Research Statement

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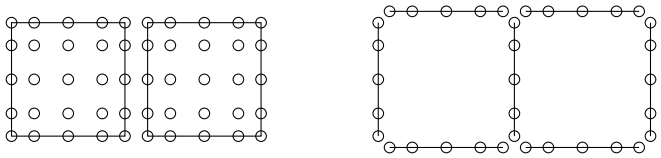
Overview. I am interested in the general realm of applied mathematics. In other words, I care about real world applications and believe that mathematics is the correct language/tool to formulate/solve the most important problems in these applications. To be more specific, my current research interests lie in the intersection of the following areas: (1) numerical methods for partial differential equations, (2) inverse and ill-posed problems, and (3) scientific machine learning and data-driven methods.

1 Numerical methods for partial differential equations

1.1 Background

The numerical methods I am primarily interested in belong to a class of finite element methods called *hybridizable discontinuous Galerkin methods*, or simply HDG methods. A significant advantage of HDG methods is that they can reduce the globally coupled DOFs by static condensation. See the following figure, HDG is able to remove all interior nodes of DOFs.



DG HDG

In addition, HDG methods lie in between the two most important groups of finite element-type methods: (1) conforming/mixed methods and (2) discontinuous Galerkin (DG) methods. This enables HDG to combine the many advantages from these two groups. Here we list a few of them:

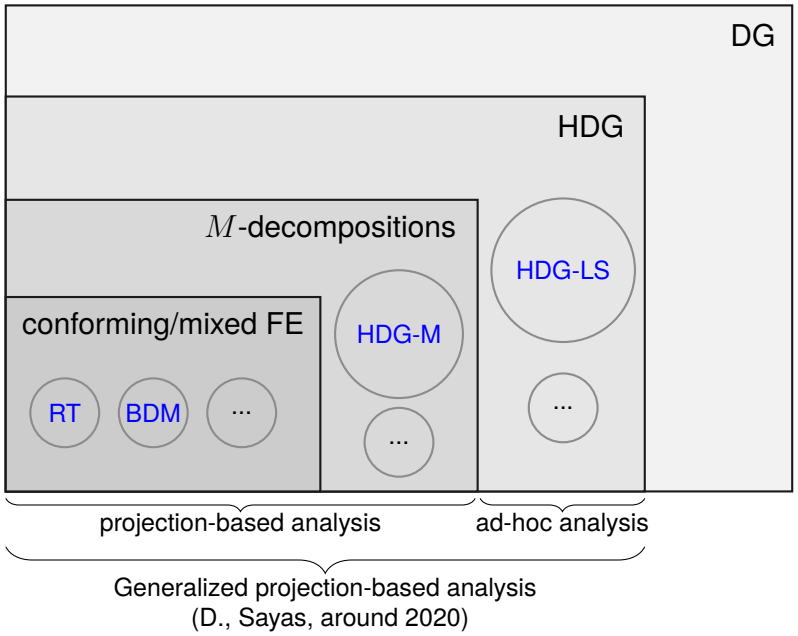
1. Naturally support static condensation for DOFs reduction (as was mentioned above)
2. Optimal accuracy and super-convergence
3. Exactly divergence free, pressure robust, locking free, spurious modes free
4. Geometric flexibility and mesh adaptation - unstructured mesh, hanging nodes, hp-adaptivity
5. Parallelization - local problem solution processes are completely independent

1.2 What I did: generalized projection-based analysis of HDG

HDG methods can be separated into two groups – (1) the HDG methods that are more alike conforming/mixed methods (the HDG methods which admit M-decomposition), and

(2) the HDG methods which are more alike nonconforming/DG methods (the HDG methods which do not admit M-decomposition). As a result, their corresponding analysis was also separated into two groups: for those more alike mixed methods, they were analyzed similar to the classical analysis of mixed methods, by the so-called *projection-based analysis*; on the other hands, for those more alike nonconforming/DG methods, they were analyzed by ad-hoc approaches. This separation of analysis has the following undesired consequences:

- Those ad-hoc analysis is not as concise and simple as the projection-based analysis
- Ad-hoc analysis becomes difficult for complicated problems (e.g., time-dependent problems, coupling problems)
- Analysis is hard to reuse because of the separation



To address this issue, we developed the so-called *generalized projection-based analysis*, extending the classical projection-based analysis to those HDG method which do not admit M-decomposition (e.g. Lehrenfeld-Schöberl HDG). What lies at the center of this framework is a mathematical object we introduced – boundary remainder δ – to quantify the nonconformity of a given projection.

