# Easy-to-implement *hp*-adaptivity for non-elliptic goal-oriented problems


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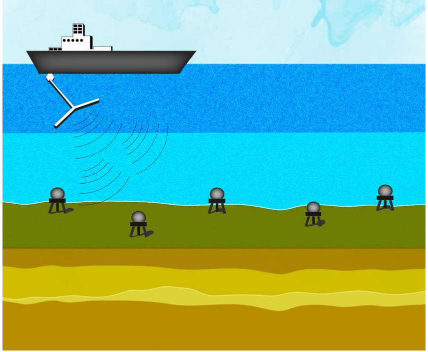
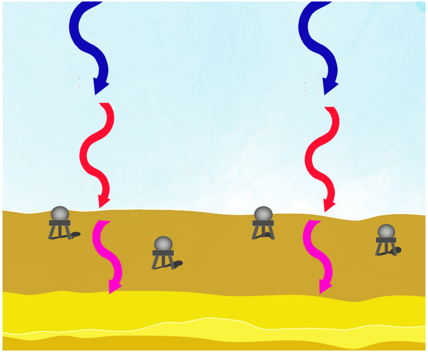
# Electromagnetic (EM) Applications



(a) CSEM (artificial source)

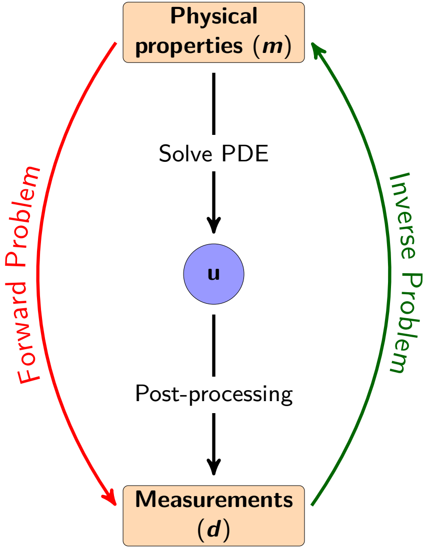


(b) MT (natural source)

## Objective

**Objective**: To obtain the **conductivity/resistivity** distribution of the Earth's subsurface.

# Overview of Forward and Inverse Problems




**Definitions**

$\mathcal{F}$ : Forward Operator
$\boldsymbol{m} \mapsto \boldsymbol{d}$

$\mathcal{I}$ : Inverse Operator
$\boldsymbol{d} \mapsto \boldsymbol{m}$

$\mathcal{I}_\phi$ : Neural Network approximation of $\mathcal{I}$

# Generation of Massive Databases

## Objective

Building the **Inverse Operator** (not just evaluating it).

## Loss Function and Training

Find $\mathcal{I}_{\phi^*}$ such that

$$\phi^* = \arg\min_{\phi \in \boldsymbol{\Phi}} \sum \|(\mathcal{F} \circ \mathcal{I}_\phi)(\boldsymbol{d}_i) - \boldsymbol{d}_i\|^2$$

where evaluating $\mathcal{F}$ is expensive!

## Difficulties

1. We need a Forward Solver $\mathcal{F}$ for any parameterization (model).
2. A huge number of evaluations needed to train the DNN.

## Solution

1. Approximate the Forward Operator with a Neural Network.

# Traditional Numerical Methods in Geophysics

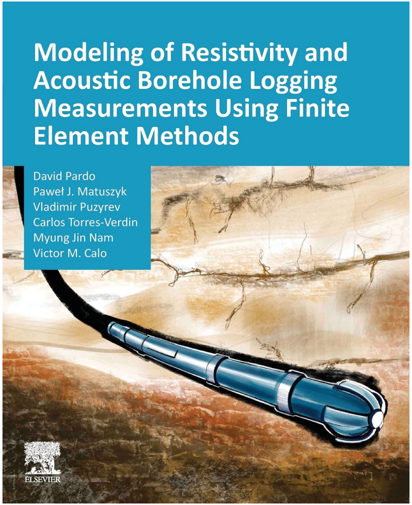



**Figure:** Published in 2021

## Numerical Methods

- Finite Element method
- Finite Difference method
- Finite Volumes method
- Integral methods
- Semi-analytical methods

