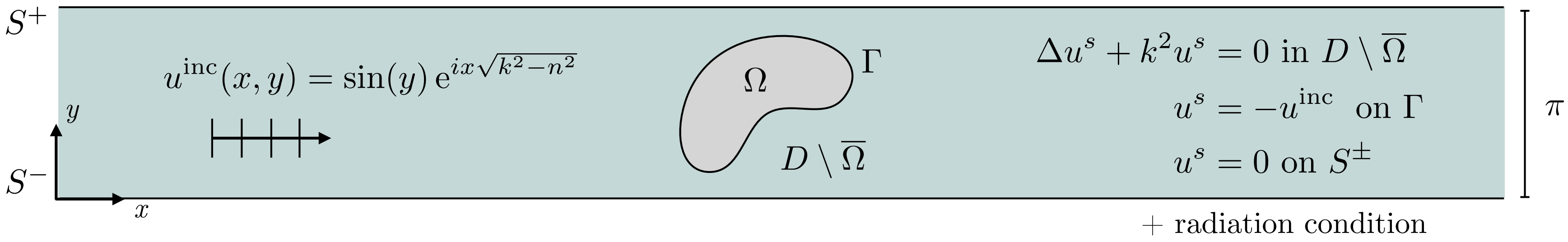

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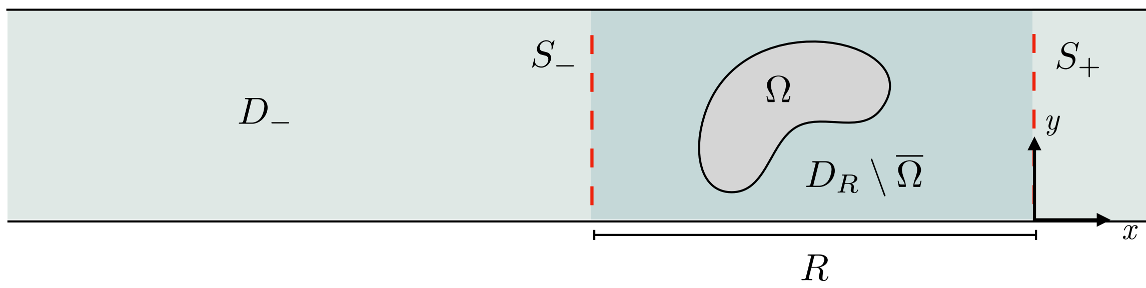

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$$\frac{\partial u^s}{\partial x}\Big|_{S_+} = \Lambda_+\big[\gamma_0^{S_+} u^s\big](y) := \frac{2i}{\pi} \sum_{n=0}^{\infty} \sqrt{k^2-n^2}\,\sin(ny) \int_0^{\pi} u^s(0,t)\sin(n\pi t)\,\mathrm{d}t, \quad \Lambda_+ : \widetilde{H}^{1/2}(S_+) \to H^{-1/2}(S_+)$$

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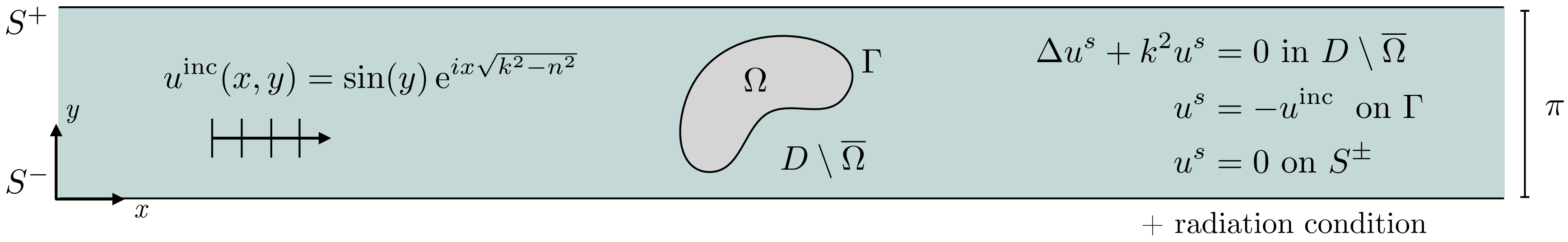

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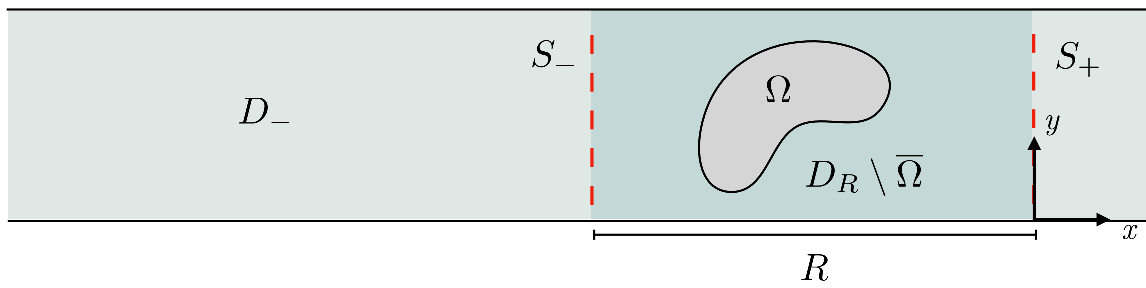
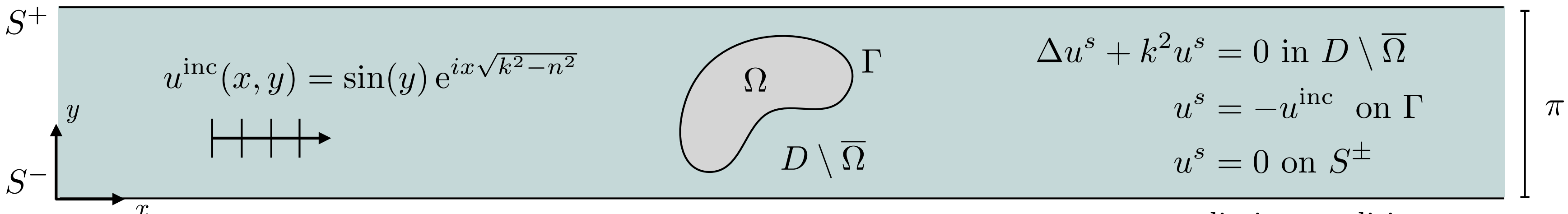


Assuming $u^s = f$ on S_-, the solution in D_- is given by: $u_-(x,y) = \dfrac{2}{\pi} \displaystyle\sum_{n=0}^{\infty} \sin(ny)\,\mathrm{e}^{-ix\sqrt{k^2-n^2}} \int_0^{\pi} f(t)\,\sin(nt)\,\mathrm{d}t.$

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

DtN Map for Waveguides



$$\Delta u^s + k^2 u^s = 0 \text{ in } D \setminus \overline{\Omega}$$
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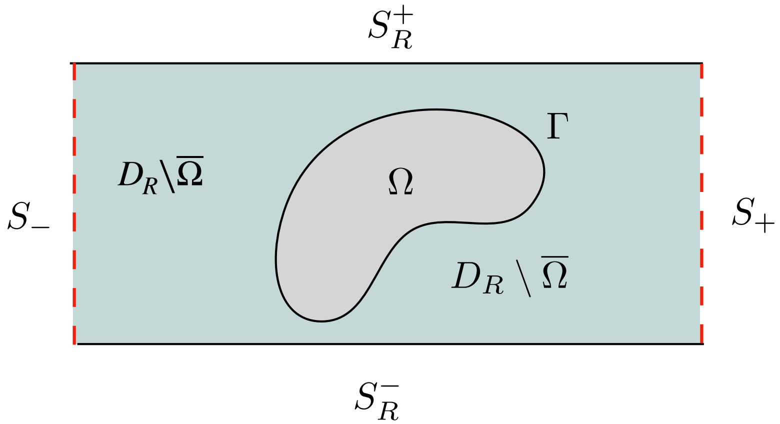
$$u^s = 0 \text{ on } S^{\pm}$$

+ radiation condition

$\Updownarrow$

Truncated waveguide problem:



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

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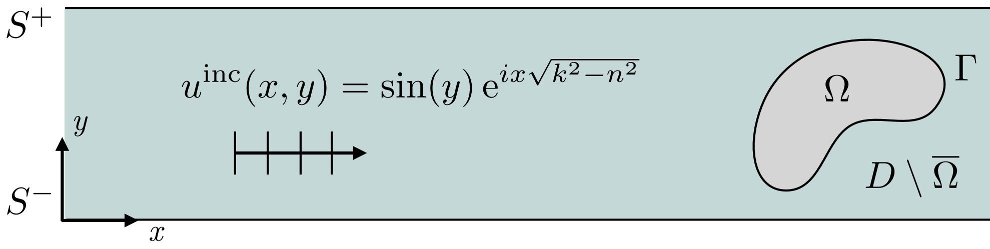

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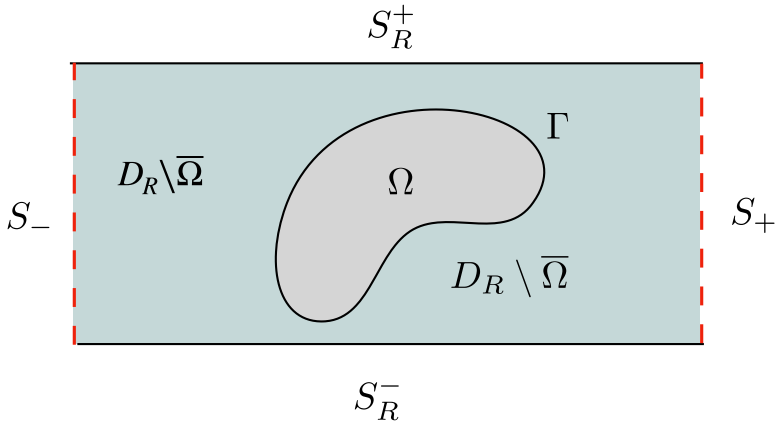

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this problem can be directly solved using standard (Lagrange) finite elements!