The following three inequalities show the abstract form of the energy identities obtained by using classical and generalized projection based analysis. It shows that the generalized projection-based analysis is a natural extension of the classical one.

(mixed methods, around 1980)	$a^2 = a * e \Rightarrow a \leqslant e$
(M-decomposition HDG, around 2010)	$a^2 + b^2 = a * e \Rightarrow a + b \leqslant e$
(our work, general HDG, around 2020)	$a^2 + b^2 = a * e + b * \delta \Rightarrow a + b \leqslant e + \delta$

With these new analysis tools, we are able to devise/analyze new HDG methods or improve the analysis of existing ones. The applications include time-harmonic and transient elastic waves [3, 5], static and time-dependent Maxwell's equations [4, 1] and Stokes equations [2].

1.3 Future research plan

M-decomposition for Maxwell's equations in 3D. The theory of M-decomposition can be used to systematically devise superconvergent HDG methods on general polyhedral elements. However, to date, the theory is still missing for the three-dimensional Maxwell's equations.

In [4], we introduced a unified analysis framework for the HDG methods for Maxwell's equations. Based on this work, I am interested in studying the M-decomposition theory for the three-dimensional Maxwell's equations.

New link between HDG and mixed methods. Recently, a new link between HDG methods and (hybridized) mixed methods was revealed in [Cockburn, Jpn. J. Ind. Appl. Math., 2023]. Here we quote from the paper:

We then uncover a new link between HM and HDG methods, namely, that any HM method can be rewritten as an HDG method by a suitable transformation of a subspace of the approximate fluxes of the HM method into a stabilization function.

This new link has opened many exciting new directions of studying HDG methods. Among them, I am especially interested in exact sequences for DG methods.

2 Inverse and ill-posed problems

2.1 Background

The inverse problems that particularly capture my interest fall under the category of inverse transport problems, or more specifically the inverse radiative transfer. These problems serve as the mathematical foundation for a wide spectrum of applications such as optical tomography and remote sensing.

Despite their broad applications, devising numerical methods for inverse radiative transfer is notoriously challenging. This is largely due to the high-dimensional nature of the forward problem. Standard discretizations that meet the accuracy standards often demand significant memory resources, making the solver inefficient and sometimes impractical. This challenge amplifies in the inverse problem scenario, where numerous iterations of the forward problems are necessary. As such, there's a pressing need to design numerical methods that are memory-efficient and have fewer degrees of freedom (DOFs) without compromising on accuracy.

2.2 What I did: adaptive-mesh inversion – a goal-oriented adaptive mesh refinement method tailored for solving inverse problems

To address the challenges previously mentioned, we introduced the so called adaptive-mesh inversion method. This is a goal-oriented hp-adaptive mesh refinement (AMR) technique tailored for solving inverse problems. A distinctive feature of the approach is the integration of two optimization processes: one for inversion and the other for mesh adaptivity. By leveraging the connections between duality-based mesh adaptivity and adjoint-based inversion techniques, we are able to devise a goal-oriented error estimator. This estimator is cost-effective to compute. The numerical tests suggest it can efficiently steer mesh-refinement to effectively address the inverse radiative transfer problem.

The main idea of the methodology can be visually represented as in Figure 1.

