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

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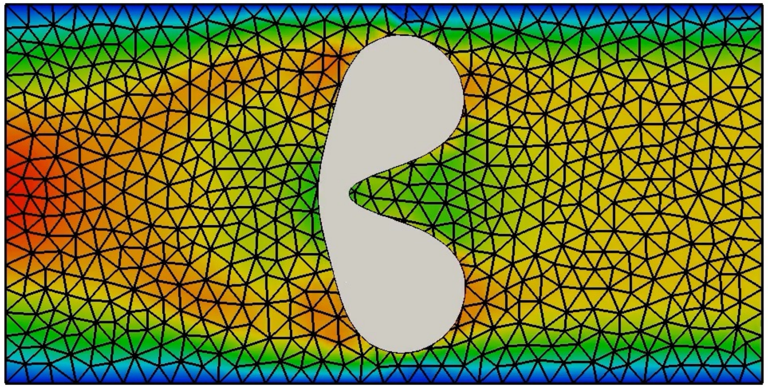
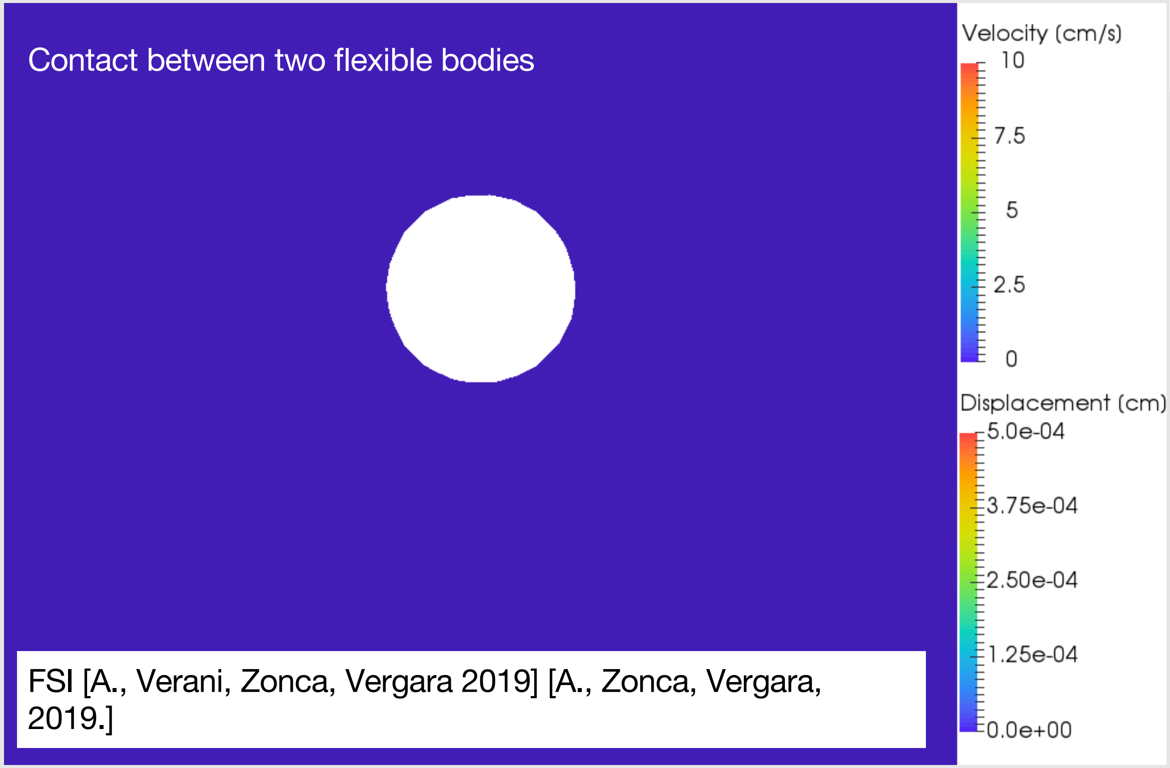
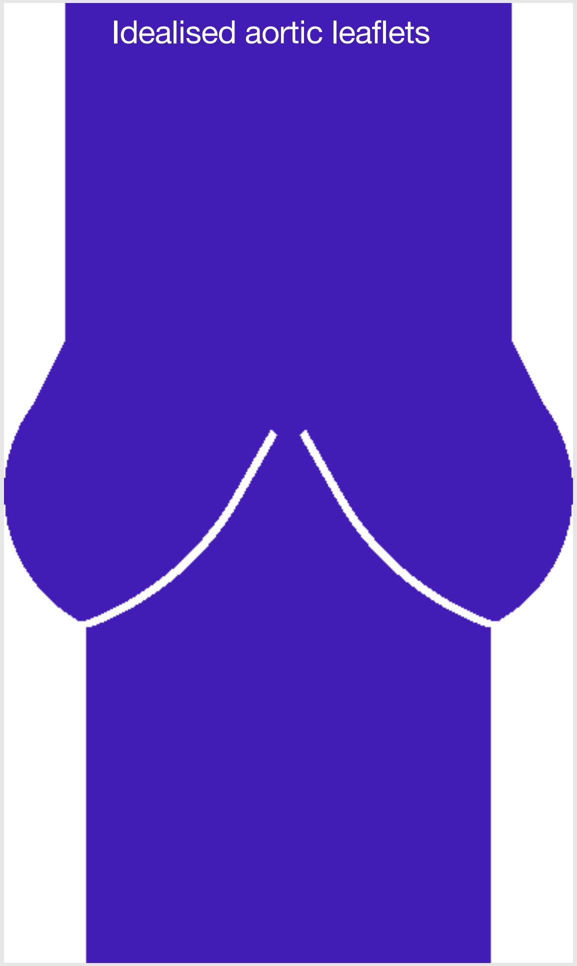
joint work with E. Manuzzi

Motivations

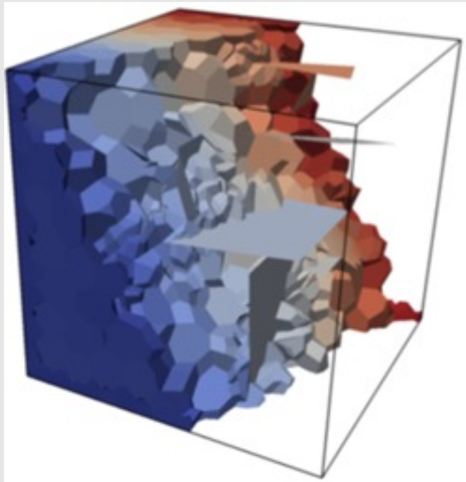
Many engineering and geophysical applications have complex physical domains (fluid-structure interaction, crack propagation, flow in fractured porous media).