Perfectly Matched Layers (PMLs)

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

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

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

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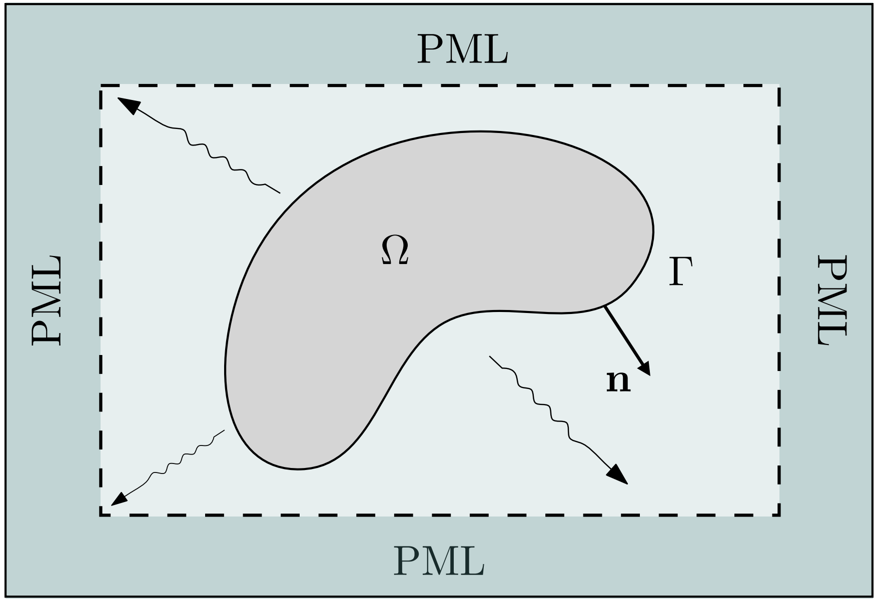

Perfectly Matched Layers (PMLs)

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

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

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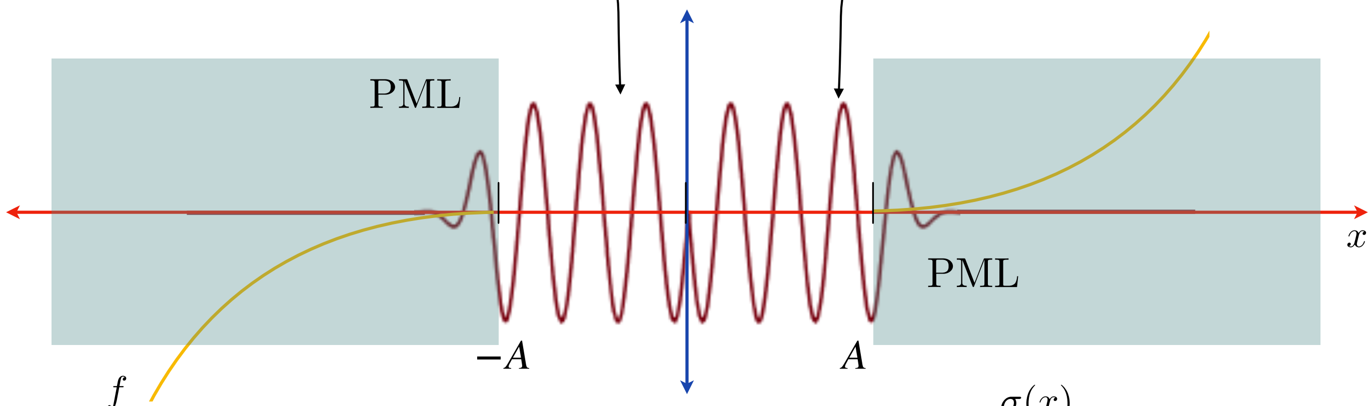
$(E\circ\tilde{x})(x)=\dfrac{i}{2k}\,\mathrm{e}^{-ikx}\,\mathrm{e}^{-k(x-A)^2}$ for $x<-A$

$(E\circ\tilde{x})(x)=\dfrac{i}{2k}\,\mathrm{e}^{ikx}\,\mathrm{e}^{-k(x-A)^2}$ for $x>A$



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

Perfectly Matched Layers (PMLs)

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

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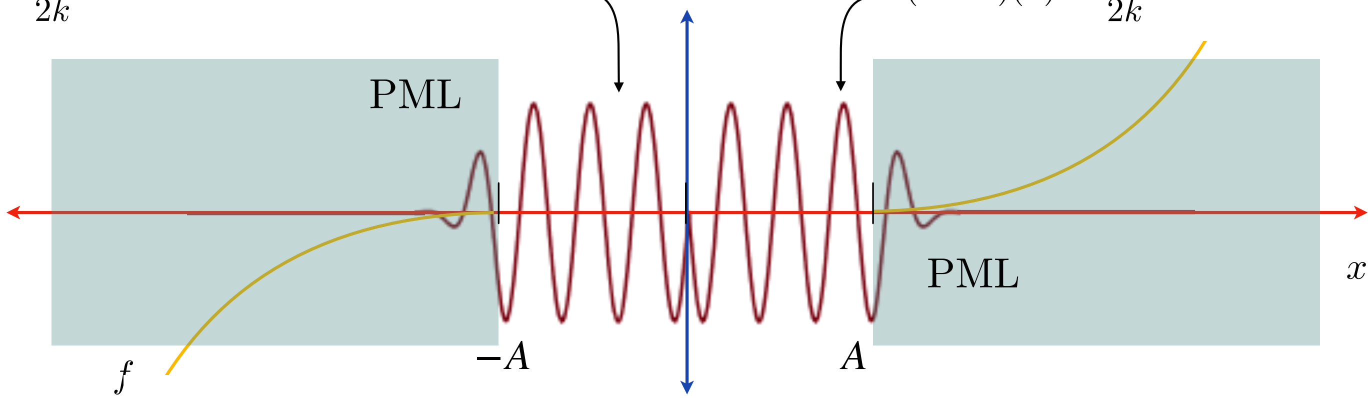

Observe that the function $\widetilde{E} := E \circ \tilde{x}$ has the following properties:

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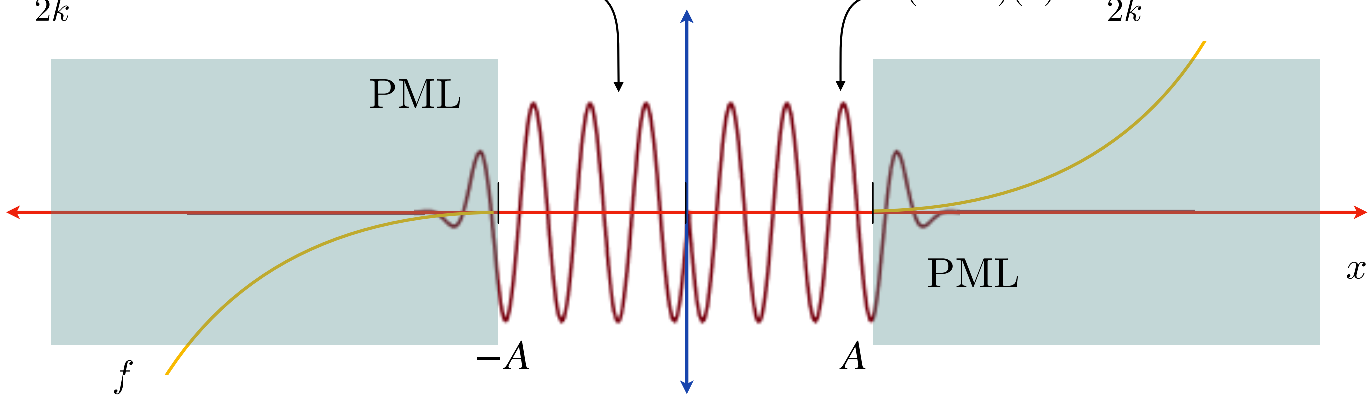

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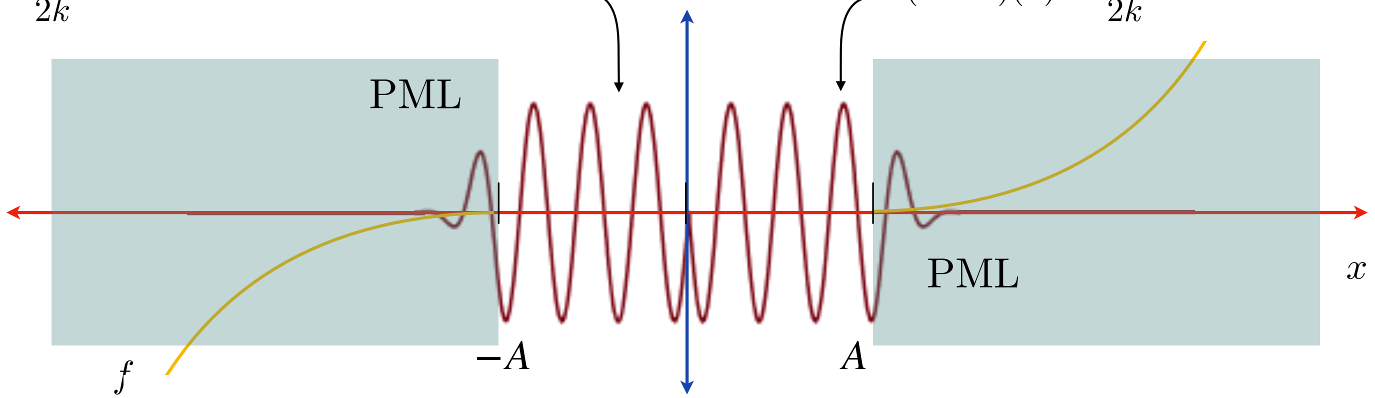

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- It coincides with E on the interval $(-A, A)$;
- It decays exponentially in the PML region, $|x| > A$.
- Since $\widetilde{E}' = E'\tilde{x}'$, $\widetilde{E}'' = E''\tilde{x}' + E'\tilde{x}'' = E''\tilde{x}' + \widetilde{E}'\frac{\tilde{x}''}{\tilde{x}'}$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

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

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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$$\tilde{u}^s(x,y) := u^s(x + if(x), y + if(y)) \implies \frac{\partial u^s}{\partial x} = \frac{1}{1 + i\frac{\sigma(x)}{k}} \frac{\partial \tilde{u}^s}{\partial x}, \quad \frac{\partial u^s}{\partial y} = \frac{1}{1 + i\frac{\sigma(y)}{k}} \frac{\partial \tilde{u}^s}{\partial y}$$

$$\implies \frac{\partial^2 u^s}{\partial x^2} = \frac{1}{1 + i\frac{\sigma(x)}{k}} \frac{\partial}{\partial x} \left(\frac{1}{1 + i\frac{\sigma(x)}{k}} \frac{\partial \tilde{u}^s}{\partial x} \right), \quad \frac{\partial^2 u^s}{\partial y^2} = \frac{1}{1 + i\frac{\sigma(y)}{k}} \frac{\partial}{\partial y} \left(\frac{1}{1 + i\frac{\sigma(y)}{k}} \frac{\partial \tilde{u}^s}{\partial y} \right)$$

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We therefore solve the following problem:

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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:

$$\tilde{u}^s(x,y) := u^s(x+if(x), y+if(y)) \implies \frac{\partial u^s}{\partial x} = \frac{1}{1+i\frac{\sigma(x)}{k}}\frac{\partial \tilde{u}^s}{\partial x}, \quad \frac{\partial u^s}{\partial y} = \frac{1}{1+i\frac{\sigma(y)}{k}}\frac{\partial \tilde{u}^s}{\partial y}$$

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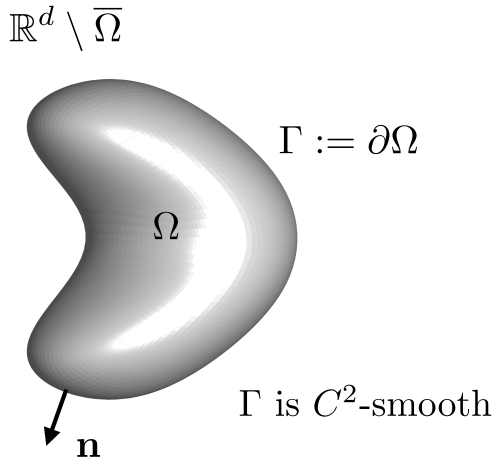
whose solution provides an accurate **approximation** of the exact analytic extension.