# Outline

1. Goal-Oriented *hp*-adaptivity for non-parametric PDEs
   - Why *hp*-Adaptivity?
   - Goal-Oriented coarsening strategy
   - 1D Numerical results for Goal-Oriented *h*- and *p*-adaptivity
   - 2D Numerical results for *hp*-adaptivity
   - 3D Numerical results for *hp*-adaptivity
2. Goal-Oriented *hp*-adaptivity for parametric PDEs.
   - Database generation for DL inversion
3. Main Achievements
4. Conclusions and Future Work

# Goal-Oriented *hp*-adaptivity for non-parametric PDEs

# Why *hp*-Adaptivity?

**Advantages**

- *hp*-adaptive FEM achieves exponential convergence rates
- Precise mesh refinement near singularities
- Smaller meshes with higher accuracy per number of degrees of freedom

**Limitations**

- Solution accuracy heavily mesh-dependent, requiring precise mesh design
- Increasing accuracy leads to prohibitive computational costs

# Main Ingredients

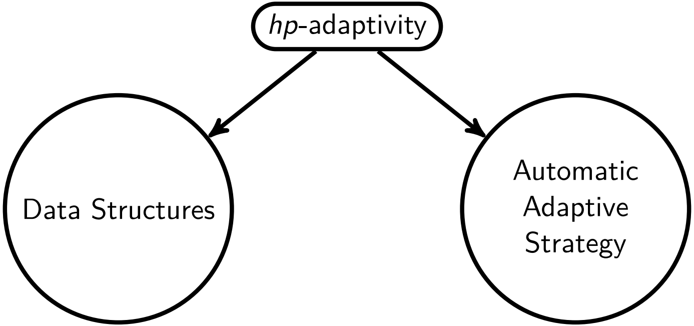
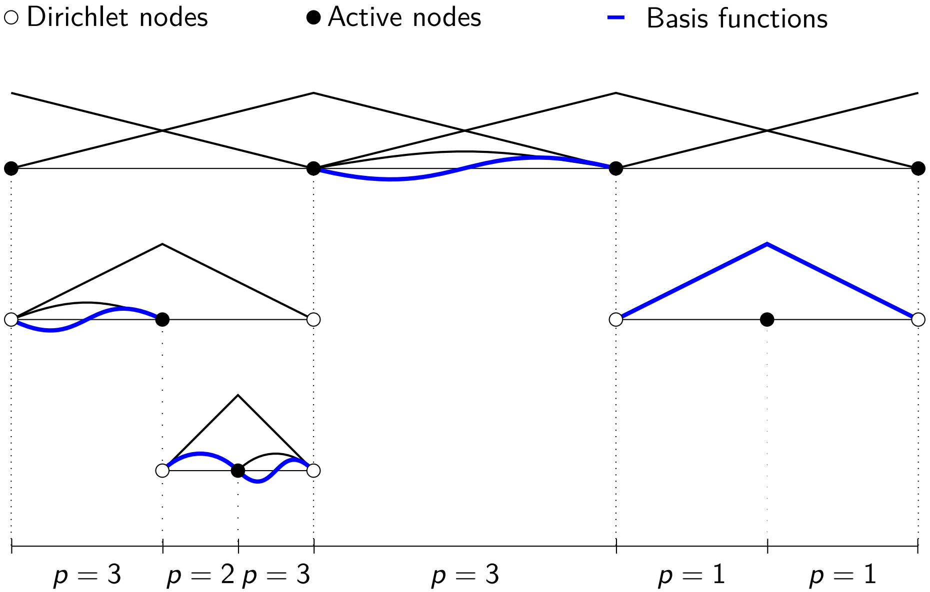