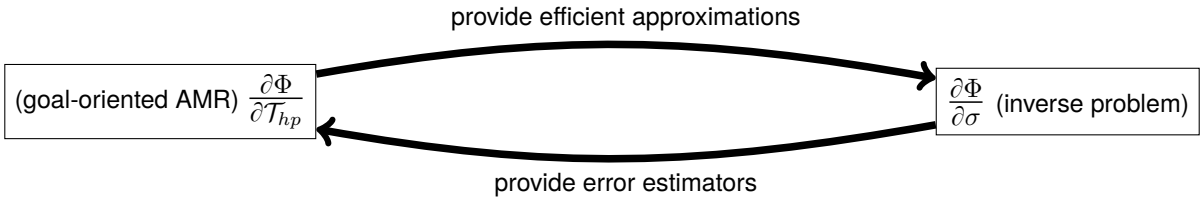


Figure 1: Core idea of adaptive-mesh inversion. Here, Φ is the typical optimization function for an inverse problem, $\mathcal{T}_{hp}$ is a finite element mesh, and σ denotes the PDE parameter that we aim to recover.

When compared with standard error reduction strategies such as uniform h-refinement, uniform p-refinement, and traditional (non-goal oriented) hp-adaptive mesh refinement, our proposed method delivers better recovered optical coefficient with a reduced count of DOFs; we refer to [8, 7] for more detail.

2.3 Future research plan

While the method is proposed for inverse radiative transfer, the general principles of devising the error estimators and the refinement algorithms should be able to be naturally extended to enable adaptive-mesh inversion for other types of inverse problems, such as the Calderón problem, inverse scattering, and remote sensing. I am interested in extending the proposed method to these other applications.

3 Scientific machine learning and data-driven methods

3.1 Background

In the past decade, (artificial) neural networks and machine learning tools have surfaced as game changing technologies across numerous fields, solving an array of challenging problems. Examples include image recognition, playing the game GO, protein folding, and large language models such as GPT3. Given these impressive results, it is reasonable to envision the potential of neural networks (NNs) for the numerical solution of partial differential equations (PDEs) or other scientific computing problems.

3.2 What I did: element learning – a systematic approach of accelerating finite element-type methods by machine learning

My research interests in this area center around the consideration of the following two closely related questions:

1. *What are the advantages and disadvantages of classical numerical methods (e.g. finite element) and machine learning based methods?*
2. *How to combine their advantages?*

Thinking about the above two questions has led to a recent discovery of a new computational framework which we call *element learning*. This new approach can be used to systematically accelerate finite element-type methods through machine learning while still retaining

the many advantages of classical finite element-type methods, such as proficient handling of complex geometry and boundary conditions, reliability, and many more. See the following Figure 2 for a visual explanation of the core idea of element learning.