Boundary Integral Equation Methods

Combined Field Integral Equation (CFIE)

Consider once again for problem of scattering:

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



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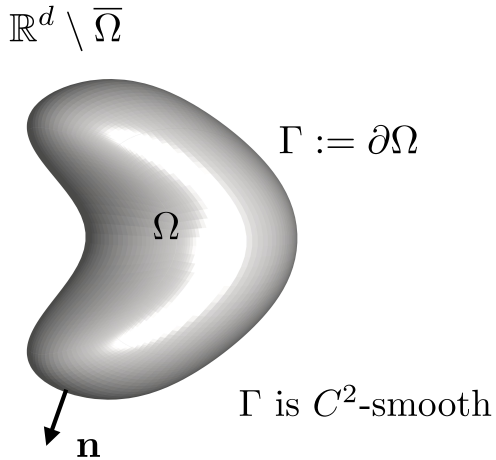

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We seek the solution given by the **combined-field potential**:

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

$$(\mathcal{S}\varphi)(\boldsymbol{x}) := \int_\Gamma G(\boldsymbol{x}, \boldsymbol{y})\varphi(\boldsymbol{y})\mathrm{d}s(\boldsymbol{y}) \qquad \text{and} \qquad (\mathcal{D}\varphi)(\boldsymbol{x}) := \int_\Gamma \frac{\partial G(\boldsymbol{x}, \boldsymbol{y})}{\partial \boldsymbol{n}(\boldsymbol{y})}\varphi(\boldsymbol{y})\mathrm{d}s(\boldsymbol{y})$$

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

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:

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

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

$$(S\varphi)(\boldsymbol{x}) = \int_\Gamma G(\boldsymbol{x},\boldsymbol{y})\varphi(\boldsymbol{y})\mathrm{d}s(\boldsymbol{y}) \qquad \text{and} \qquad (K\varphi)(\boldsymbol{x}) = \int_\Gamma \frac{\partial G(\boldsymbol{x},\boldsymbol{y})}{\partial \boldsymbol{n}(\boldsymbol{y})}\varphi(\boldsymbol{y})\mathrm{d}s(\boldsymbol{y}), \quad \boldsymbol{x} \in \Gamma$$

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

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

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Can we numerically solve this BIE?

Boundary Element Method (BEM)

Suppose we wish to solve:

$$\varphi(\boldsymbol{x}) + \int_\Gamma L(\boldsymbol{x},\boldsymbol{y})\varphi(\boldsymbol{y})\,\mathrm{d}s(\boldsymbol{y}) = f(\boldsymbol{x}), \quad \boldsymbol{x} \in \Gamma,$$

where $\quad L(\boldsymbol{x},\boldsymbol{y}) := 2\left\{\dfrac{\partial G(\boldsymbol{x},\boldsymbol{y})}{\partial n(\boldsymbol{y})} - i\eta G(\boldsymbol{x},\boldsymbol{y})\right\} \quad$ and $\quad f(\boldsymbol{x}) := -2u^{\mathrm{inc}}(\boldsymbol{x})$

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

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

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

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

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double surface integral with a singular kernel!

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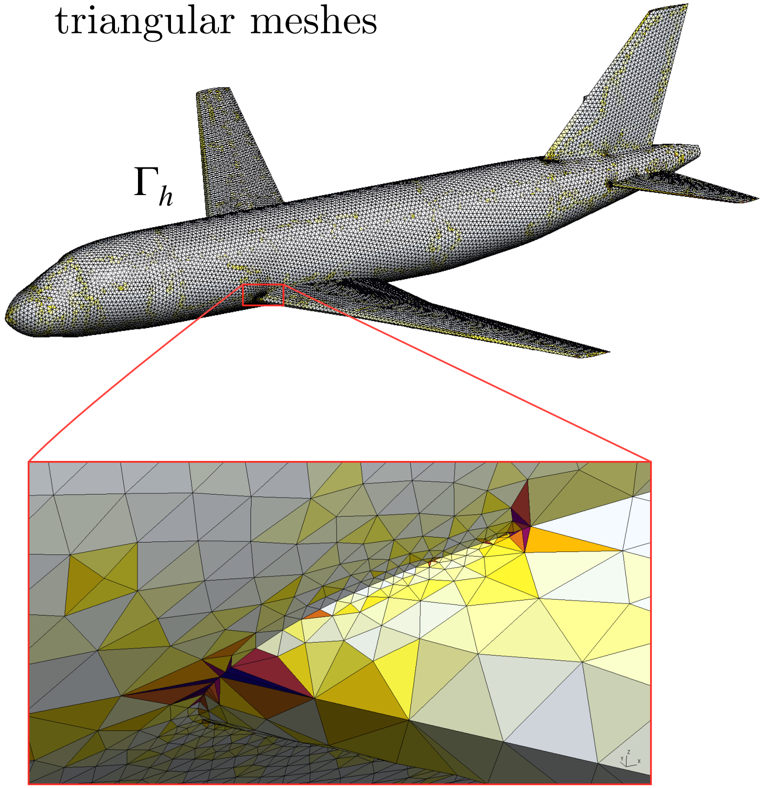
In the BEM, surfaces are most commonly represented by triangular meshes



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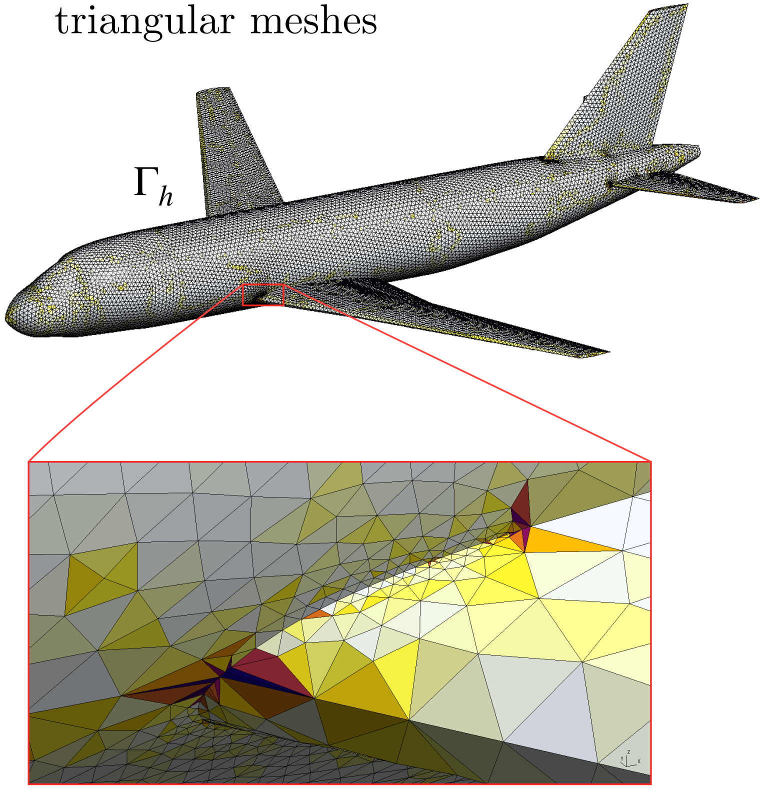

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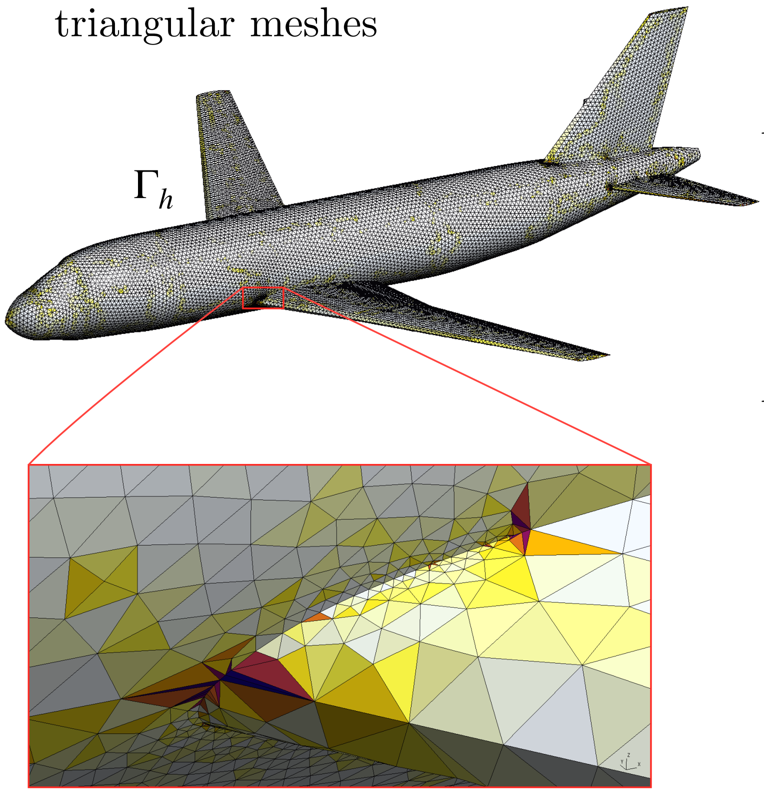

