Machine Learning-aided enhancement and acceleration techniques for Polyhedral Finite Element Methods

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joint work with E. Manuzzi
Motivations

Many engineering and geophysical applications have complex physical domains (fluid-structure interaction, crack propagation, flow in fractured porous media).

Contact between two flexible bodies

Evolution of an ideal red blood cell experiencing very large displacements

Development of numerical methods that use general polygonal and polyhedral mesh elements (es. Virtual Element Method, Polygonal Discontinuous Galerkin, HDG, Weak Galerkin, Mimetic Finite Differences, Hybrid High Order, etc...).
Objective
- Develop effective algorithms to handle polygonal and polyhedral grids, in particular mesh refinement and agglomeration, based on employing Machine Learning techniques.
- Enhance the performance and accuracy of Polyhedral Finite Element methods based on employing ML-aided strategies.
ML-enhanced mesh refinement (2D)

Refinement strategies for triangles and quadrilaterals.
<table>
<thead>
<tr>
<th>initial polygons</th>
<th>Voronoi</th>
<th>midpoint</th>
<th>preferential direction*</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image1" alt="Initial Polygon" /></td>
<td><img src="image2" alt="Voronoi" /></td>
<td><img src="image3" alt="Midpoint" /></td>
<td><img src="image4" alt="Direction" /></td>
</tr>
<tr>
<td><img src="image5" alt="Initial Polygon" /></td>
<td><img src="image6" alt="Voronoi" /></td>
<td><img src="image7" alt="Midpoint" /></td>
<td><img src="image8" alt="Direction" /></td>
</tr>
</tbody>
</table>

*S. Berrone, A. Borio, and A. D’Auria 2021*
"Ideal" strategy

1. Classify the "shape" of a polygon.
2. Apply a suitable refinement for that specific shape.

Step 1 can be learned from a database of examples using Machine Learning (ML).

[A., Manuzzi, JCP, 2022]
Image classification using Convolutional Neural Networks (CNNs)

Network training is the process of tuning the neurons parameters, in order to correctly classify a given database of samples.

It is expensive but it can be done offline once and for all, while online classification is very fast.
Algorithm 1: CNN-enhanced Reference Polygon (CNN-RP) strategy

Strategies for regular polygons are extended to arbitrary polygons by exploiting the CNN information about the "shape".
Algorithm 2: CNN-enhanced Mid-Point (CNN-MP) strategy

The MP strategy can be enhanced by classifying polygons using a CNN and choosing refinement connections according to the label.
Automatic dataset generation

Reference polygon
Label: "Triangle"

Small distortions applied
Label: "Triangle"

Binary image 64x64 pixels
Label: "Triangle"
Refined grids obtained after three steps of uniform refinement based on employing the MP, the CNN-RP and the CNN-MP strategies.
Effects of CNN-enhanced refinement strategies on Quality Metrics

Uniformity Factor = \( \frac{\text{element size}}{\text{mesh size}} \)

Circle Ratio = \( \frac{\text{inscribed circle radius}}{\text{circumscribed circle radius}} \)
Effects of CNN-enhanced refinement strategies on accuracy of polyhedral Finite Element Methods

- **PolyDG methods** [A. Brezzi, Marini, 2009], [Bassi et al, 2012], [A., Giani, Houston, 2013], [Cangiani, Geourgolis, Houston, 2014], [A., Cangiani, Collis, Dong, Georgoulis, Giani, Houston, 2016], [Cangiani, Dong, Geourgolis, Houston, 2017], ......


Given $\Omega \subset \mathbb{R}^d$, $d = 2, 3$, and $f \in L_2(\Omega)$: find $u$ such that

$$-\nabla \cdot (\rho \nabla u) = f \text{ in } \Omega, \quad u = 0 \text{ on } \partial \Omega,$$

where $0 < \rho_0 \leq \rho$. 
PolyDG formulation

We consider a tessellation of the domain into polygonal/polyhedral elements

We set

\[ V_h = \{ u \in L_2(\Omega) : u|_{\kappa} \in P_{p,\kappa}(\kappa) \ \forall \kappa \in T_h \}, \]

where \( P_{p,\kappa}(\kappa) \) denotes the set of polynomials of degree at most \( p \geq 1 \) over \( \kappa. \)

find \( u_h \in V_h \) such that

\[ A_h(u_h, v_h) = \int_\Omega f v_h \, dx \]

for all \( v_h \in V_h. \)
PolyDG formulation

Find \( u_h \in V_h \) such that

\[
A_h(u_h, v_h) = \int_{\Omega} f v_h \, dx
\]

for all \( v_h \in V_h \), where

\[
A_h(u, v) = \sum_{k \in T_h} \int_{k} \rho \nabla u \cdot \nabla v \, dx + \sum_{F \in F_h} \int_{F} \sigma \, [u] \cdot [v] \, ds
\]

\[
- \sum_{F \in F_h} \int_{F} (\{\rho \nabla_h v\}_{\omega} \cdot [u] + \{\rho \nabla_h u\}_{\omega} \cdot [v]) \, ds
\]

\( \{ \cdot \}_{\omega} \) : \( \rho \)-Weighted Average Operator \quad \[ \cdot \] : Jump Operator
Virtual Element formulation

We will build a **discrete problem** in following form

\[
\begin{aligned}
\text{find } u_h \in V_h \text{ such that } \\
a_h(u_h, v_h) = \langle f_h, v_h \rangle \quad \forall v_h \in V_h,
\end{aligned}
\]

where

- \( V_h \subset V \) is a finite dimensional space;
- \( a_h(\cdot, \cdot) : V_h \times V_h \to \mathbb{R} \) is a discrete bilinear form approximating the continuous form \( a(\cdot, \cdot) \);
- \( \langle f_h, v_h \rangle \) is a right hand side term approximating the load.