**Figure:** Main ingredients

# Multi-Level Mesh Data Structure 1D



# Multi-Level Mesh Data Structure 2D

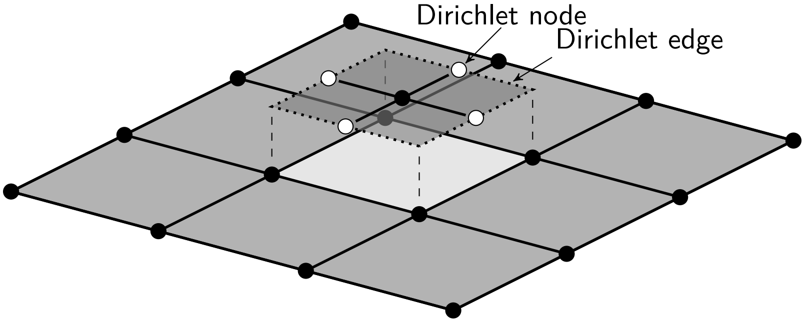
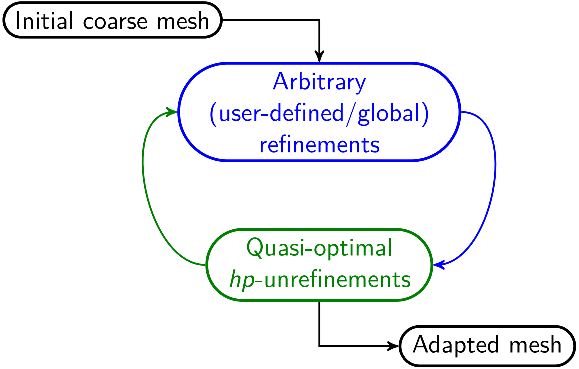



**Figure:** Multi-level 2D mesh without constraints on hanging nodes using Dirichlet nodes. The bubble basis functions are at the lowest level of each family


N. Zander, T. Bog, S. Kollmannsberger, D. Schillinger, and E. Rank
Multi-level *hp*-adaptivity: high-order mesh adaptivity without the difficulties of constraining hanging nodes
*Computational Mechanics*, 55(3):499–517, Mar 2015

# A Painless Automatic Adaptive Strategy





V. Darrigrand, D. Pardo, T. Chaumont-Frelet, I. Gómez-Revuelto, L. E. García-Castillo
A painless automatic *hp*-adaptive strategy for elliptic problems
*Finite Elements in Analysis and Design*, 2020.

F. V. Caro, V. Darrigrand, J. Alvarez-Aramberri, E. Alberdi, D. Pardo
A painless multi-level automatic goal-oriented *hp*-adaptive coarsening strategy for elliptic and non-elliptic problems
*Computer Methods in Applied Mechanics and Engineering*, 2022.

# Adaptive Mesh Refinement Algorithm

**Algorithm 1:** Adaptive process

**Input:** A given initial mesh

**Output:** A final *hp*-adapted mesh

**while** *error above tolerance* **do**

  Perform a global and uniform ($h$ or $p$) refinement;

  Execute a (quasi)-optimal *hp*-coarsening step (Algorithm 2) to the mesh;

  Update error;

**end**

# *hp*-Unrefinement Policy

**Algorithm 2:** *hp*-unrefinement policy

**Input:** A given mesh

**Output:** An *hp*-unrefined mesh

**do**

Compute the solution on the current mesh;

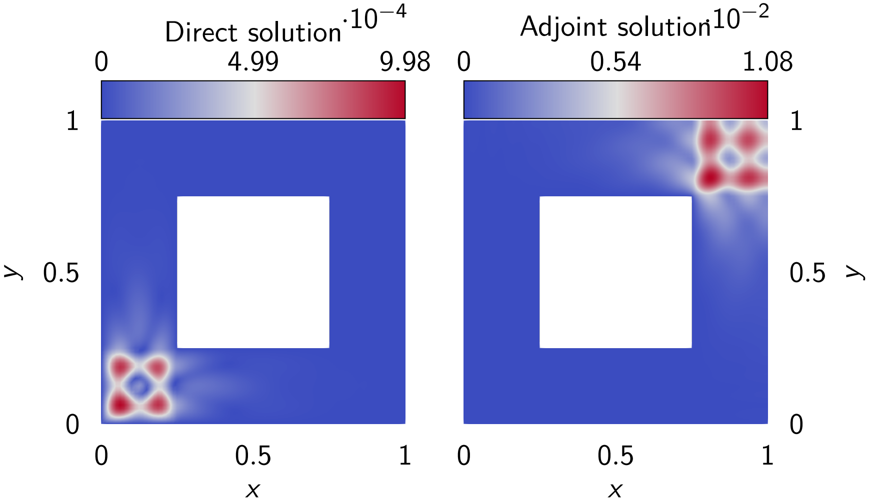
Compute the element-wise error indicators;