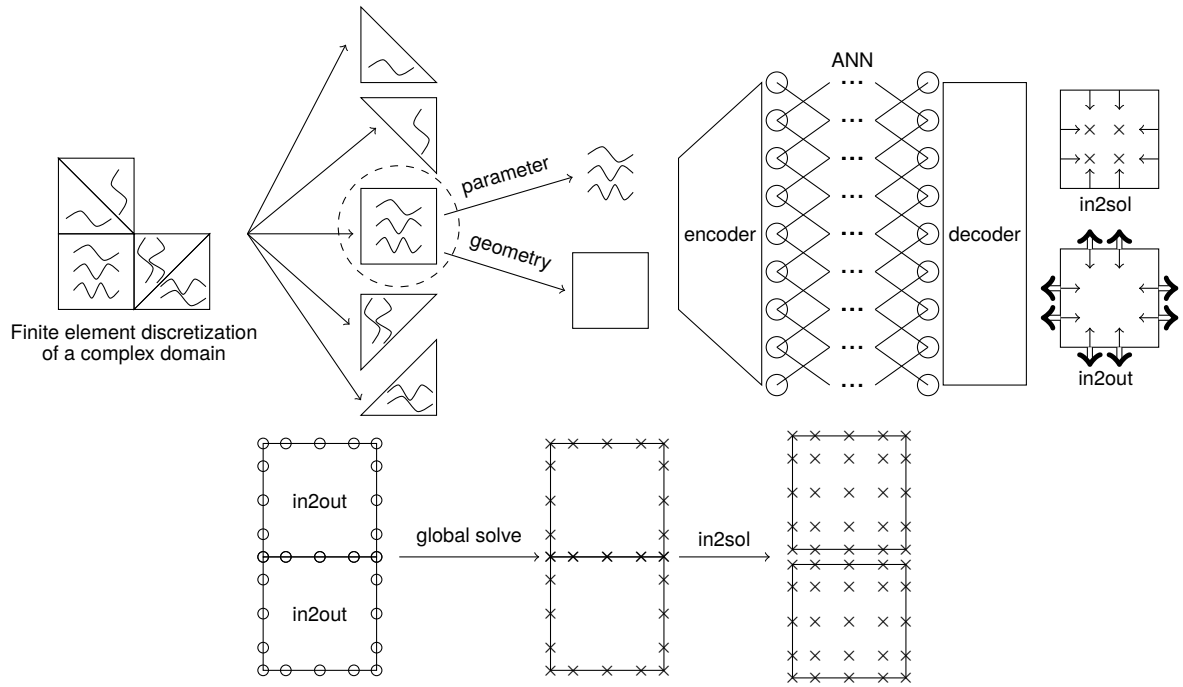


Figure 2: A finite element mesh is broken down element by element. For each element, a neural network takes the element geometry and PDE parameters as inputs, and returns the *in2sol* and *in2out* operators as outputs. Here *in2out* is for inter-element communication, *in2sol* is for element-wise solution recovery. Then, these operators are coupled globally to find the global solution using the HDG local-global solver strategy.

Our preliminary numerical results for radiative transfer equation show that element learning can generally achieve at least 5-10 times speed-up compared to a classical finite element-type method while retaining the same accuracy requirement. We refer to [6] for more detail on our discovery.

Element learning can be derived from two perspectives: (1) accelerating HDG methods by machine learning, (2) mitigate the difficulties of operator learning by using an elementwise approach. We next explain this with more detail.

3.2.1 Element learning: accelerating HDG methods by machine learning

One of the most attractive properties of HDG methods is that they support static condensation for DOFs reduction. Generally speaking, the DOFs reduction ratio is proportional to the polynomial degree k:

$$\text{reduction ratio} = \frac{\text{DOFs of DG methods}}{\text{DOFs of HDG methods}} \approx \frac{k}{d},$$

where d is the problem dimension. Thus, naturally, one would aim for choosing a large k for more DOFs reduction.

On the other hand, a fundamental dilemma here is that, increasing the polynomial degree k would make the calculation of the HDG local solver significantly more expensive. Note

that we will need to precompute the solution for *all* possible combinations of the boundary conditions to apply the static condensation. To see this more clearly, let A_K be the assembled matrix for the local system on the element K, then we need to invert

$$\text{not} \quad A_K^{-1} f \qquad \text{but} \quad A^{-1}[f, \widehat{u}_1, \widehat{u}_2, ..., \widehat{u}_N],$$

where $\{\widehat{u}_i\}_{i=1}^N$ are a basis for the boundary condition space on an element. Generally speaking, $N = \mathcal{O}(k^{d-1})$.

To resolve this dilemma, we propose to use a neural network (NN) to accelerate the calculation of the local system inversion:

$$\text{(Element learning)} \qquad (\sigma, K) \xrightarrow{\text{NN}} A^{-1}[f, \widehat{u}_1, \widehat{u}_2, ..., \widehat{u}_N].$$

This is how element learning is derived from the first perspective.

3.2.2 Element learning: mitigate the difficulties of operator learning by using an elementwise approach

To help explain the main idea we consider the abstract form of a general PDE

$$\mathcal{L}(\sigma)[u] = f \qquad \text{in } \Omega,$$

where $\mathcal{L}$ represents the differential/integral operator. The PDE has four basic components: (1) PDE parameter σ, (2) u as the solution, (3) f as the boundary/forcing data, and (4) Ω as the domain.