[Beirão da Veiga, Brezzi, Cangiani, Manzini, Marini, Russo, 2013]
The local spaces $V_{h|E}$

For all $E \in \Omega_h$:

$$V_{h|E} = \{ v \in H^1(E) : -\Delta v \in \mathbb{P}_{k-2}(E), \quad v|_e \in \mathbb{P}_k(e) \quad \forall e \in \partial E \}.$$  

- the functions $v \in V_{h|E}$ are continuous (and known) on $\partial E$;
- the functions $v \in V_{h|E}$ are unknown inside the element $E$!
- it holds $\mathbb{P}_k(E) \subseteq V_{h|E}$

The **global space** $V_h$ is built by assembling the local spaces $V_{h|E}$ as usual:

$$V_h = \{ v \in H^1_0(\Omega) : v|_E \in V_{h|E} \quad \forall E \in \Omega_h \}$$

The choice of degrees of freedom guarantees the **global continuity** of the functions in $V_h$. 
The degrees of freedom for $V_{h|E}$

- Red dots stand for pointwise evaluation, at vertexes and on edges ($k-2$ per edge)
- Blue dots represent internal (volume) moments

\[
\int_E v_h \cdot p_{k-2} \quad \forall p_{k-2} \in P_{k-2}(E).
\]
The bilinear form $a_h(\cdot, \cdot)$

The bilinear form $a_h(\cdot, \cdot)$ is built element by element

$$a_h(v_h, w_h) = \sum_{E \in \Omega_h} a_h^E(v_h, w_h) \quad \forall \; v_h, w_h \in V_h,$$

where

$$a_h^E(\cdot, \cdot) : V_{h|E} \times V_{h|E} \rightarrow \mathbb{R}$$

are symmetric bilinear forms that mimic

$$a_h^E(\cdot, \cdot) \simeq a(\cdot, \cdot)|_E$$

by satisfying stability and consistency conditions.
Solving the Poisson problem using the VEM (uniform refinement)

- Triangular grid
- Voronoi grid
- Smoothed-Voronoi grid
- Non-convex grid
Solving the Poisson problem using the PolyDG method (uniform refinement)

Analogous results for advection-diffusion and Stokes problems.
Solving the Poisson problem using the VEM (adaptive refinement)

**Triangular grid**

- MP
- CNN-RP
- CNN-MP

**Voronoi grid**

- MP
- CNN-RP
- CNN-MP

**Smoothed-Voronoi grid**

- MP
- CNN-RP
- CNN-MP

**Non-convex grid**

- MP
- CNN-RP
- CNN-MP
ML-enhanced mesh refinement (3D)

with E. Manuzzi and F. Dassi (U. Milano Bicocca)

Challenges in 3D:

• high geometrical complexity: need to design of simple and robust refinement strategies

• high computational costs: need for fast algorithms (e.g. CNNs)

• high shape variability: need to tackle unknown shapes explicitly
3D refinement strategies for general polyhedra

- **Diameter strategy**: cut the element perpendicular to its diameter.
- **K-means strategy**: cut the element balancing the volume distribution.
- **"Classical" strategies**: if the element has a specific shape refine it using a predefined strategy.
The CNN classifies the 3D image of the input polyhedron according to its shape, in order to apply suitable refinement strategies. Elements in class "other" are refined using the k-means strategy.
Refined grids obtained after three steps of uniform refinement based on employing the diameter, the k-means and the CNN strategies.
Quality Metrics

Uniformity Factor = \( \frac{\text{element size}}{\text{mesh size}} \)

Circle Ratio = \( \frac{\text{inscribed circle radius}}{\text{circumscribed circle radius}} \)
Effects of ML-based refinement strategies on statistics of computational complexity
Solving the Poisson problem with the VEM (3D)

Analogous results for the VEM of order higher than 1.
ML-enhanced agglomeration strategies

Merging neighboring mesh elements to obtain a coarser grid.

- Design of multilevel solvers
- Defeaturing of complex geometries
Objective:
Find a partition with minimal interconnections between sets, while keeping errors (volumes) balanced.

Advantages:
Fast inference and full exploitation of both graph and geometrical features.
Agglomerated grids based on employingmetis. Metis is «standard» for graph partitioning.
GNN-based method can be competitive wrt SotA methods (Metis, Kmeans, ...)?

- Implement different model architectures
- Optimize model’s runtime
Conclusions

1. ML can be employed to learn the "shape" of mesh elements within (adaptive) refinement strategies
   - Allows to extend or boost existing refinement strategies.
   - Improves the performance in terms of accuracy and quality of the underlying mesh.
   - It is fully automatic, and it has a low computational cost for online classification.
   - It is independent of the underlying differential model and of the numerical method used.

2. GNN can be employed to drive agglomeration procedures
   - Design of multilevel solvers
   - Defeaturing of complex geometries
1. Optimal estimate of the PolyDG/VEM stabilization parameters using CNNs (with E. Manuzzi, S. Bonetti)
2. Development 3D ML-enhanced agglomeration strategies for multigrid solvers (with E. Manuzzi)
3. Improving efficiency of algebraic multigrid methods through artificial neural networks: choosing the strong threshold parameter $\theta$ as the one the ANN predicts to give the best performance.
4. Application of the described algorithms in the context of
   - Modelling neurodegenerative diseases
   - Geophysical applications, including fluid-structure interaction with complex and moving geometries.

Ongoing
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