Unrefine the mesh by eliminating the *removable* basis functions with low error indicators;

When no contributions are below a given tolerance, exit;

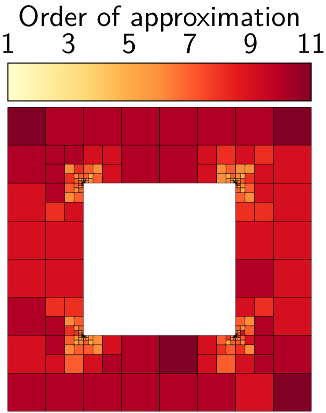
**end**;

# Illustrating the Goal-Oriented *hp*-Adaptive Strategy

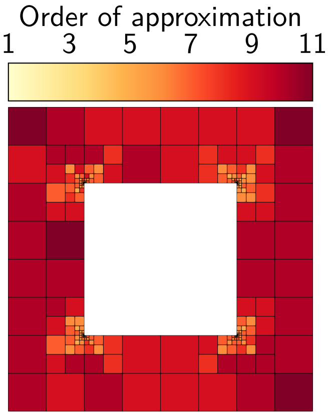



**(a)** Solution to the direct problem. **(b)** Solution to the adjoint problem.

# Illustrating the Goal-Oriented *hp*-Adaptive Strategy




**(a)** Polynomial orders $p$ in the x-direction




**(b)** Polynomial orders $p$ in the y-direction

**Figure:** Final *hp*-adapted meshes after the adaptivity

## Goal-Oriented coarsening strategy

# The Variational Formulation

## The Abstract Variational Formulation

Find $u_{\mathcal{F}} \in \mathbb{H}_{\mathcal{F}}$ such that

$$b\left(u_{\mathcal{F}}, \phi_{\mathcal{F}}\right) = f\left(\phi_{\mathcal{F}}\right), \quad \forall \phi_{\mathcal{F}} \in \mathbb{H}_{\mathcal{F}}, \tag{1}$$

with the following specifications:

- $f(\cdot)$ is a linear form,
- $b$ represents a bilinear form defined on $\mathbb{H} \times \mathbb{H}$,
- $\mathbb{H}_{\mathcal{F}} := \mathrm{span}\{\phi_1, \ldots, \phi_{n_{\mathcal{F}}}\}$ denotes the finite element space,
- $\mathcal{T}$ represents the discretization of $\mathbb{H}$ into finite elements, where $\mathbb{H}_{\mathcal{F}} \subset \mathbb{H}$,
- $\mathcal{F} = \{\phi_i\}_{i=1}^{n_{\mathcal{F}}}$ is the set of basis functions defining $\mathbb{H}_{\mathcal{F}}$,
- $n_{\mathcal{F}}$ is the dimension of $\mathbb{H}_{\mathcal{F}}$, i.e., $n_{\mathcal{F}} = \dim(\mathbb{H}_{\mathcal{F}})$,
- $u_{\mathcal{F}}$ is the Galerkin approximation of $u$ within $\mathbb{H}_{\mathcal{F}}$.

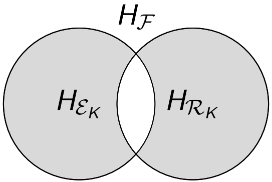
# Basis Function Decomposition

## Decomposition into Essential and Removable Basis Functions

For any element $K$, consider the following sets and spaces:

- $\mathcal{R}_K$: the set of *removable* basis functions associated to $K$ and $|\mathcal{R}_K|$ its cardinality.
- $\mathbb{H}_{\mathcal{R}_K}$: the space generated by $\mathcal{R}_K$.
- $\mathcal{E}_K := \mathcal{F} \setminus \mathcal{R}_K$: the set of *essential* basis functions.
- $\mathbb{H}_{\mathcal{E}_K}$: the space associated with $\mathcal{E}_K$.

