

Boundary integral based neural networks to learn solutions of elliptic PDEs

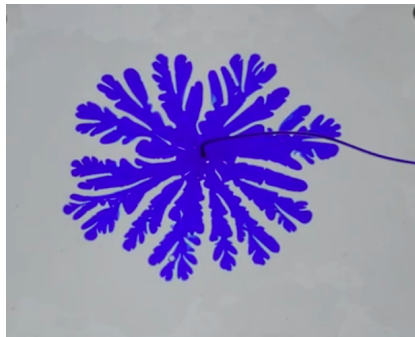
Pawan Negi
pnegi@iit.edu

Applied Mathematics Department, Illinois Institute of Technology

Wednesday, November 20, 2024

Moving interface problem

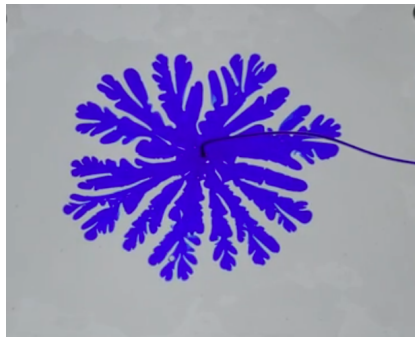
- Saffman-Taylor instability $\rightarrow$ Viscous fingering



Source: www.youtube.com/watch?v=9F1sy0sc_cg

Moving interface problem

- Saffman-Taylor instability → Viscous fingering
 - Crude oil extraction
 - Tumor growth
 - Ice crystal formation
(Mullins-Sekerka Instability)

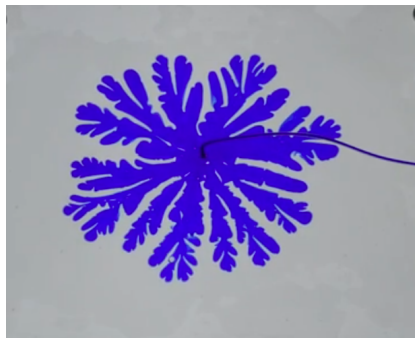


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Moving interface problem

- Saffman-Taylor instability $\rightarrow$ Viscous fingering
 - Crude oil extraction
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(Mullins-Sekerka Instability)
- Both region satisfy elliptic PDE of the form

$$-\left(\nabla \cdot (\sigma(\mathbf{x})\nabla) + \kappa^2(\mathbf{x})\right) u(\mathbf{x}) = f(\mathbf{x})$$



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Target problem

- Solution of variable coefficient elliptic PDEs

$$-\left(\nabla \cdot (\sigma(\mathbf{x})\nabla) + \kappa^2(\mathbf{x})\right) u(\mathbf{x}) = \mathcal{L}_{\mathbf{x}} u(\mathbf{x}) = f(\mathbf{x})$$

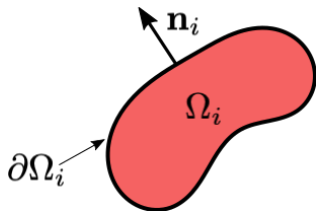
$x \in \Omega$, $\kappa, \sigma \in C^2$ are variable coefficients

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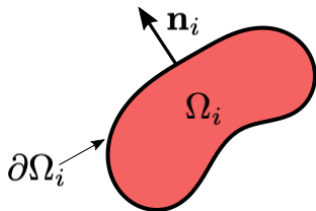
Interior problem

Target problem

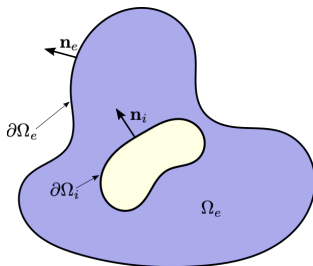
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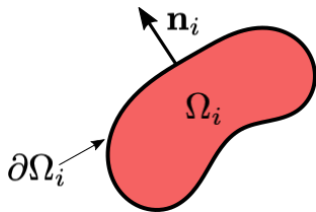
Exterior problem