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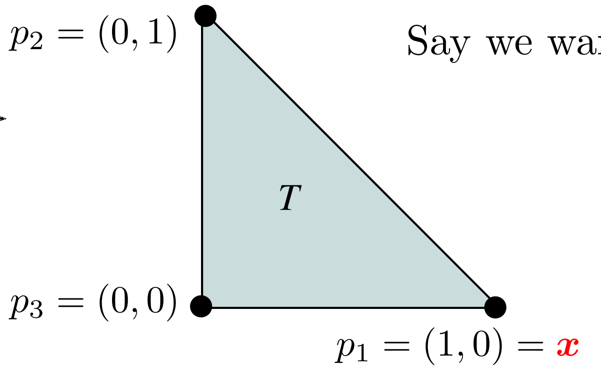

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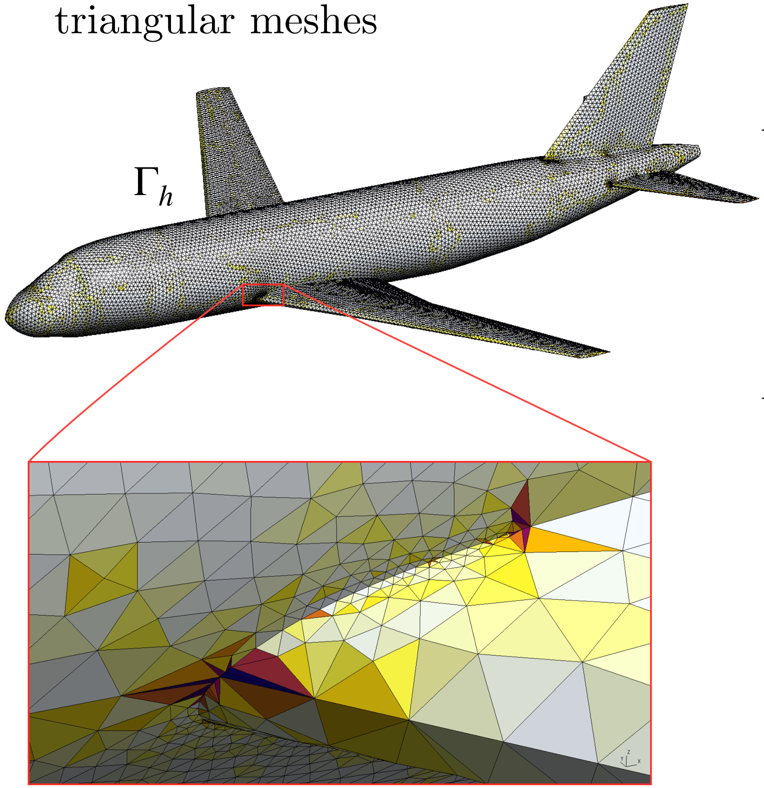

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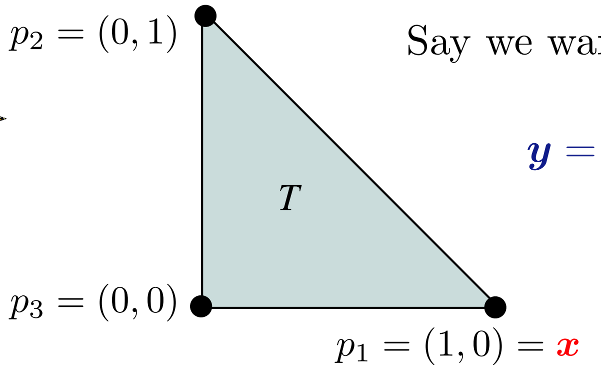

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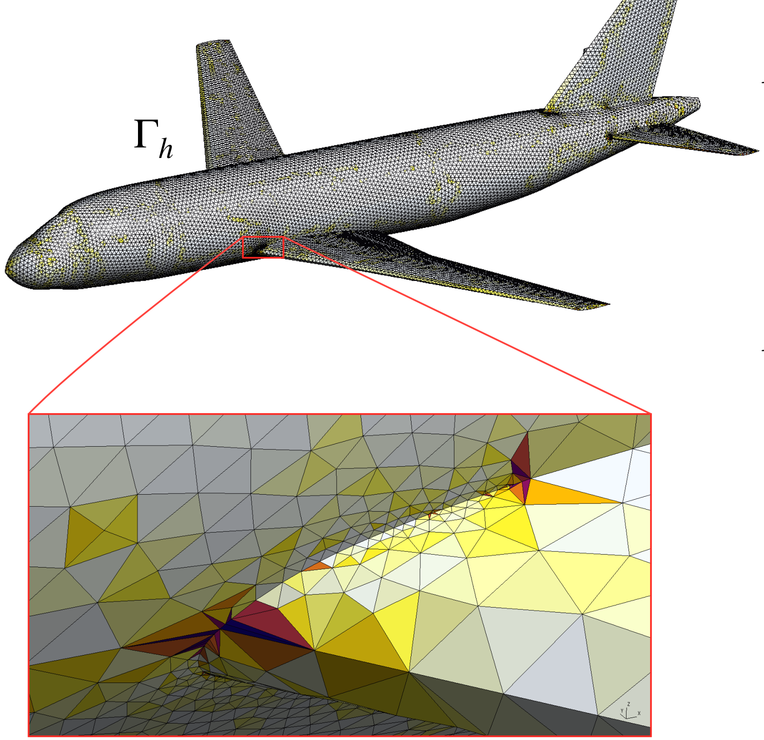

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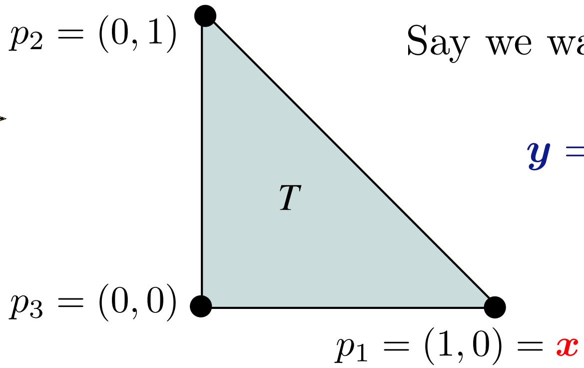

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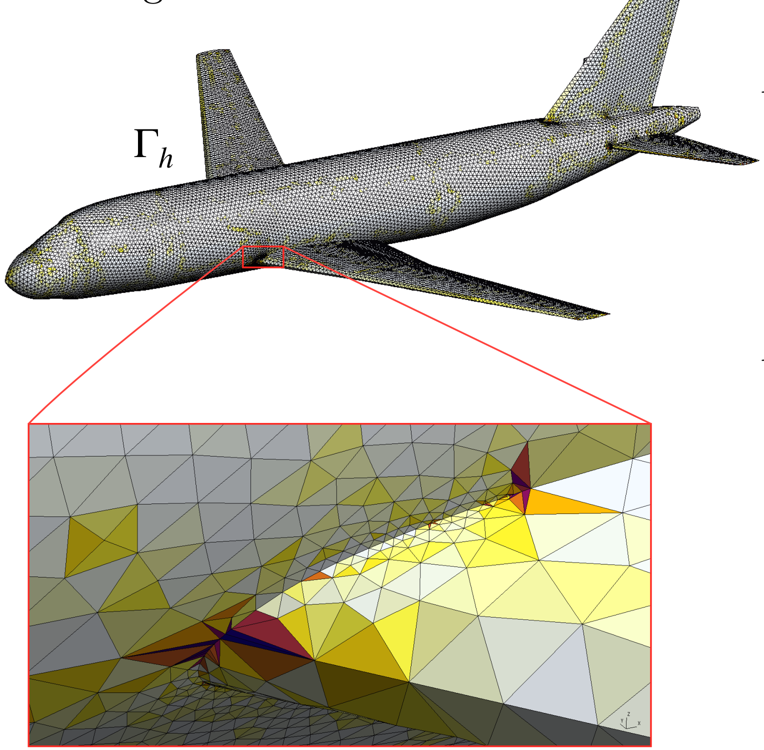

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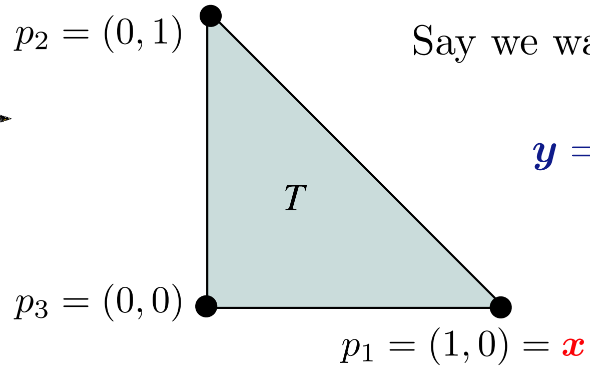

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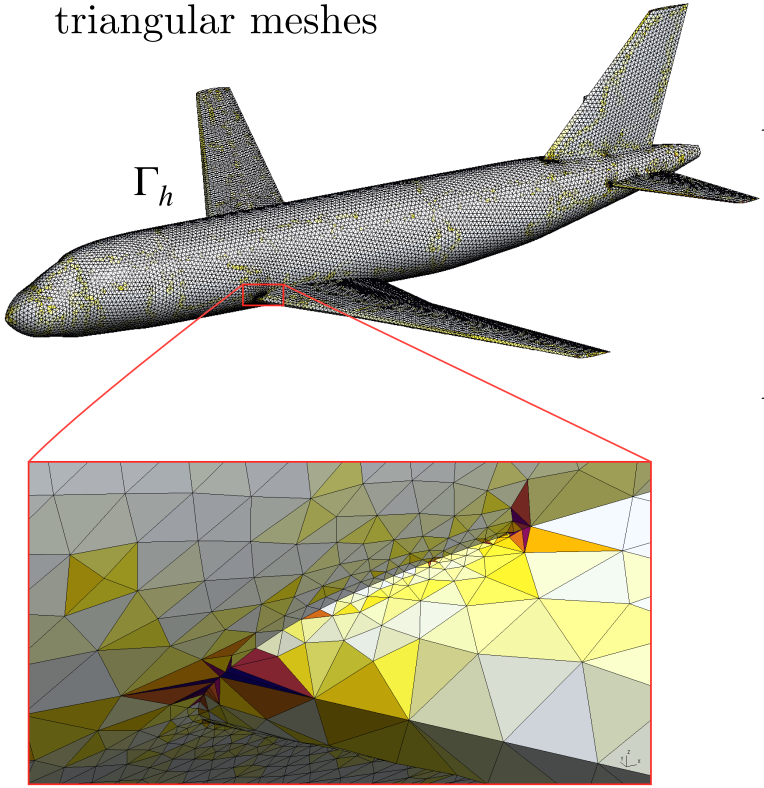