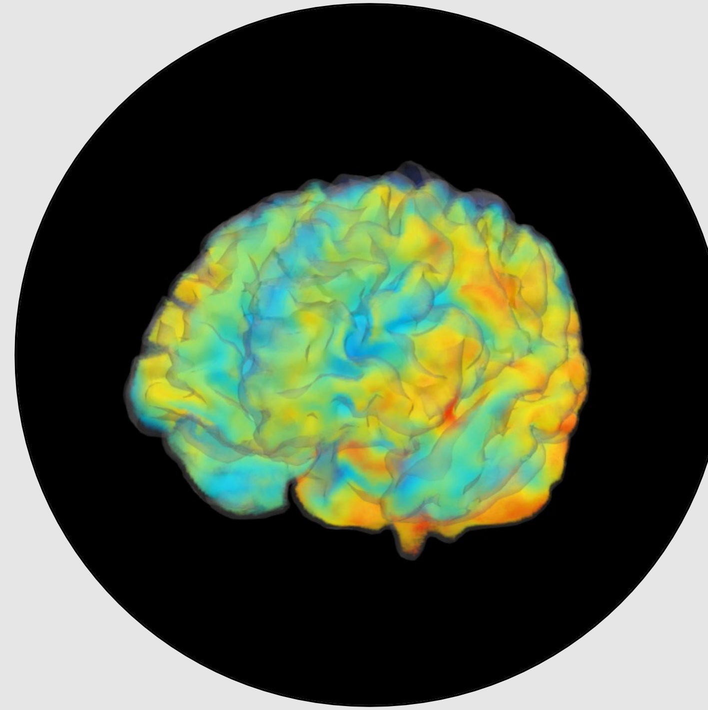

Evolution of an ideal red blood cell experiencing very large displacements





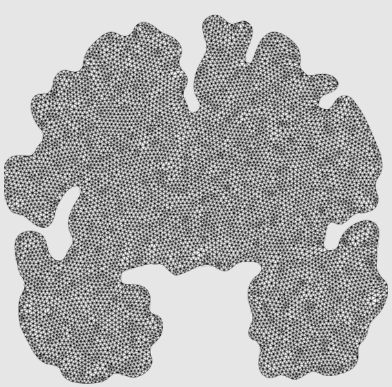
Development of numerical methods that use general polygonal and polyhedral mesh elements (es. **Virtual Element Method**, **Polygonal Discontinous Galerkin**, HDG, Weak Galerkin, Mimetic Finite Differences, Hybrid High Order, etc…).