Target problem

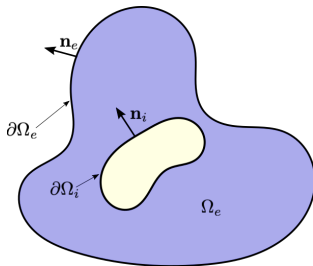
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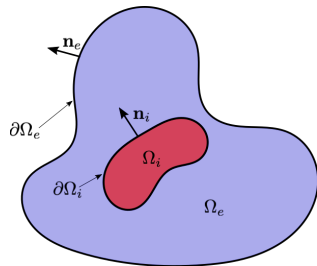
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Interior problem



Exterior problem



Interface problem

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- Learn fundamental solution $\tilde{G}(\mathbf{x}, \mathbf{y})$ for an elliptic PDE

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- Use learned fundamental solution to solve interior, exterior and interface problems

Generalized boundary integral equation

- Solution in terms of boundary integrals

$$u(\mathbf{x}) = \int_{\Omega} f(\mathbf{y}) \tilde{G}(\mathbf{x}, \mathbf{y}) dy - \int_{\partial\Omega} \sigma u(\mathbf{y}) \frac{\partial \tilde{G}}{\partial \mathbf{n}}(\mathbf{x}, \mathbf{y}) dS(y) + \int_{\partial\Omega} \sigma \nabla_{\mathbf{n}} u(\mathbf{y}) \tilde{G}(\mathbf{x}, \mathbf{y}) dS(y)$$

where

$$f(\mathbf{x}) = - \left(\nabla \cdot (\sigma \nabla) + \kappa^2 \right) u(\mathbf{x}) = \mathcal{L}_{\mathbf{x}} u(\mathbf{x})$$

where $\kappa \in C^2$ is variable “reaction” coefficient

Boundary integral (BI) $\rightarrow$ Neural network

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$$\begin{aligned} u(\mathbf{x}; \Theta, \theta) = & \sum_{i \in N_i} a_i f(\mathbf{x}_i) \text{KNN}_{\tilde{G}}(\|\mathbf{x} - \mathbf{x}_i\|; \Theta) \\ & - \sum_{i \in N_b} d_i u(\mathbf{x}_i^b; \theta) \mathbf{n}_i \cdot \nabla \text{KNN}_{\tilde{G}}(\|\mathbf{x} - \mathbf{x}_i\|; \Theta) \\ & + \sum_{i \in N_b} d_i \mathbf{n}_i \cdot \nabla u(\mathbf{x}_i^b; \theta) \text{KNN}_{\tilde{G}}(\|\mathbf{x} - \mathbf{x}_i\|; \Theta) \end{aligned}$$

Results: Helmholtz equation

$$\nabla^2 u(\mathbf{x}) + k^2 u(\mathbf{x}) = 0$$

describes the wave propagation in areas
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$k = 20$: the wave number

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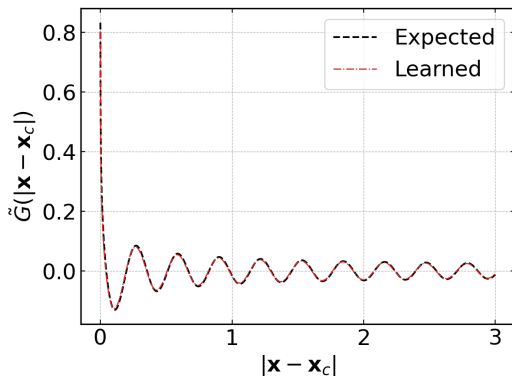
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Fundamental solution for Helmholtz equation:

$$\tilde{G}_o(r) = -\frac{1}{4} Y_0(kr)$$

Y_0 : Bessel function of the second kind of order 0



Results: variable coefficient equation

$$\nabla \cdot (\sigma \nabla u) + \kappa^2 u = f$$

$$\sigma(x, y) = 1.5 + 0.5(\sin(x) + \cos(y))$$

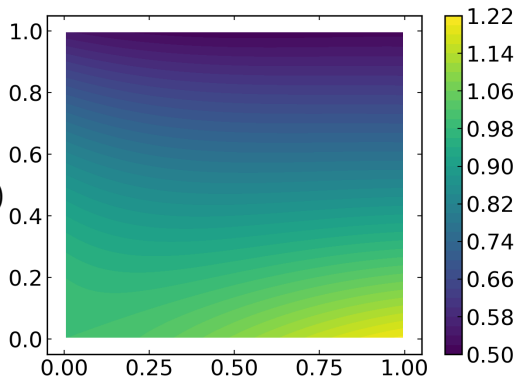
$$\kappa^2(x, y) = 20 + \exp(0.8x + 0.6y)$$

Use a test function:

$$u_o(x, y) = \exp(-x) \cos(y) + \exp(-y) \sin(x)$$

Relative L_2 error:

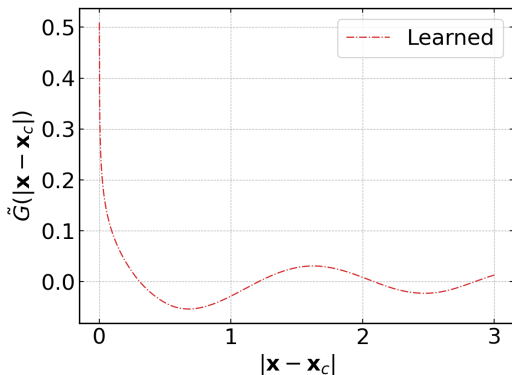
$$L_2 = \frac{\sqrt{\sum_j (u(\mathbf{x}_j) - u_o(\mathbf{x}_j))^2}}{\sqrt{\sum_j u_o(\mathbf{x}_j)^2}}$$



Results: variable coefficient equation (contd.)

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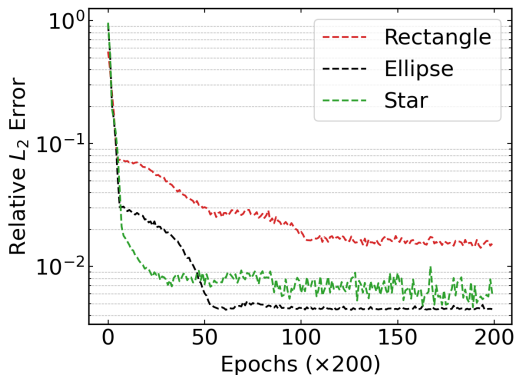
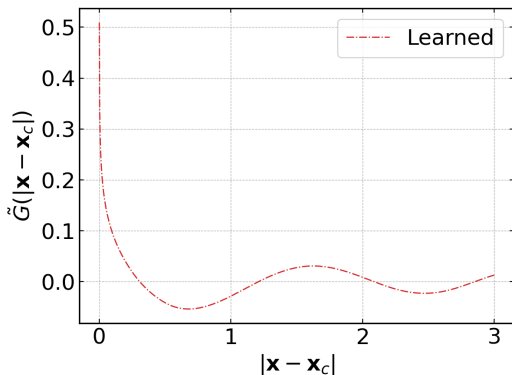
$$\sigma(x, y) = 1.5 + 0.5(\sin(x) + \cos(y)) \text{ and } \kappa^2(x, y) = 20 + \exp(0.8x + 0.6y)$$



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- Extend this model to 3D elliptic PDEs

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- Allow mixed boundary condition: part Dirichlet and part Neumann

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- Allow mixed boundary condition: part Dirichlet and part Neumann
- Write unit tests for existing code base

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- Working understanding of neural networks

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- Comfortable with pytorch and python
- Comfortable working with large code base

Question?

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