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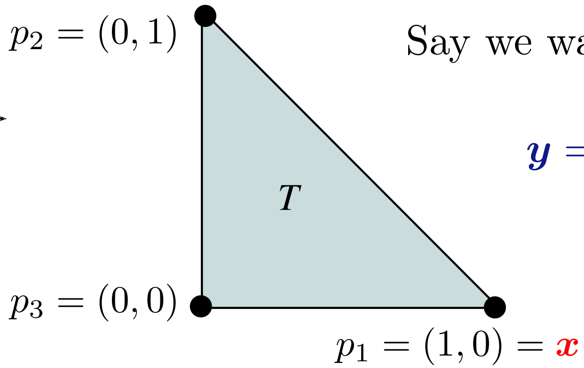

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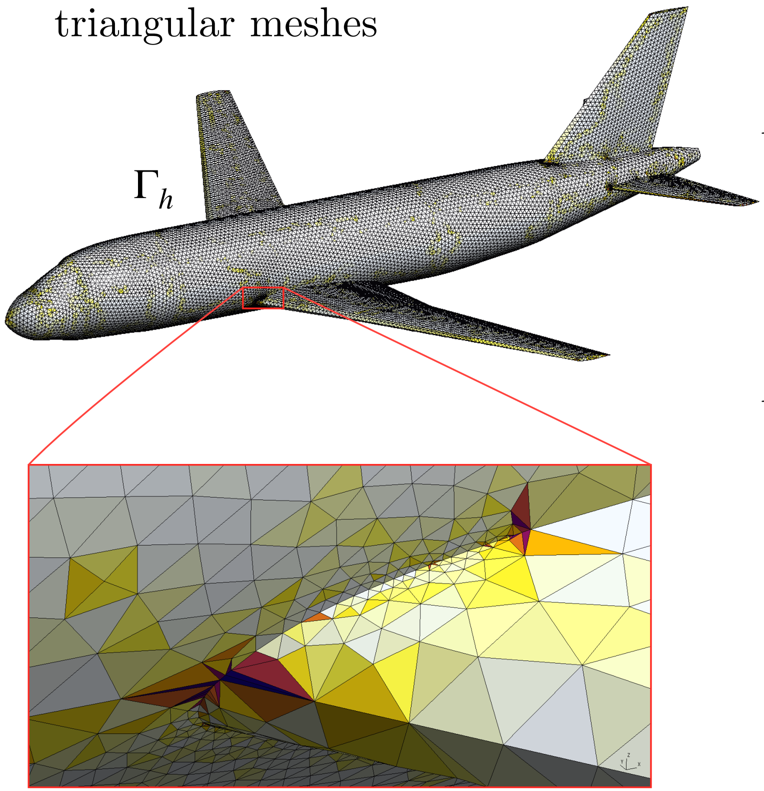
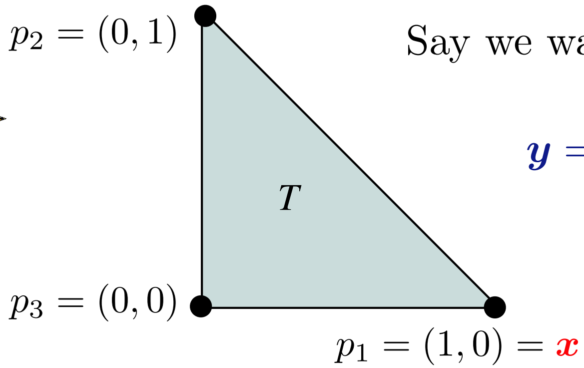


To compute $\mathsf{A} \in \mathbb{C}^{N\times N}$, it is necessary to evaluate weakly singular kernel integrals over triangles

The Duffy transformation:



Say we want to evalute: $I := \displaystyle\int_T \frac{\mathrm{d}s(\boldsymbol{y})}{|\boldsymbol{x} - \boldsymbol{y}|}$

$\boldsymbol{y} = (u,v), 0 \le u, v \le 1, u + v \le 1$

$$I = \int_0^1 \int_0^{1-u} \frac{\mathrm{d}v\,\mathrm{d}u}{\sqrt{(1-u)^2 + v^2}}$$

Change of variables $u = \xi,\ v = (1-\xi)\,\eta,$ with $\xi, \eta \in [0,1]$.

$$I = \int_0^1 \int_0^1 \frac{J(\xi,\eta)}{(1-\xi)\sqrt{1+\eta^2}}\,\mathrm{d}\xi\,\mathrm{d}\eta = \int_0^1 \int_0^1 \frac{\mathrm{d}\xi\,\mathrm{d}\eta}{\sqrt{1+\eta^2}}$$

since $\quad J(\xi,\eta) = \left| \det \left[\begin{array}{ccc} 1 & 0 & \\ -\eta & 1 & -\xi \end{array} \right] \right| = 1 - \xi$

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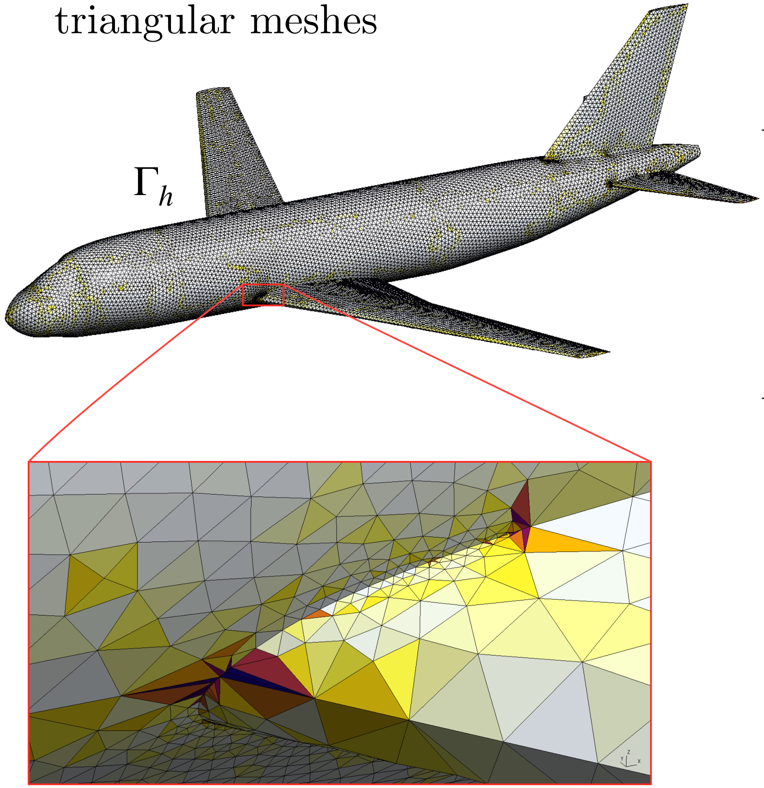

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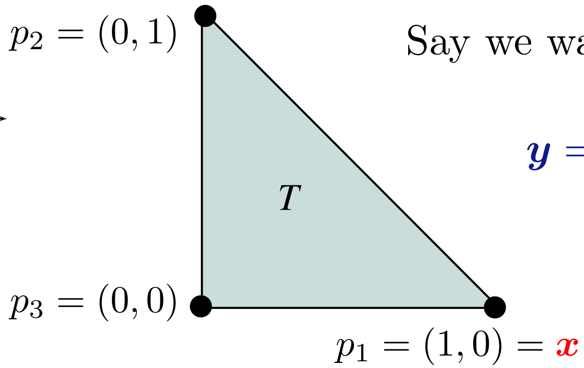

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since $\quad J(\xi,\eta) = \left|\det\begin{bmatrix} 1 & 0 \\ -\eta & 1-\xi \end{bmatrix}\right| = 1-\xi$ **smooth integrand!**

Nyström Method

Suppose we wish to solve:

$$\varphi(\boldsymbol{x}) + \int_\Gamma L(\boldsymbol{x},\boldsymbol{y})\varphi(\boldsymbol{y})\,\mathrm{d}s(\boldsymbol{y}) = f(\boldsymbol{x}), \quad \boldsymbol{x} \in \Gamma,$$

where $\quad L(\boldsymbol{x},\boldsymbol{y}) := 2\left\{\dfrac{\partial G(\boldsymbol{x},\boldsymbol{y})}{\partial n(\boldsymbol{y})} - i\eta G(\boldsymbol{x},\boldsymbol{y})\right\}\quad$ and $\quad f(\boldsymbol{x}) := -2u^{\mathrm{inc}}(\boldsymbol{x})$

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

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

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

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

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

where $\varphi_j = \widetilde{\varphi}(\mathsf{x}(t_j))$, 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:

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

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

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

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Nyström Method: Surface Representation

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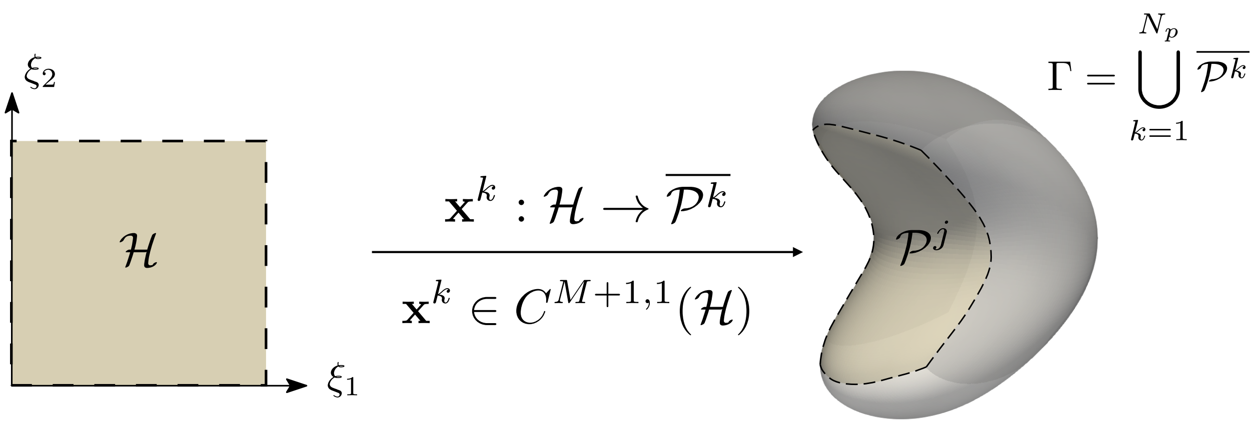
- Parametrizing the surface via disjoint smooth coordinate charts (patches):