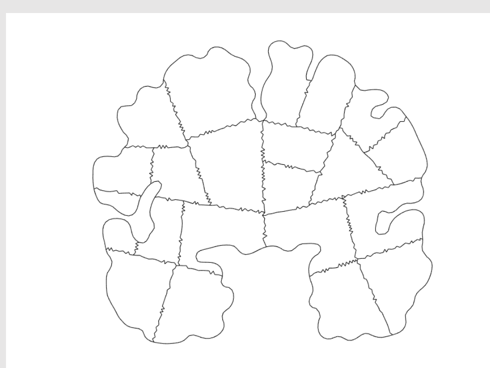


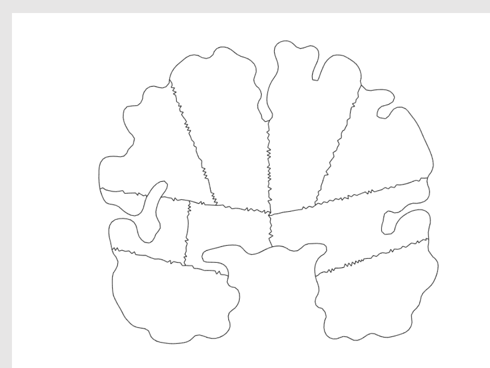


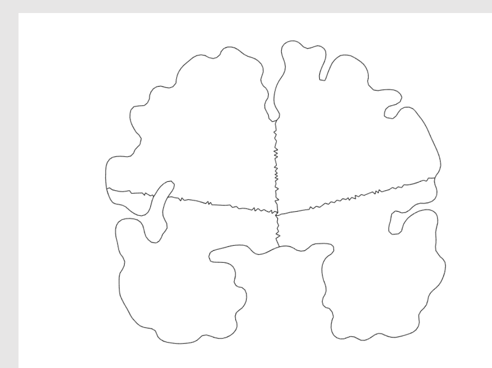
Objective

- 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

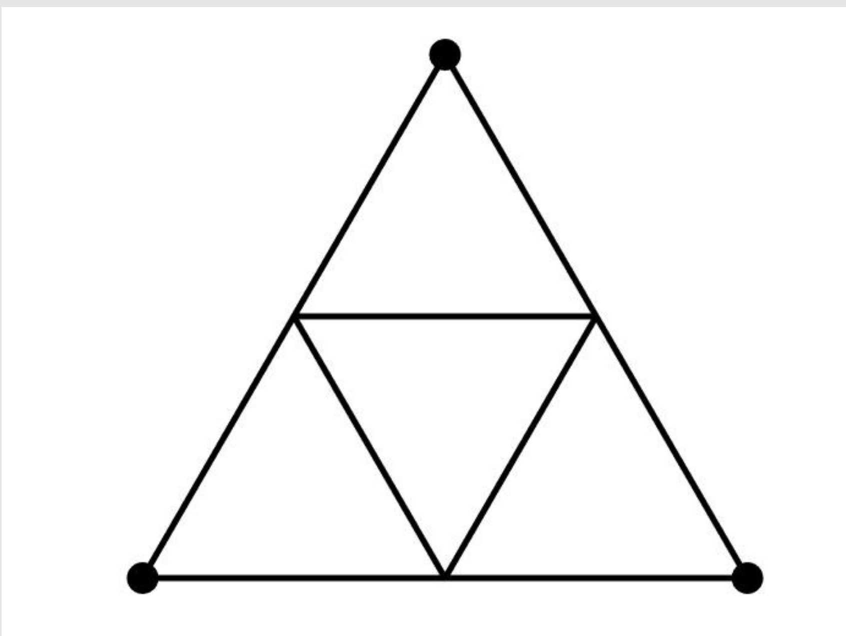


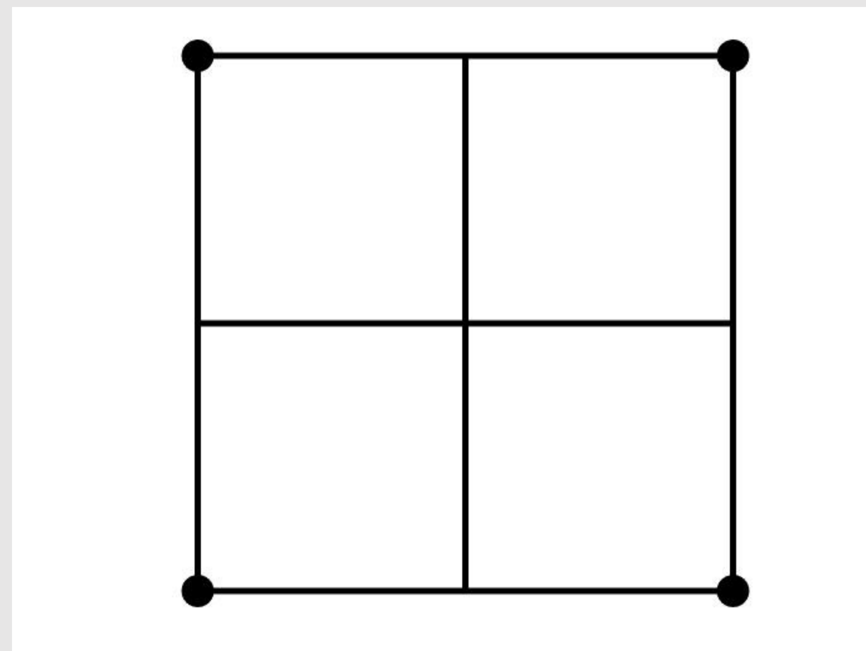






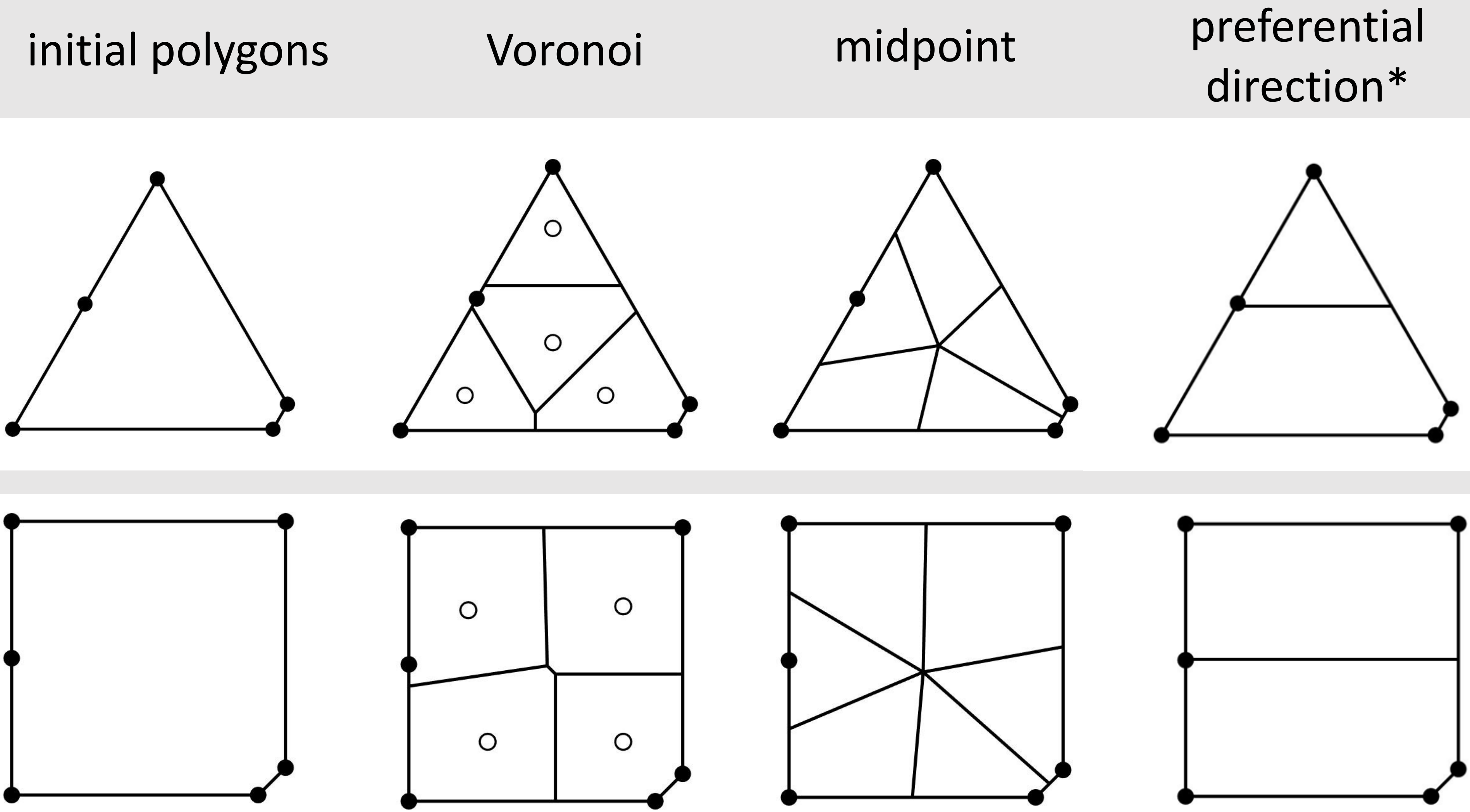
ML-enhanced mesh refinement (2D)





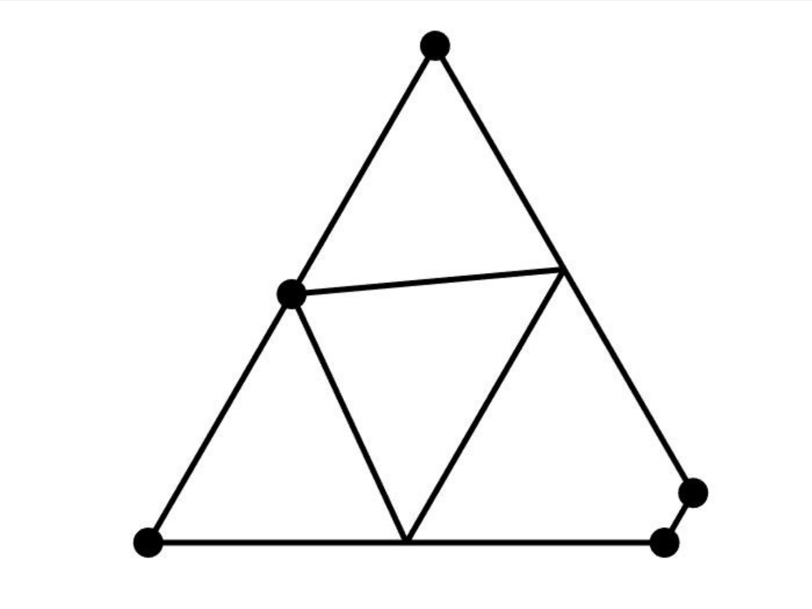
Refinement strategies for triangles and quadrilaterals.

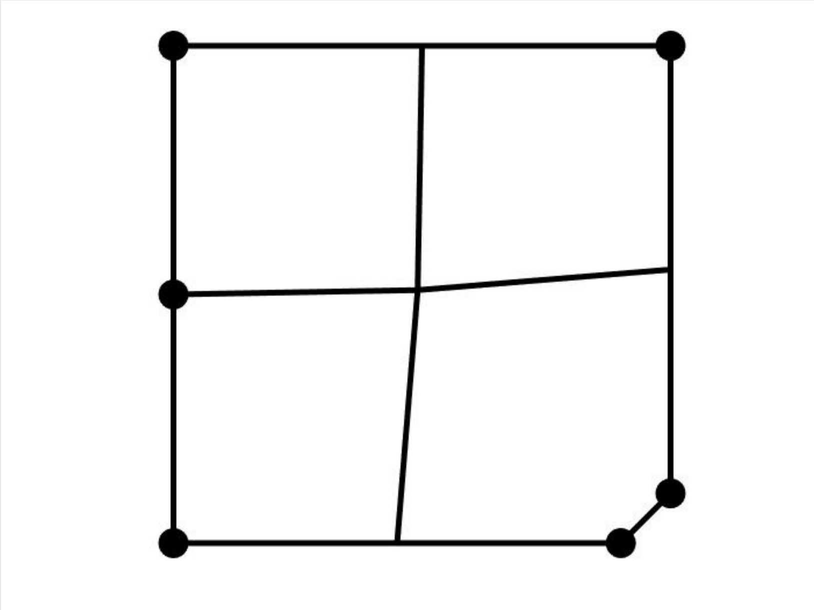
Refinement strategies for general polygons