These satisfy the following properties:



# Projection Operator

## Definition of the Projection Operator

For a given subset of basis functions $\mathcal{S} \subset \mathcal{F}$ that generates the space $\mathbb{H}_{\mathcal{S}} \subset \mathbb{H}_{\mathcal{F}}$, we define our *projection operator* $\Pi_{\mathcal{F}}^{\mathcal{S}}$: $\mathbb{H}_{\mathcal{F}} \longrightarrow \mathbb{H}_{\mathcal{S}}$ as

$$\Pi_{\mathcal{F}}^{\mathcal{S}} u_{\mathcal{F}} := \sum_{\phi_i \in \mathcal{S}} u_i \phi_i, \tag{2}$$

where we extract the coefficients of $u_{\mathcal{F}}$ corresponding to the basis functions in $\mathcal{S}$, and we set the others to zero.

Hence, any function $u_{\mathcal{F}} \in \mathbb{H}_{\mathcal{F}}$ can be decomposed as:

$$u_{\mathcal{F}} = \Pi_{\mathcal{F}}^{\mathcal{E}_K} u_{\mathcal{F}} + \Pi_{\mathcal{F}}^{\mathcal{R}_K} u_{\mathcal{F}}. \tag{3}$$

Note: For a single mesh, the solution $u_{\mathcal{E}_K}$ in $\mathcal{E}_K$ associated with Equation (3) is not computed explicitly. Instead, the projection of $u_{\mathcal{F}}$ onto $\mathcal{E}_K$ is used to approximate it.

# Error indicators in our Strategy

Let $\|\cdot\|_e$ be the *energy norm* associated with the Hilbert space $\mathbb{H}$.
**For Elliptic Problems:** The energy norm is defined from the bilinear form of the problem $b$, that is,

$$\|\cdot\|_e^2 = b\left(\cdot,\cdot\right).$$

**For Non-Elliptic Problems:** We define an alternative operator $a$, not necessarily the original bilinear form, such that

$$\left|b\left(\phi,\psi\right)\right| \leq \left|a\left(\phi,\psi\right)\right|, \forall \phi,\psi \in \mathbb{H}$$

and the energy norm is

$$\|\cdot\|_e^2 = a\left(\cdot,\cdot\right).$$

The choice of these operators might highly influence the results of the adaptive process, an essential ingredient of adaptive strategies.

# Energy-norm based Elliptic Problems

For a given element $K \in \mathcal{T}$, our goal is to quantify the energy lost in the solution when removing a subset of basis functions from the set of *removable* basis functions $\mathcal{R}_K$.

$$\|u_{\mathcal{F}} - u_{\mathcal{E}_K}\|_e^2 .$$

**Mathematical Derivation:** Analogously to Cea's lemma proof, we derive:

$$\begin{aligned}
\|u_{\mathcal{F}} - u_{\mathcal{E}_K}\|_e^2 &= b\left(u_{\mathcal{F}} - u_{\mathcal{E}_K}, u_{\mathcal{F}} - u_{\mathcal{E}_K}\right) && (4)\\
&= b\left(u_{\mathcal{F}} - u_{\mathcal{E}_K}, u_{\mathcal{F}} - \Pi_{\mathcal{F}}^{\mathcal{E}_K} u_{\mathcal{F}}\right) + b\left(u_{\mathcal{F}} - u_{\mathcal{E}_K}, \Pi_{\mathcal{F}}^{\mathcal{E}_K} u_{\mathcal{F}} - u_{\mathcal{E}_K}\right) && (5)\\
&\leq \|u_{\mathcal{F}} - u_{\mathcal{E}_K}\|_e \left\|u_{\mathcal{F}} - \Pi_{\mathcal{F}}^{\mathcal{E}_K} u_{\mathcal{F}}\right\|_e , && (6)
\end{aligned}$$

where we use the $b$-orthogonality of $u_{\mathcal{F}} - u_{\mathcal{E}_K}$ with $\mathbb{H}_{\mathcal{E}_K}$ and the Cauchy-Schwarz inequality. Hence,

$$\|u_{\mathcal{F}} - u_{\mathcal{E}_K}\|_e \leq \left\|u_{\mathcal{F}} - \Pi_{\mathcal{F}}^{\mathcal{E}_K} u_{\mathcal{F}}\right\|_e = \left\|\Pi_{\mathcal{F}}^{\mathcal{R}_K} u_{\mathcal{F}}\right\|_e . \tag{7}$$