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

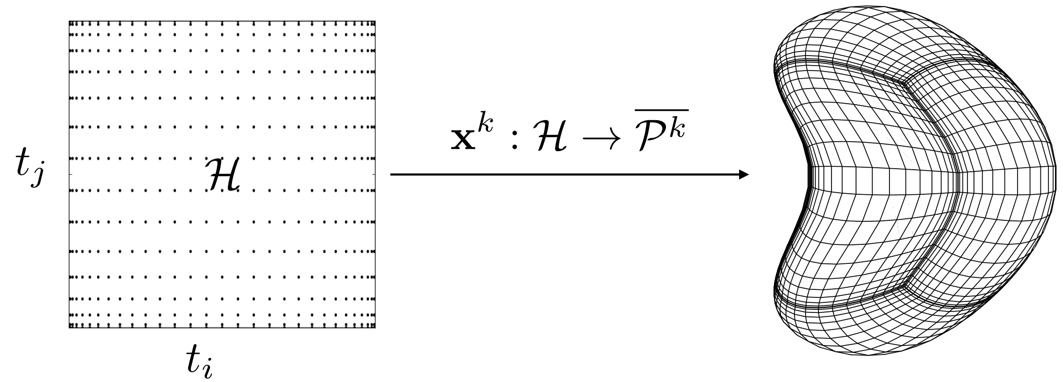
Nyström Method: High-Order Quadratures

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

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

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

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



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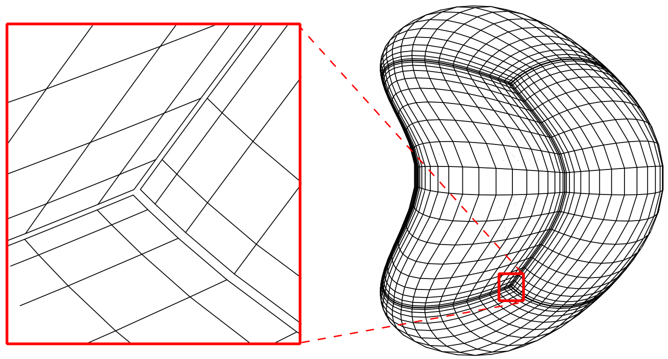
no quadrature nodes lie on the edges of the patch



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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:

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

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

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

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

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- The matrix $\mathsf{E} + \mathsf{A}$ is **dense** (again, unlike in finite element or finite difference methods).
- 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 $\mathsf{E} + \mathsf{A}$ may become too large to fit in memory!

GMRES (Generalized Minimal Residual Method)

- Iterative solver for linear systems $\mathsf{M}\mathbf{x} = \mathbf{b}$, particularly suitable for **non-symmetric matrices**.

- Constructs approximations $\mathbf{x}_m$ by minimizing the residual $\|\mathbf{b} - \mathsf{M}\mathbf{x}_m\|$ over the Krylov subspace
$$\mathcal{K}_m(\mathsf{M}, \mathbf{r}_0) = \mathrm{span}\{\mathbf{r}_0, \mathsf{M}\mathbf{r}_0, \ldots, \mathsf{M}^{m-1}\mathbf{r}_0\}.$$
Only the action of M as a linear mapping (i.e., matrix-vector products) is required, rather than explicit access to all entries of 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.

- Convergence depends on the spectrum of M; **clustering of eigenvalues away from the origin in the complex plane generally leads to faster convergence.**

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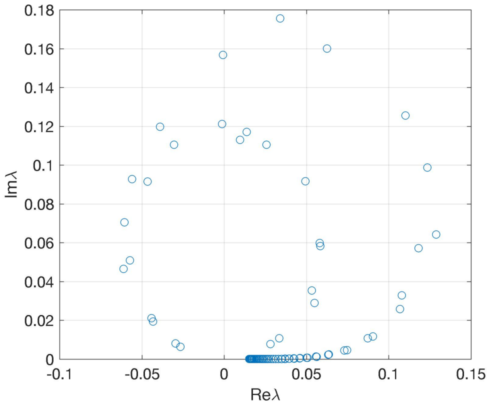
... in our case

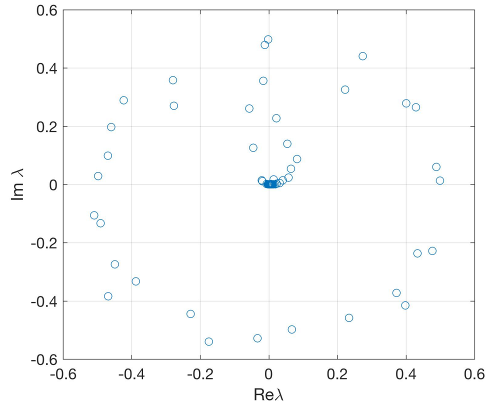
Linear System Solution and Fast BIE Methods

- 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 discretized operator K



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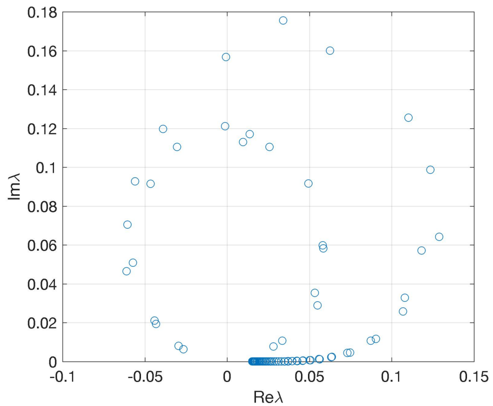

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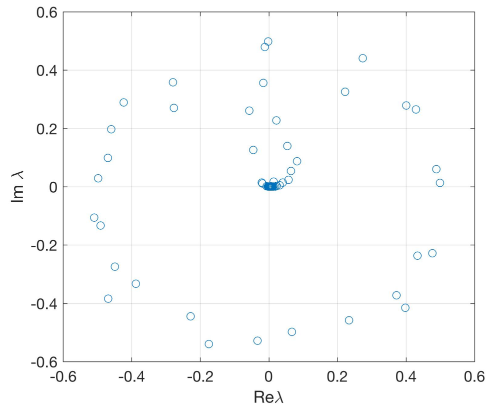

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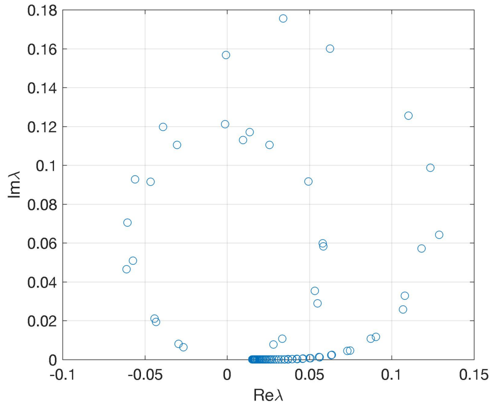

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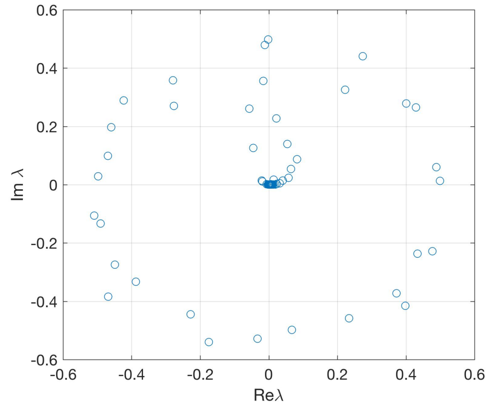

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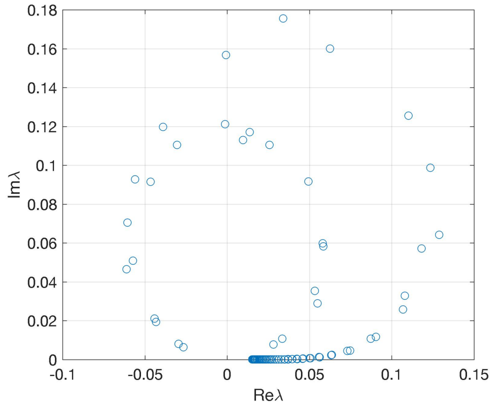

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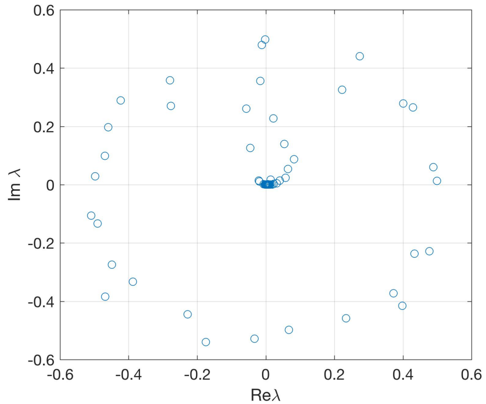

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$$(\mathsf{E} + \mathsf{A})\mathbf{x} = \mathbf{b}$$

from $O(N^3)$ (LU) to $O(N^2)$, i.e., $O(1)$ **matrix-vector products per iteration.**

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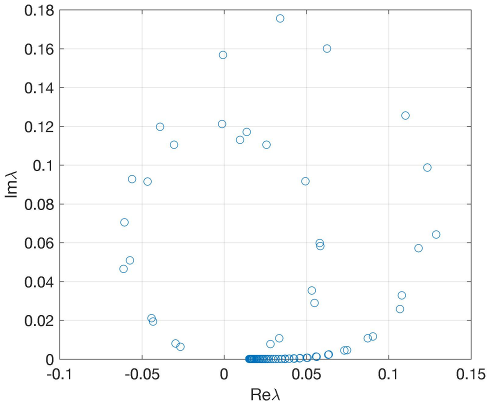

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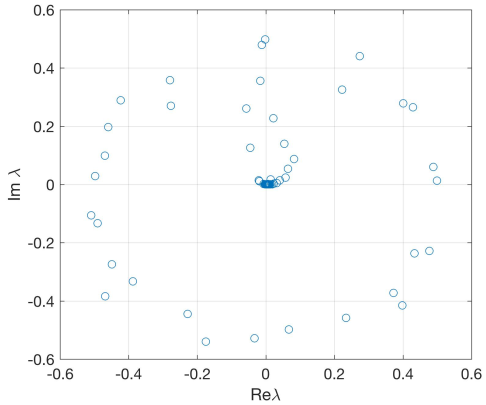

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can we do even better?