*S. Berrone, A. Borio, and A. D'Auria 2021

"Ideal" strategy



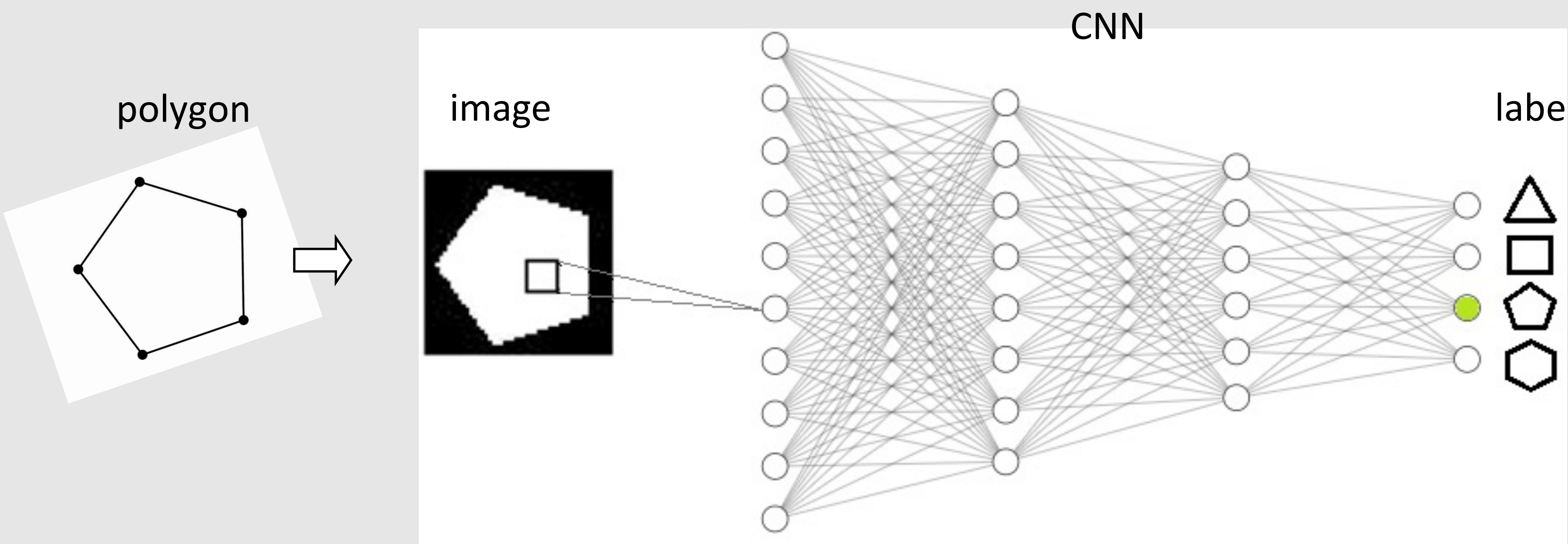


1. Classify the "**shape**" of a polygon.
2. Apply a suitable refinement for that specific shape.

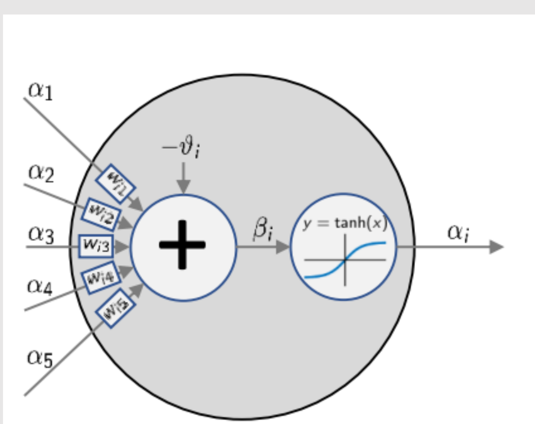
Step 1 can be learned from a database of examples using Machine Learning (ML).

[A., Manuzzi, JCP, 2022]

Image classification using Convolutional Neural Networks (CNNs)