**Error Indicator:** We define the element-wise error indicator as

$$\eta_K := \left\|\Pi_{\mathcal{F}}^{\mathcal{R}_K} u_{\mathcal{F}}\right\|_e^2, \quad \forall K \in \mathcal{T}. \tag{8}$$

# Energy-Based Non-Elliptic Problems

- **Discrete Inf-Sup Condition:**
  - We assume that $b$ satisfies the discrete inf-sup condition:

$$\exists \gamma > 0, \quad \inf_{\phi \in \mathbb{H}_{\mathcal{E}_K}} \sup_{\psi \in \mathbb{H}_{\mathcal{E}_K}} \frac{b(\phi, \psi)}{\|\phi\|_e \|\psi\|_e} \geq \gamma. \tag{9}$$

- **Utilizing $b$-Orthogonality:**
  - We use the $b$-orthogonality of $u_{\mathcal{F}} - u_{\mathcal{E}_K}$ with respect to $\mathbb{H}_{\mathcal{E}_K}$.

$$\gamma \left\| \Pi_{\mathcal{F}}^{\mathcal{E}_K} u_{\mathcal{F}} - u_{\mathcal{E}_K} \right\|_e \leq \sup_{\psi \in \mathbb{H}_{\mathcal{E}_K}} \frac{b\left(\Pi_{\mathcal{F}}^{\mathcal{E}_K} u_{\mathcal{F}} - u_{\mathcal{E}_K}, \psi\right)}{\|\psi\|_e} \tag{10}$$

$$\leq M_b \left\| u_{\mathcal{F}} - \Pi_{\mathcal{F}}^{\mathcal{E}_K} u_{\mathcal{F}} \right\|_e, \tag{11}$$

  where $M_b$ is the continuity constant of $b$.

- **Concluding Inequality:**
  - Hence, we derive the following bound:

$$\|u_{\mathcal{F}} - u_{\mathcal{E}_K}\|_e^2 \lesssim \left\| u_{\mathcal{F}} - \Pi_{\mathcal{F}}^{\mathcal{E}_K} u_{\mathcal{F}} \right\|_e^2 = \left\| \Pi_{\mathcal{F}}^{\mathcal{R}_K} u_{\mathcal{F}} \right\|_e^2. \tag{12}$$

# Extension to Goal-Oriented Adaptivity

## The Adjoint Problem

Find $v_{\mathcal{F}} \in \mathbb{H}_{\mathcal{F}}$ such that

$$b\left(\phi_{\mathcal{F}}, v_{\mathcal{F}}\right) = l\left(\phi_{\mathcal{F}}\right), \quad \forall \phi_{\mathcal{F}} \in \mathbb{H}_{\mathcal{F}}, \tag{13}$$

with the following specifications:

- the objective is to produce a space $\mathbb{H}_{\mathcal{F}}$ with minimal dimension such that the error in the Quantity of Interest (QoI) is below a user-defined tolerance,
- the QoI of the solution $u_{\mathcal{F}}$ is expressed as $l(u_{\mathcal{F}})$,
- $v_{\mathcal{F}}$ is the Galerkin approximation of $v$ within $\mathbb{H}_{\mathcal{F}}$,
- $v_{\mathcal{E}_K}$ in $\mathcal{E}_K$ is considered for analysis purposes, but not computed in practice.