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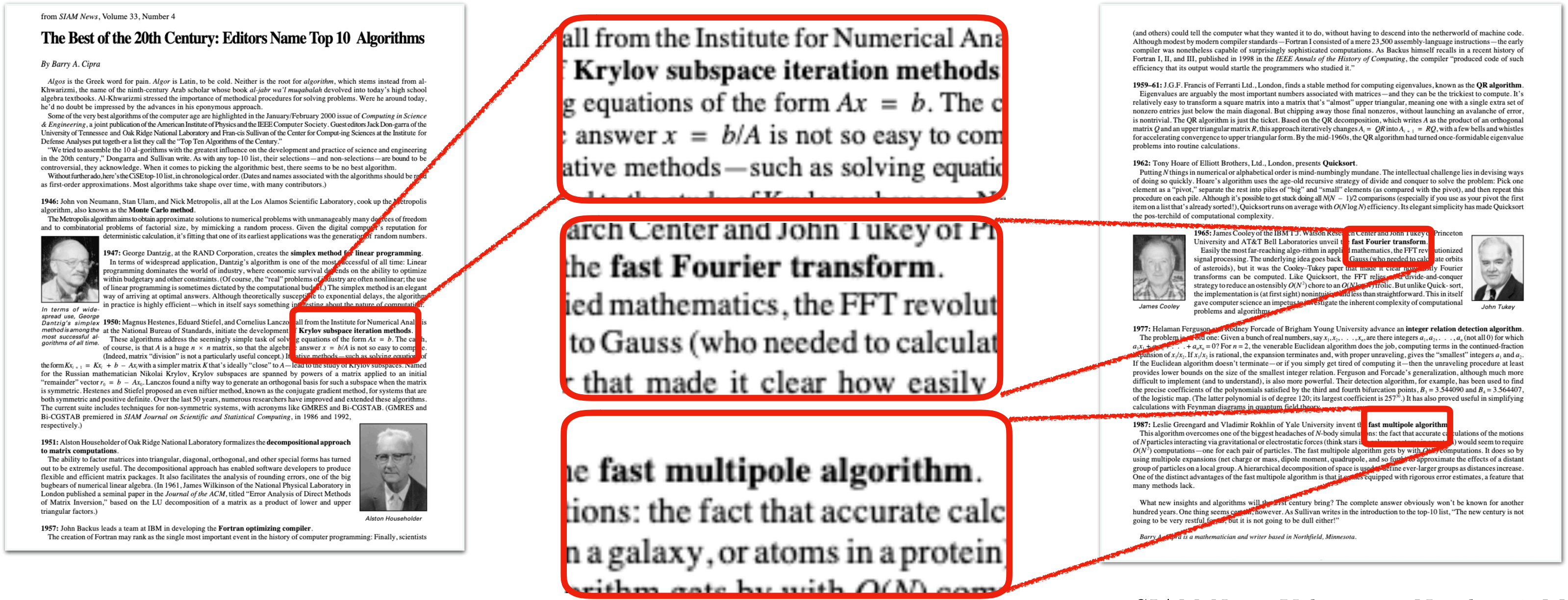
Linear System Solution and Fast BIE Methods

- 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.

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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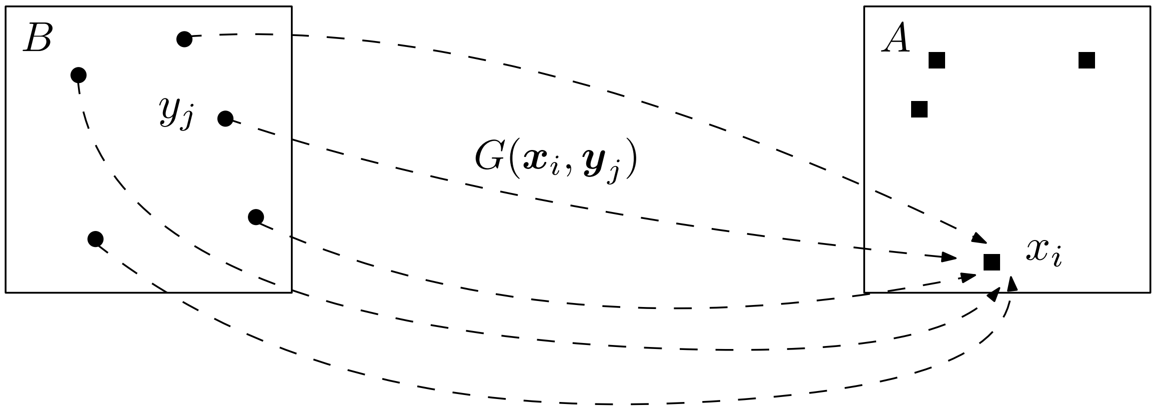
Ideas Behind the Fast Multipole Method (FMM)

Point sources $\{\boldsymbol{y}_j, q_j\}_{j=1}^{N_B}$. Target points $\{\boldsymbol{x}_i\}_{i=1}^{N_A}$.



Problem: Evaluate the potentials

$$u_i = \sum_j G\left(\boldsymbol{x}_i, \boldsymbol{y}_j\right) q_j, \quad i = 1, \ldots, N_A$$

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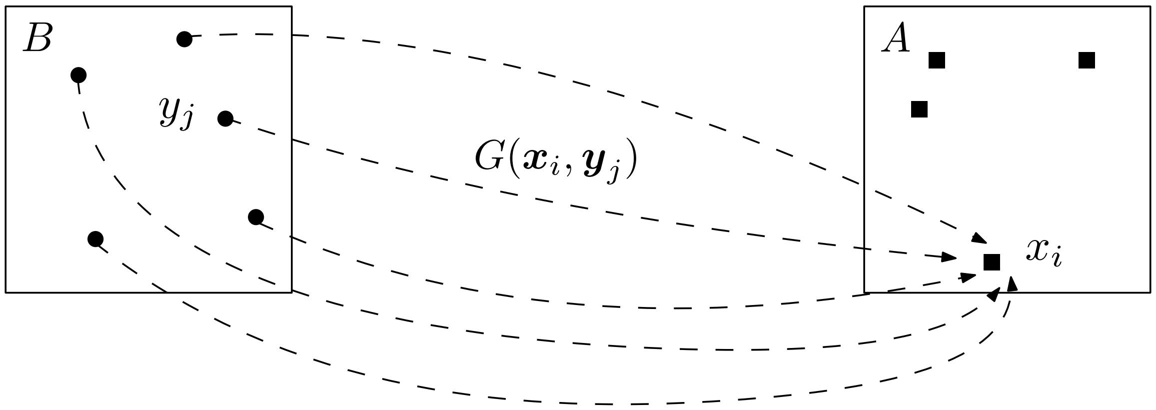
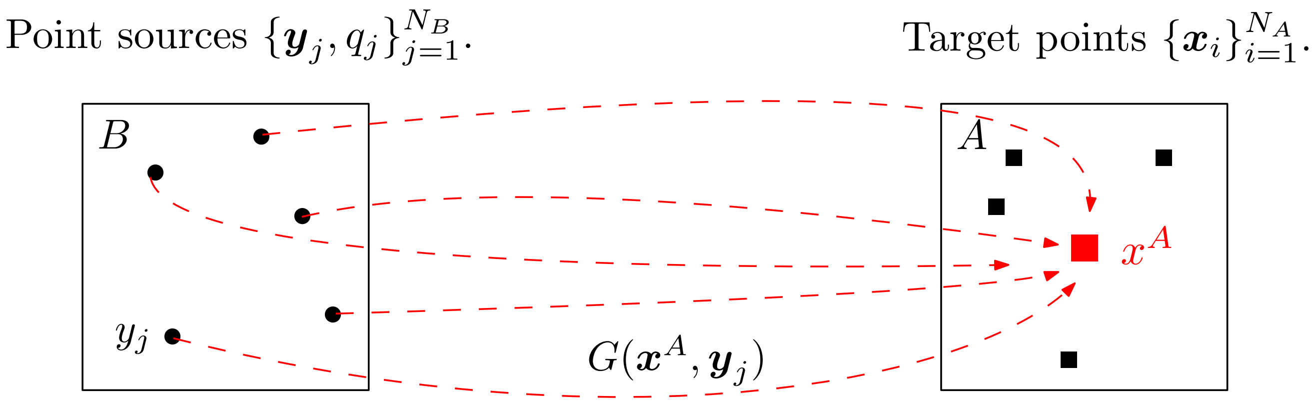


Problem: Evaluate the potentials

$$u_i = \sum_j G\left(\boldsymbol{x}_i, \boldsymbol{y}_j\right) q_j, \quad i = 1, \ldots, N_A$$

Computational cost: $O\left(N_A N_B\right)$

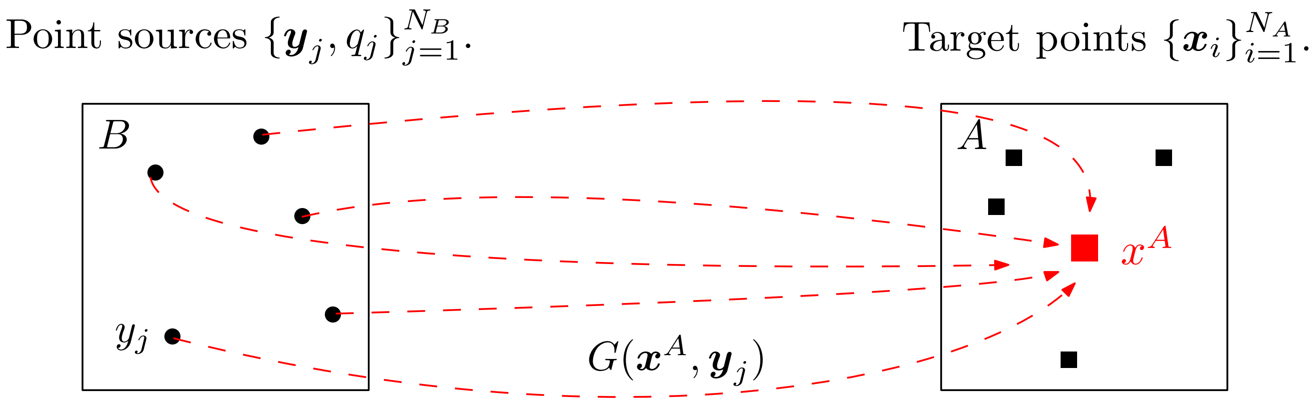
FMM: Via Interpolation



- Evaluate potentials at a small set of convenient locations

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

FMM: Via Interpolation



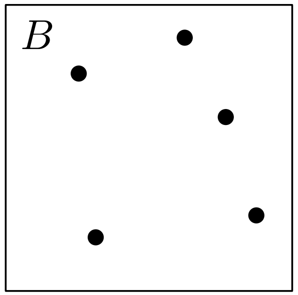
- Evaluate potentials at a small set of convenient locations