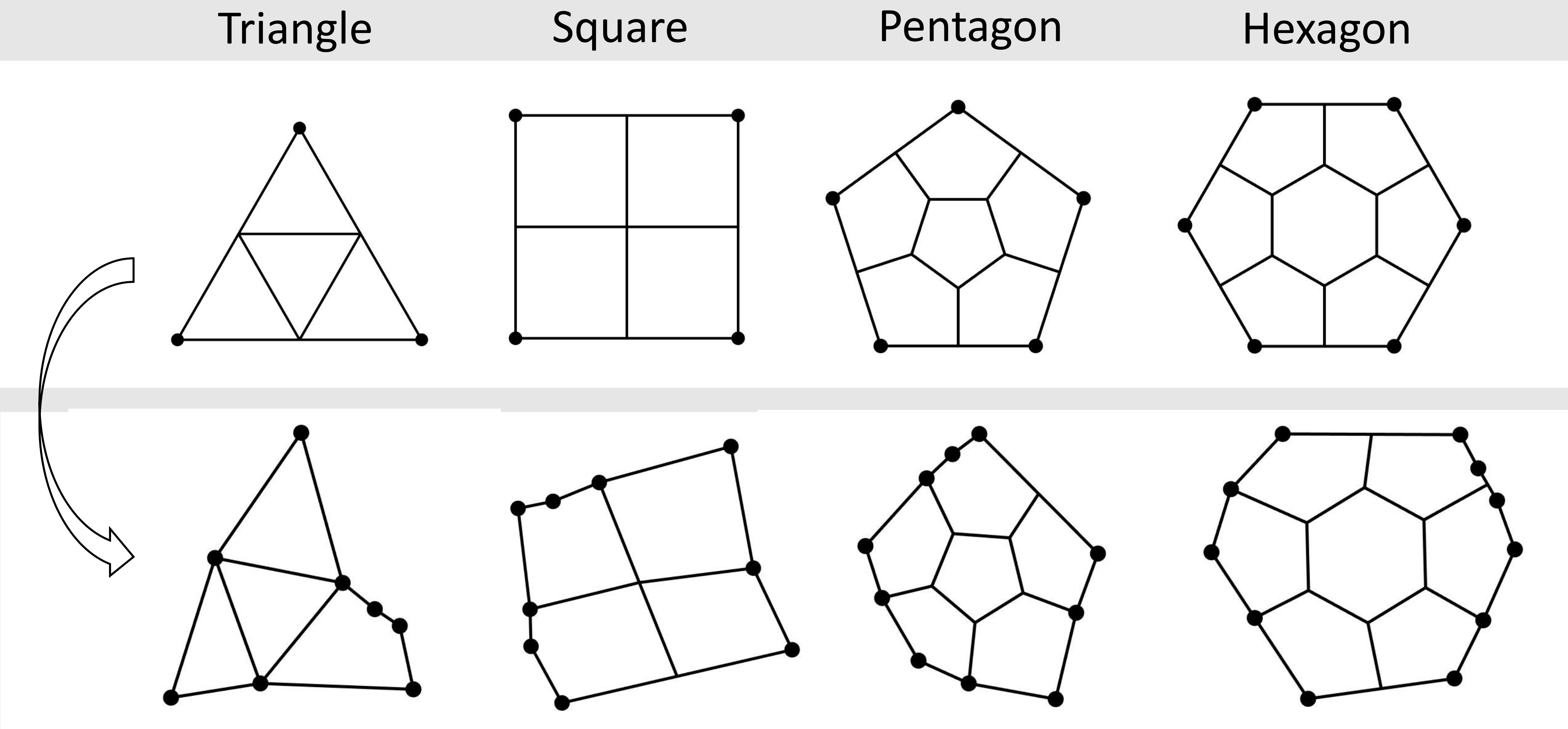
neuron



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

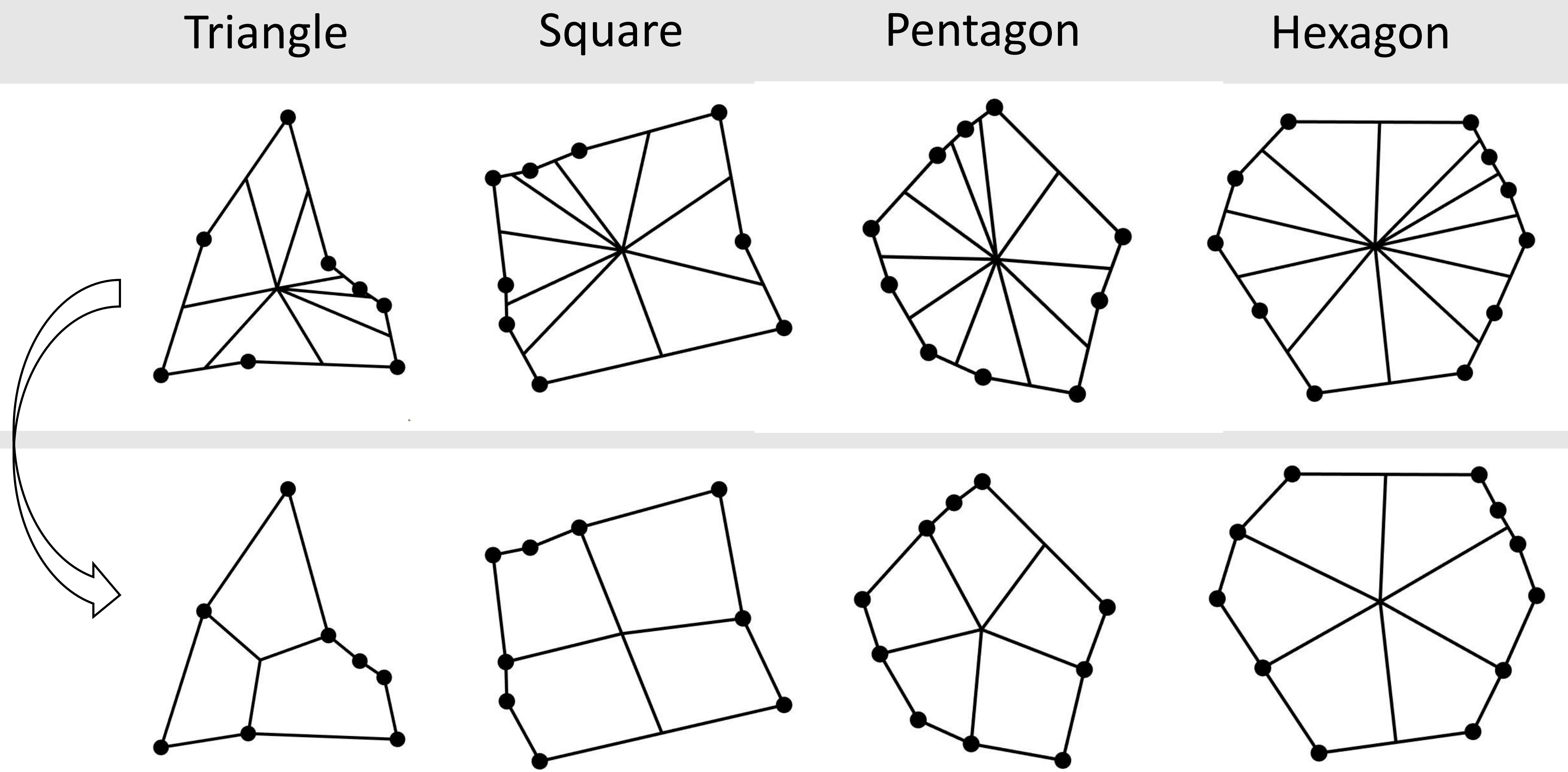
It is expensive but it can be done offline once and for all, while online classification is very fast.

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



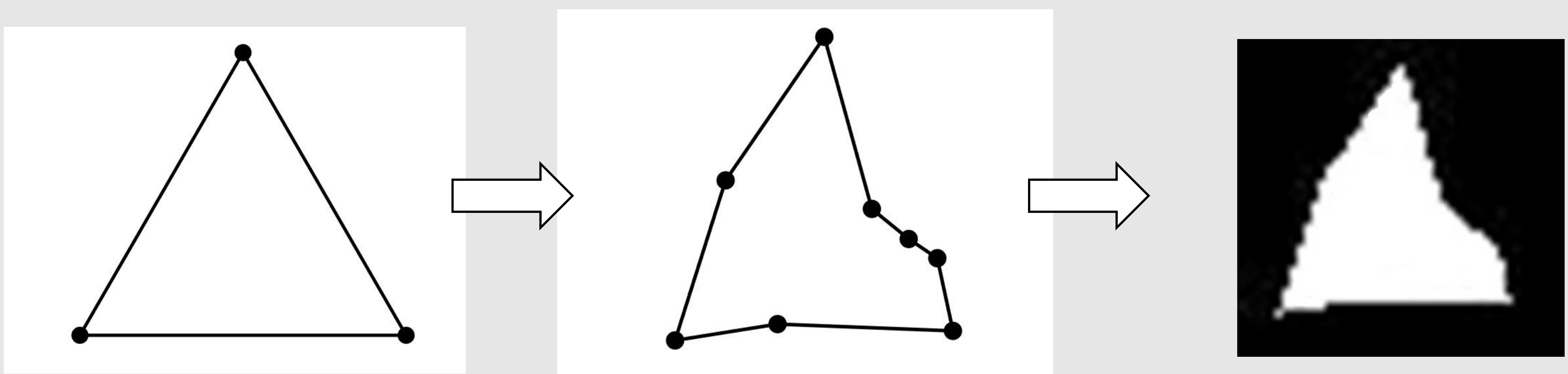
The MP strategy can be enhanced by classifying polygons using a CNN and chosing refinement connections according to the label.