# Quantifying Changes in the Quantity of Interest (QoI)

For a given element $K \in \mathcal{T}$, we control $\left| l\left(u_{\mathcal{F}}\right) - l\left(u_{\mathcal{E}_K}\right)\right|$, $\forall K \in \mathcal{T}$.
**Using Galerkin Orthogonality:** Since $\mathbb{H}_{\mathcal{E}_K} \subset \mathbb{H}_{\mathcal{F}}$, we have

$$b\left(u_{\mathcal{F}} - u_{\mathcal{E}_K}, \phi\right) = 0, \quad \forall \phi \in \mathbb{H}_{\mathcal{E}_K}. \tag{14}$$

**Decomposing the Change in QoI:**

$$\begin{aligned} l\left(u_{\mathcal{F}}\right) - l\left(u_{\mathcal{E}_K}\right) &= b\left(u_{\mathcal{F}} - u_{\mathcal{E}_K}, v_{\mathcal{F}} - v_{\mathcal{E}_K}\right) & (15)\\ &= b\left(u_{\mathcal{F}} - u_{\mathcal{E}_K}, \Pi_{\mathcal{F}}^{\mathcal{R}_K} v_{\mathcal{F}}\right) \quad \text{(second term vanishes)} & (16)\end{aligned}$$

**Applying Decomposition and Orthogonality:**

$$\left| l\left(u_{\mathcal{F}}\right) - l\left(u_{\mathcal{E}_K}\right)\right| \simeq \left| b\left(\Pi_{\mathcal{F}}^{\mathcal{R}_K} u_{\mathcal{F}}, \Pi_{\mathcal{F}}^{\mathcal{R}_K} v_{\mathcal{F}}\right)\right| \leq \left| a\left(\Pi_{\mathcal{F}}^{\mathcal{R}_K} u_{\mathcal{F}}, \Pi_{\mathcal{F}}^{\mathcal{R}_K} v_{\mathcal{F}}\right)\right|. \tag{17}$$

**Defining Element-wise Indicators:**

$$\eta_K := \left| a\left(\Pi_{\mathcal{F}}^{\mathcal{R}_K} u_{\mathcal{F}}, \Pi_{\mathcal{F}}^{\mathcal{R}_K} v_{\mathcal{F}}\right)\right|, \quad \forall K \in \mathcal{T}. \tag{18}$$

# Error Indicators Using a Pseudo-Dual Operator

## The Adjoint Problem

Find $\tilde{\epsilon}$ such that

$$\hat{b}\left(\phi_{\mathcal{F}}, \tilde{\epsilon}\right) = l\left(\phi_{\mathcal{F}}\right) - b\left(\phi_{\mathcal{F}}, \Pi_{\mathcal{F}}^{\mathcal{E}_K} v_{\mathcal{F}}\right), \quad \forall \phi \in \mathbb{H}, \tag{19}$$

with the following specifications:

- $\eta_K$ is defined as the error indicator associated with the element $K$

$$\eta_K := \left| \hat{b}\left(\Pi_{\mathcal{F}}^{\mathcal{R}_K} u_{\mathcal{F}}, \tilde{\epsilon}\right) \right|, \quad \forall K \in \mathcal{T}, \tag{20}$$

- where, the operator $a\left(\cdot,\cdot\right)$ is defined as $a\left(\cdot,\cdot\right) = \hat{b}\left(\cdot,\cdot\right)$.

# Main Achievements

# Main Achievements

## Peer-Reviewed Publications


- F. V. Caro, V. Darrigrand, J. Alvarez-Aramberri, and D. Pardo. "A Multi-Adaptive-Goal-Oriented Strategy to Generate Massive Databases of Parametric PDEs," To be submitted to *Computer Methods in Applied Mechanics and Engineering*, December 2023.
- F. V. Caro, V. Darrigrand, J. Alvarez-Aramberri, E. Alberdi, and D. Pardo. "A Painless Multi-Level Automatic Goal-Oriented *hp*-Adaptive Coarsening Strategy for Elliptic and Non-Elliptic Problems," *Computer Methods in Applied Mechanics and Engineering*, vol. 401, 115641, 2022. `https://doi.org/10.1016/j.cma.2022.115641`
- F. V. Caro, V. Darrigrand, J. Alvarez-Aramberri, E. A. Celaya, and D. Pardo. "1D Painless Multi-Level Automatic Goal-Oriented $h$ and $p$ Adaptive Strategies Using a Pseudo-Dual Operator," In *Computational Science – ICCS 2022*, pp. 347–357, 2022. `https://doi.org/10.1007/978-3-031-08754-7_43`

## Conference Talks

[1] F. V. Caro, V. Darrigrand, J. Alvarez-Aramberri, and D. Pardo. *Databases for Deep Learning Inversion Using A Goal-Oriented hp-Adaptive Strategy.* XI International Conference on Adaptive Modeling and Simulation, Gothenburg, Sweden, June 19-21, 2023.