Past approaches of operator learning typically fix two of the above four components. Then, one seeks to the "learn" the relation between the rest two components. For instance, to learn the dynamics of evolutionary equations, we

$$\text{fix } \Omega \text{ and } \sigma. \text{ Then learn the map } f\big|_{\Omega \times \{t=0\}} = u(t=0) \mapsto u(t=T).$$

In the inverse problem setting, we

$$\text{fix } \Omega \text{ and } f. \text{ Then learn the map } \sigma \mapsto u.$$

There are several difficulties of these two approaches. First, retrain/transfer-learning is required if either (Ω, σ) (for the first approach) or (Ω, f) (for the second approach) are changed. Also, the learning becomes difficult if the PDE contains multi-scale features, since then it would require a high-resolution mesh to resolve these features.

To mitigate these difficulties, we propose the following learning paradigm:

$$(\sigma, K) \xrightarrow{\text{NN}} [f \mapsto u].$$

Namely, we aim to learn the full mechanism of a given PDE, instead of fixing some of the four components. In addition, we restrict the domain geometry to only finite element objects (e.g., triangle, tetrahedron, prism, pyramid). As a result, the learning becomes much easier.

Once we obtain the oprator $[f \mapsto u]_K$ on each element K, we then use the HDG local-global-solver technique to couple them together to recover the global solution. This is how element learning is derived from the second perspective.

3.3 Future research plan

A major part of my future research goal is to (1) build the theoretical foundation and (2) explore the maximal applicability for element learning. We next discuss these two directions with more detail.

3.3.1 Theoretical foundation of element learning

The main idea of element learning is to use a neural network (NN) to approximate the map from element geometry and PDE parameter to the elementwise solution operator. An important topic to be studied is the numerical analysis of element learning. We are interested in the following two related questions:

1. How well the NN can approximate the map? (approximation error, generalization error, optimization error)
2. How to improve the approximation capability and efficiency of the NN to the map?

Answers to the above questions can help us resolve the following problems.

Larger p. Even greater speed-up can be expected if a higher order polynomial degree p is used. At the same time, for larger p, it becomes more difficult to train the neural network. How to choose the polynomial degree for a good balance between the efficiency of the method (for which we aim to increase p), and the reliability of the method (for which we aim to decrease p), remains to be studied.

Neural network with a priori structure. The current approach uses a fully connected neural network without any a priori structures. It remains to be studied that whether better approximation of the networks can be achieved by introducing additional structures, such as convolutional layers (CNN), attention mechanism (transformer), or shortcut connections (ResNet).

3.3.2 Extend the applicability of element learning

Another direction is to explore more applications of element learning. Several topics can be considered.

More PDEs. The element learning method is closely related to hybridizable discontinuous Galerkin methods in the sense that the local solvers are replaced by machine learning approaches. As a result, all hybridizbale discontinuous Galerkin methods, hybridized mixed method, and hybridized continuous Galerkin methods, can be potentially accelerated by element learning. This generality suggests the potential of element learning to be applied to more PDEs that have been studied with HDG discretizations. Examples include but are not limited to Maxwell's equations, linear elasticity, convection-diffusion, and Stokes/Navier-Stokes equations.

Purely data-driven element learning. In some applications, a desirable property of data-driven approaches is the ability to learn a data-driven solver without knowing the underlying PDE or dynamical equations. Here, for element learning, the underlying PDE does not necessarily need to be known. Knowledge of boundary conditions is still needed for an appropriate definition of the local operators in element learning, in order to ensure a well-posed problem, and to allow the coupling of local solvers in creating the global solver. It would be interesting in the future to investigate the ideas of element learning in scenarios where the underlying PDE or dynamical equations are unknown due to the complexity of the system, or

are computationally intractable due to the high dimensionality of the true system. For example, such a situation arises in physics parameterizations or subgrid-scale parameterizations in atmospheric, oceanic, and climate dynamics and other complex systems.

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