Automatic dataset generation

Reference polygon

Small distortions applied

Binary image 64x64 pixels



Label: "Triangle"

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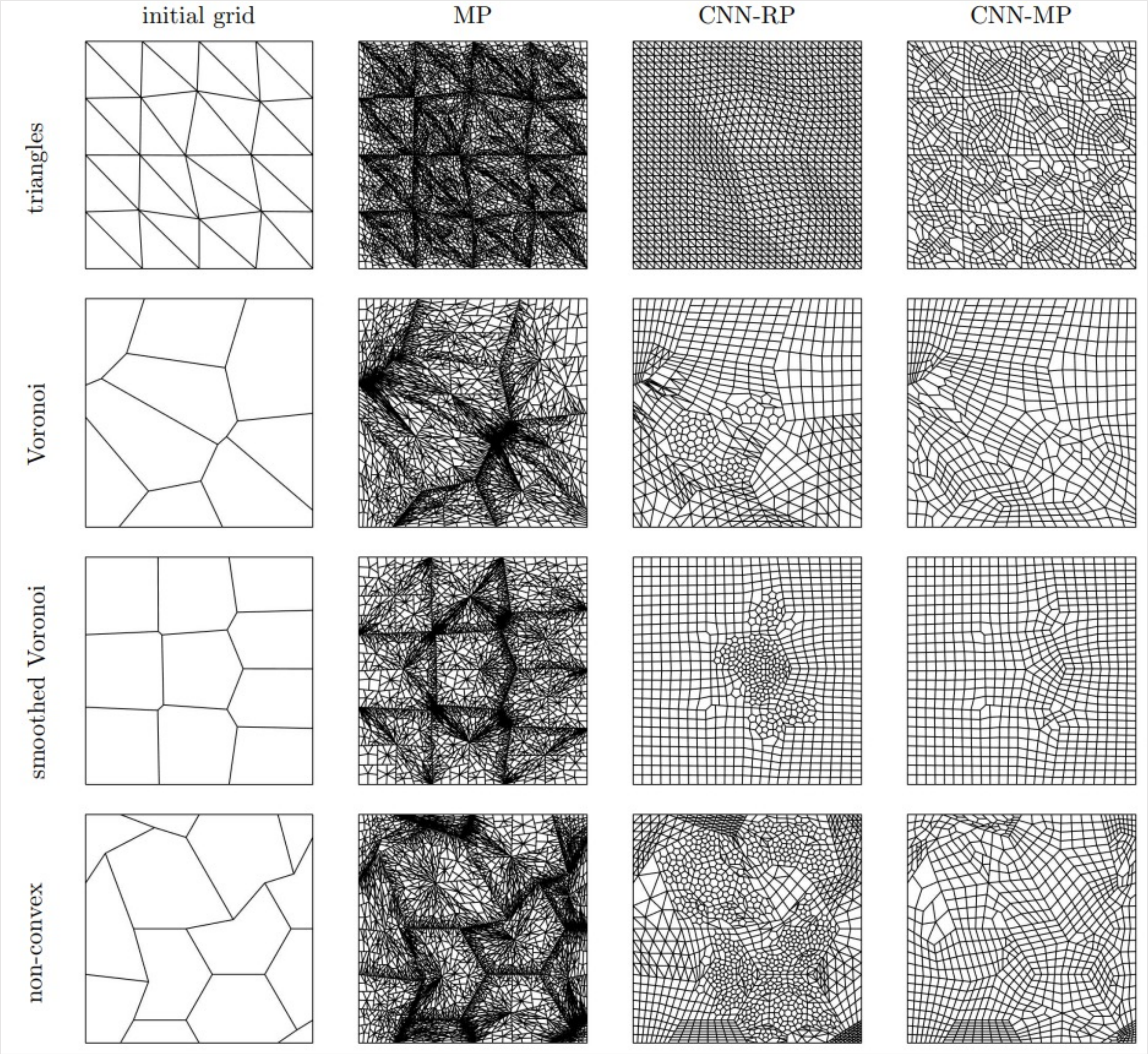
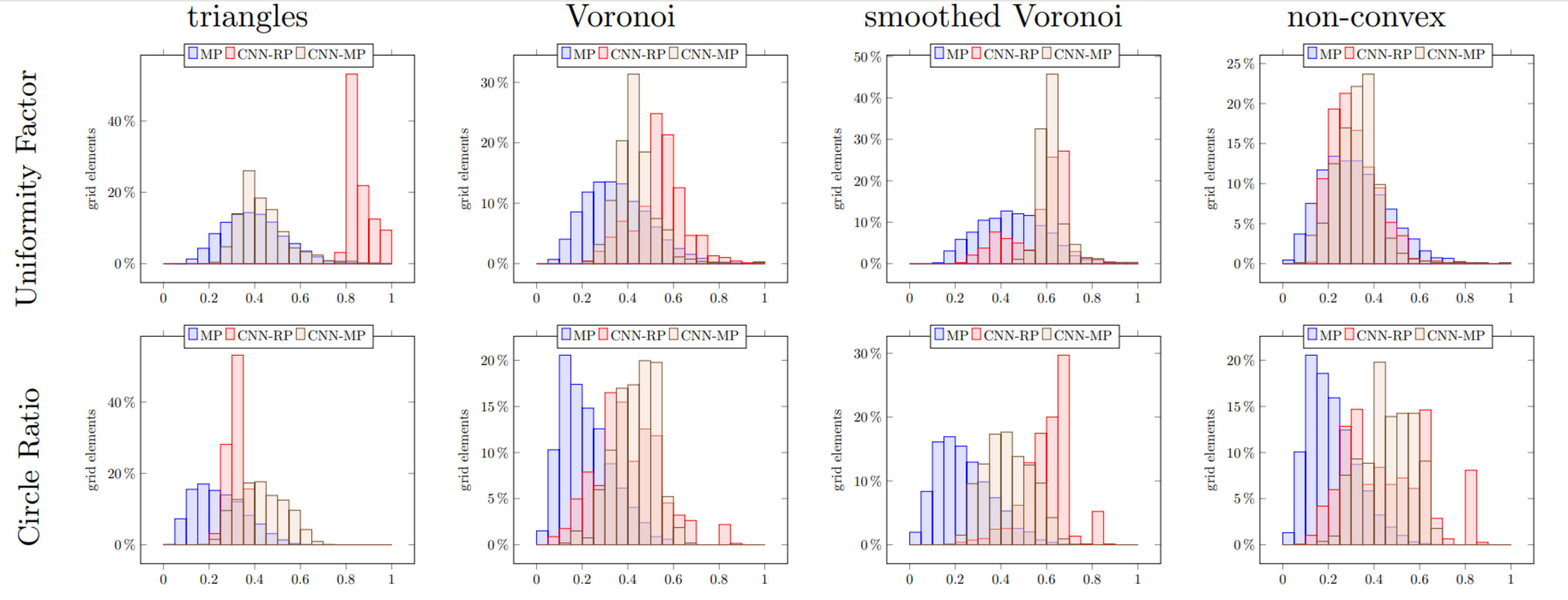


Refined grids obtained after three steps of uniform refinement based on employing the MP, the CNN-RP and the CNN-MP strategies.