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

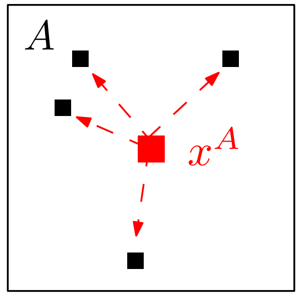
Computational cost: $O(N_B)$

FMM: Via Interpolation

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



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



- Evaluate potentials at a small set of convenient locations

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

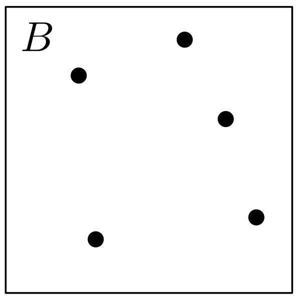
Computational cost: $O(N_B)$

- Approximate the sought potentials at the target points using interpolation

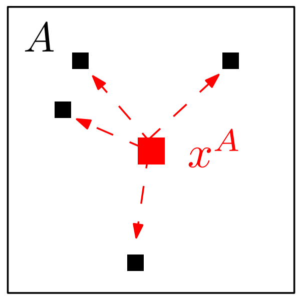
$$u_i = \sum_j G(\boldsymbol{x}^A, \boldsymbol{y}_j) q_j, \quad i = 1, \ldots, N_A$$

FMM: Via Interpolation

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



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



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Computational cost: $O(N_B)$

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

Computational cost: $O(N_A)$

FMM: Via Interpolation

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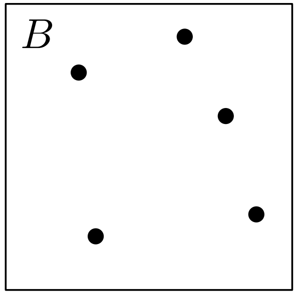

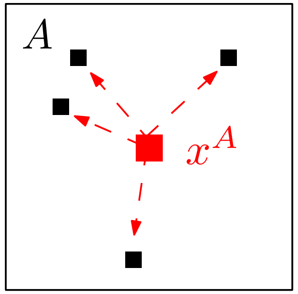

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$$\sum_j G(\boldsymbol{x}^A, \boldsymbol{y}_j) q_j$$

Computational cost: $O(N_B)$

- Approximate the sought potentials at the target points using interpolation

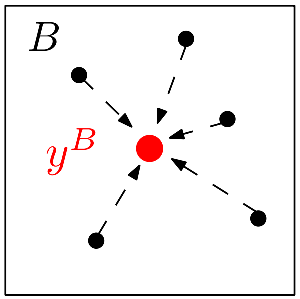
$$u_i = \sum_j G(\boldsymbol{x}^A, \boldsymbol{y}_j) q_j, \quad i = 1, \ldots, N_A$$

Computational cost: $O(N_A)$

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

FMM: Via Projection

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



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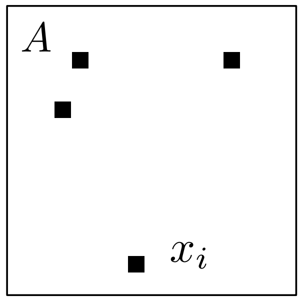
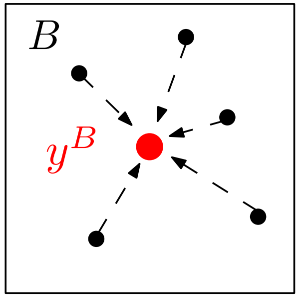


- Project "charge" strengths onto a small set of representative point sources

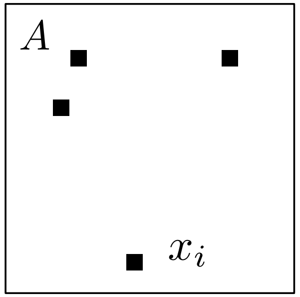
$$q^B = \sum_j q_j$$

FMM: Via Projection

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



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

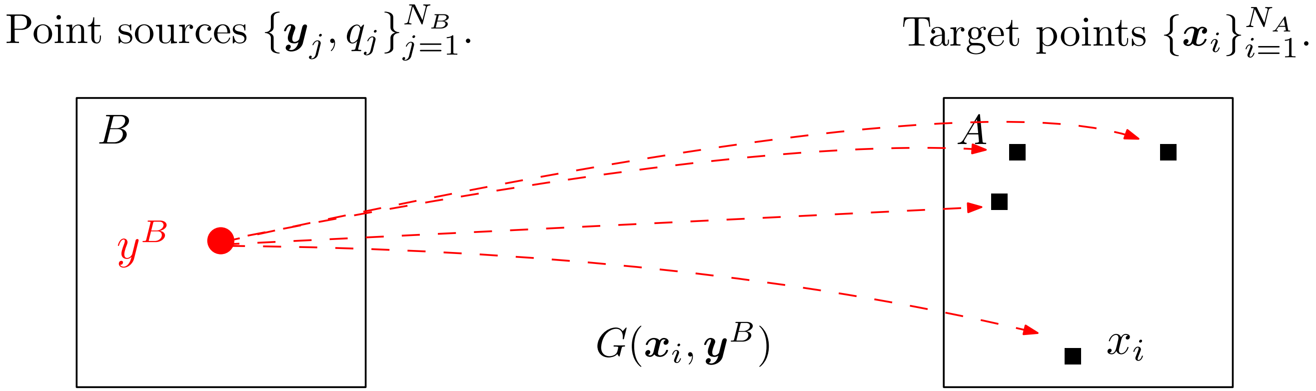


- Project "charge" strengths onto a small set of representative point sources

$$q^B = \sum_j q_j$$

Computational cost: $O(N_B)$

FMM: Projecting



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

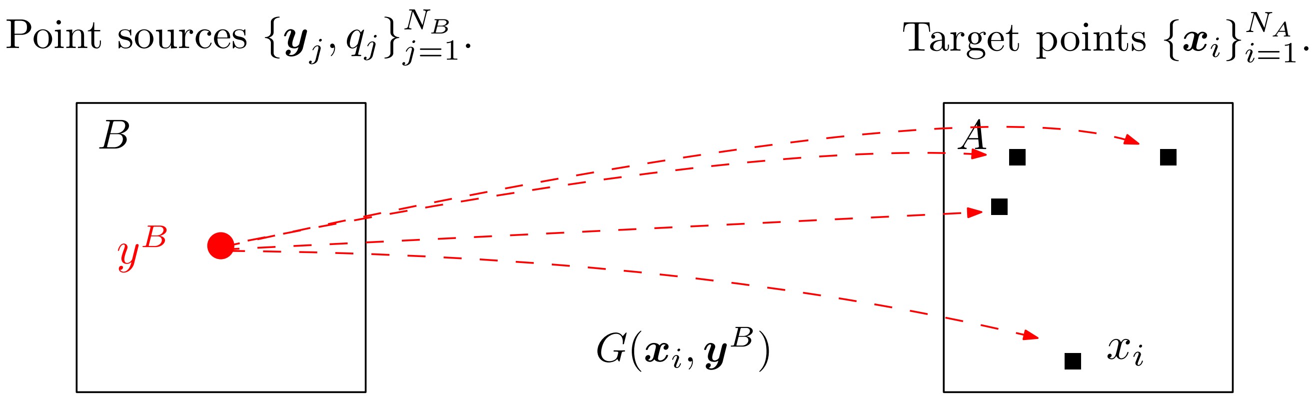
$$q^B = \sum_j q_j$$

Computational cost: $O\left(N_B\right)$

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

$$u_i = G\left(\boldsymbol{x}_i, \boldsymbol{y}^B\right) q^B, \quad i = 1, \ldots, N_A$$

FMM: Projecting



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

$$q^B = \sum_j q_j \qquad \textbf{Computational cost: } O(N_B)$$

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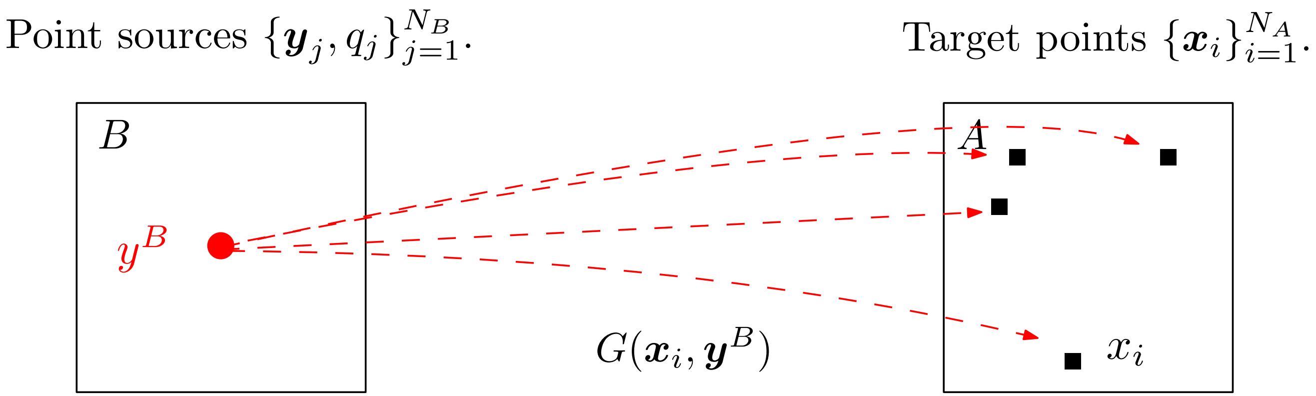
FMM: Projecting



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

$$q^B = \sum_j q_j$$

Computational cost: $O\left(N_B\right)$

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

$$u_i = G\left(\boldsymbol{x}_i, \boldsymbol{y}^B\right) q^B, \quad i = 1, \ldots, N_A$$

Computational cost: $O\left(N_A\right)$

Total computational cost: $O\left(N_A + N_B\right)$

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Thank you for your attention