[2] F. V. Caro, V. Darrigrand, J. Alvarez-Aramberri, E. Alberdi, and D. Pardo. *A Painless Automatic hp-Adaptive Coarsening Strategy For Non-SPD problems: A Goal-Oriented Approach.* 15th World Congress on Computational Mechanics & 8th Asian Pacific Congress on Computational Mechanics, Yokohama, Japan, July 31 - August 5, 2022.

[3] F. V. Caro, V. Darrigrand, J. Alvarez-Aramberri, E. Alberdi, and D. Pardo. *1D Painless Multi-Level Automatic Goal-Oriented h and p Adaptive Strategies using a Pseudo-Dual Operator.* 22nd International Conference on Computational Science, London, United Kingdom, June 21-23, 2022.

## Conference Talks

[4] F. V. Caro, V. Darrigrand, J. Alvarez-Aramberri, E. Alberdi, and D. Pardo. *Goal-Oriented hp-Adaptive Finite Element Methods: A Painless Multilevel Automatic Coarsening Strategy For Non-SPD Problems.* 8th European Congress on Computational Methods in Applied Sciences and Engineering, Oslo, Norway, June 5-9, 2022.

[5] F. V. Caro, V. Darrigrand, J. Alvarez-Aramberri, E. Alberdi, and D. Pardo. *A Painless Goal-Oriented hp-Adaptive Strategy for Indefinite Problems.* 16th U.S. National Congress on Computational Mechanics, Chicago, U.S.A, July 25-29, 2021.

[6] F. V. Caro, V. Darrigrand, J. Alvarez-Aramberri, E. Alberdi, and D. Pardo. *Goal-Oriented hp-Adaptive Finite Element Methods: A Painless Multi-level Automatic Coarsening Strategy.* 10th International Conference on Adaptive Modeling and Simulation, Gothenburg, Sweden, June 21-23, 2021.

# Main Achievements

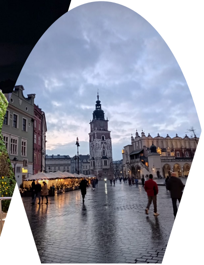
## Research Stays

| | |
|---|---|
| Feb. 2023 – Mar. 2023 (2 months) | University of Science and Technology (AGH), Krakow (Poland). **Supervisor:** Maciej Paszynski. |
| Sep. 2021 – Nov. 2021 (2 months) | CNRS-IRIT-ENSEEIHT (N7), Toulouse (France). **Supervisor:** Vincent Darrigrand. |
| Nov. 2020 – Dec. 2020 (1 month) | CNRS-IRIT-ENSEEIHT (N7), Toulouse (France). **Supervisor:** Vincent Darrigrand. |

# Main Achievements


Bilbao

Kraków



Toulouse

# Conclusions and Future Work

# Conclusions

- We employ hierarchical basis functions that effectively address the challenge of *hanging nodes*.
- We have developed **simple-to-implement** $h$- and $p$-GOA strategies that use an unconventional symmetric and positive definite bilinear form for possibly non-elliptic goal-oriented problems.
- We have expanded upon a painless automatic $hp$ strategy, initially developed for energy-norm adaptivity, to both non-elliptic and goal-oriented problems.
- We have extended the applicability of a coarsening strategy to encompass parametric PDEs.

# Future Work

- Extend algorithms to address multi-physics problems, notably $H(\text{curl})$ and $H(\text{div})$.
- Validate the efficacy of our algorithms in real-world scenarios such as Magnetotellurics, Controlled Sources, and Logging While Drilling.
- Analyze the impact of the nature and distribution of various random samples on DL inversion for optimization.
- Enhance parallelization and factorization techniques to reduce computational resource requirements in future applications.