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

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

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

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

- **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], ……

- **Virtual Element Methods** [Beirão da Veiga , Brezzi, Cangiani, Manzini, Marini, Russo, 2013], [Beirão da Veiga, Brezzi, Marini 2013], [Brezzi, Marini, 2013], [Ahmad, Alsaedi, Brezzi, Marini, Russo 2013], [Brezzi, Falk, Marini , 2014], [Beirao da Veiga, Brezzi, Marini, Russo, 2014],………

PolyDG formulation

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

We set

$$V_h = \{u \in L_2(\Omega) : u|_\kappa \in \mathcal{P}_{p_\kappa}(\kappa)\ \forall \kappa \in \mathcal{T}_h\},$$

where $\mathcal{P}_p(\kappa)$ denotes the set of polynomials of degree at most $p \geq 1$ over κ.

find $u_h \in V_h$ such that

$$\mathcal{A}_h(u_h, v_h) = \int_\Omega f v_h \mathrm{d}\mathbf{x}$$

for all $v_h \in V_h$.

PolyDG formulation

Find $u_h \in V_h$ such that

$$\mathcal{A}_h(u_h, v_h) = \int_\Omega f v_h \, dx$$

for all $v_h \in V_h$, where

$$\begin{aligned}\mathcal{A}_h(u,v) \quad = \quad & \sum_{\kappa \in \mathcal{T}_h} \int_\kappa \rho \nabla u \cdot \nabla v \, dx + \sum_{F \in \mathcal{F}_h} \int_F \sigma \, [\![u]\!] \cdot [\![v]\!] \, ds \\ & - \sum_{F \in \mathcal{F}_h} \int_F \left(\{\!\{\rho \nabla_h v\}\!\}_\omega \cdot [\![u]\!] + \{\!\{\rho \nabla_h u\}\!\}_\omega \cdot [\![v]\!] \right) ds\end{aligned}$$

$\{\!\{\cdot\}\!\}_\omega$: ρ–Weighted Average Operator $\quad [\![\cdot]\!]$: Jump Operator

Virtual Element formulation

We will build a discrete problem in following form

$$\begin{cases} \text{find } u_h \in V_h \text{ such that} \\ a_h(u_h, v_h) =< f_h, v_h > \qquad \forall\, v_h \in V_h, \end{cases}$$

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 $a(\cdot,\cdot)$;
- $< \mathbf{f}_h, \mathbf{v}_h >$ 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 $E \in \Omega_h$:

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

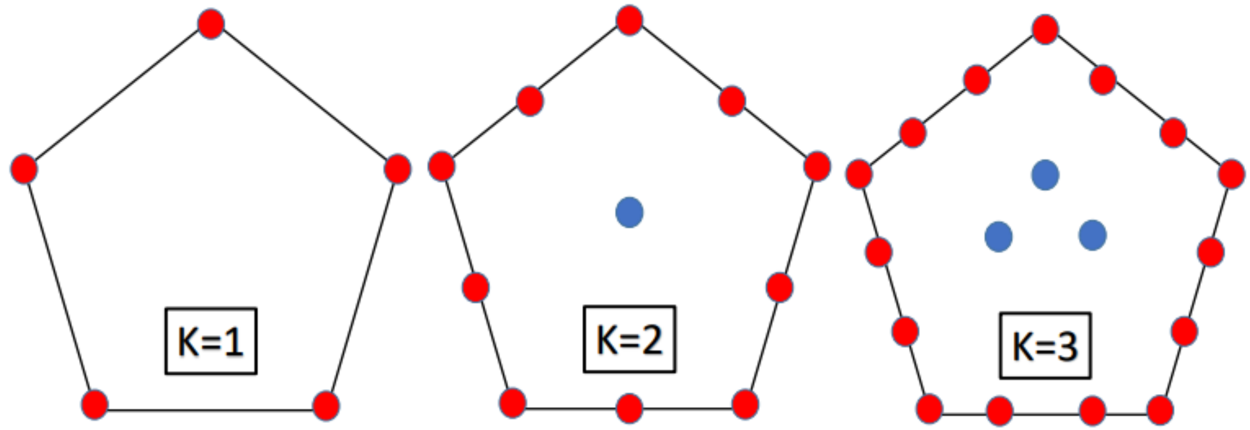
- the functions $v \in V_{h|E}$ are continuous (and known) on ∂E;
- the functions $v \in V_{h|E}$ are unknown inside the element E!
- it holds $\mathbb{P}_k(E) \subseteq V_{h|E}$

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

$$V_h = \{v \in H_0^1(\Omega) \ : \ v|_E \in V_{h|E} \, \forall E \in \Omega_h\}$$

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

$$\int_E v_h \cdot p_{k-2} \qquad \forall p_{k-2} \in \mathbb{P}_{k-2}(E)\,.$$

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

$$a_h^E(\cdot,\cdot) \;:\; V_{h|E} \times V_{h|E} \longrightarrow \mathbf{R}$$

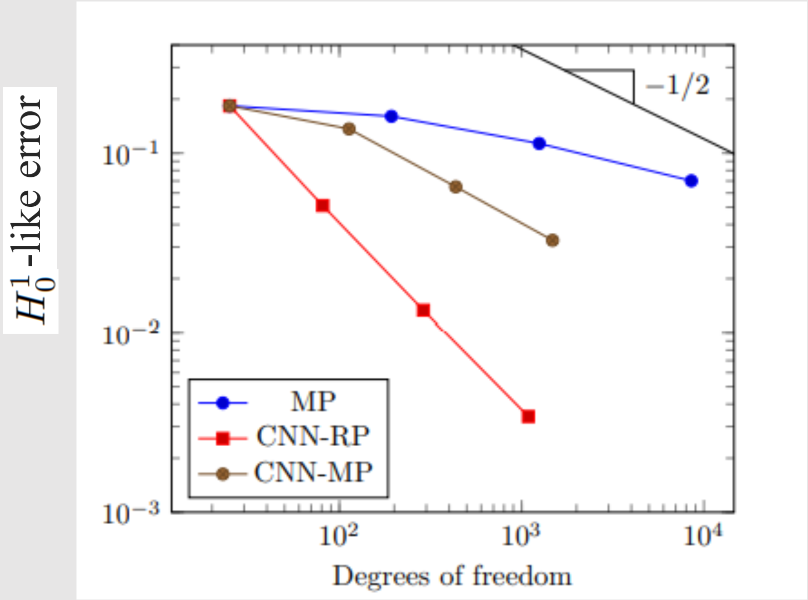
are symmetric bilinear forms that mimic

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

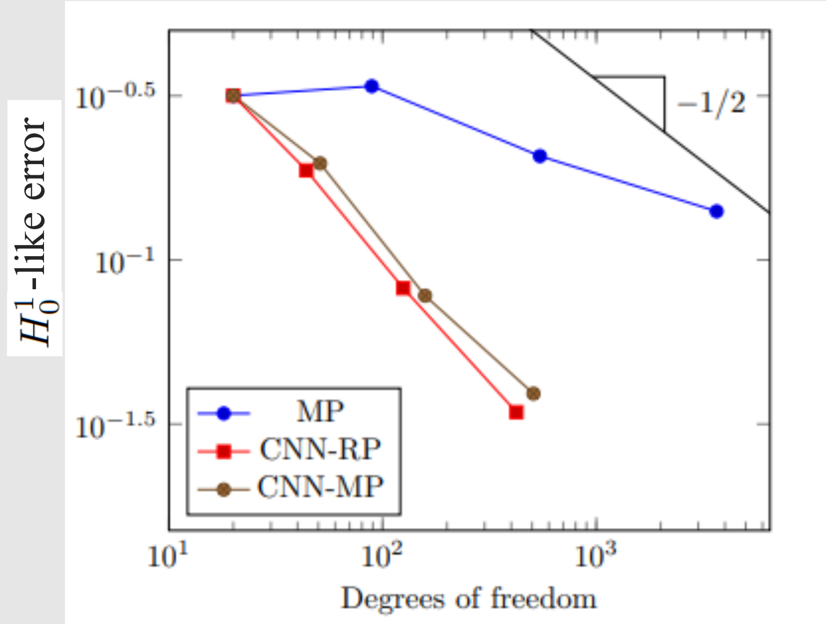
by satisfying stability and consistency conditions.

Solving the Poisson problem using the VEM (uniform refinement)

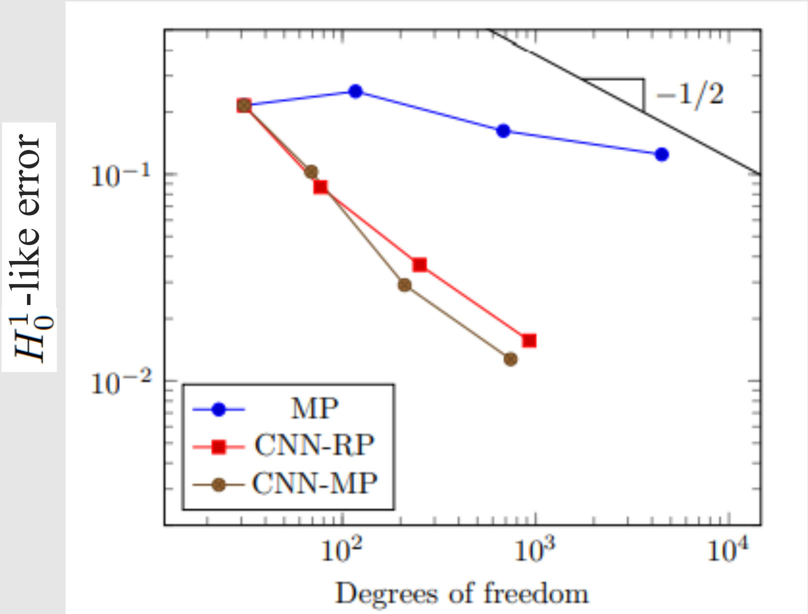
Triangular grid



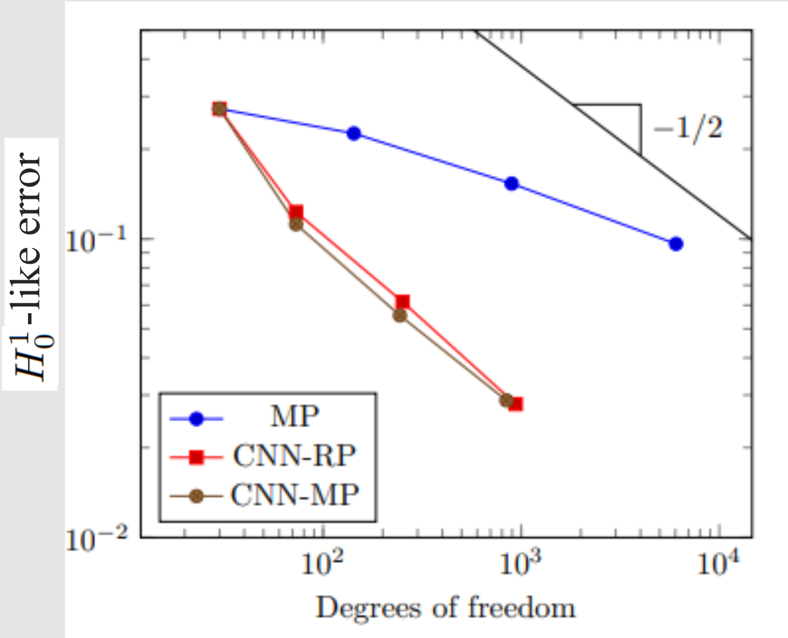
Voronoi grid



Smoothed-Voronoi grid

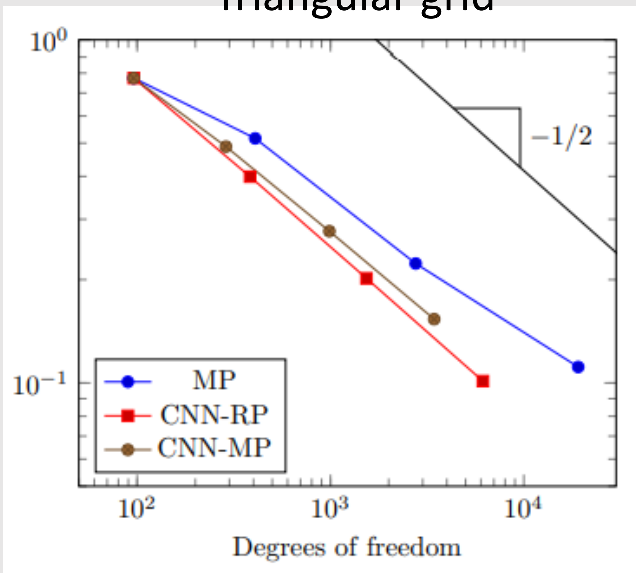


Non-convex grid

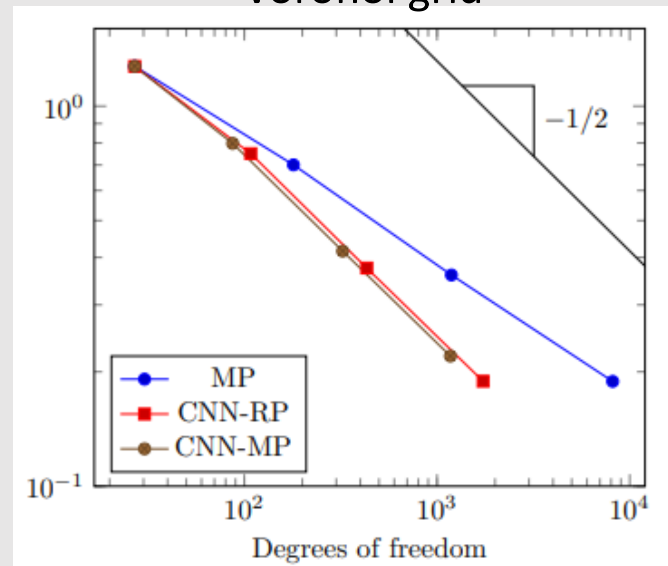


Solving the Poisson problem using the PolyDG method (uniform refinement)

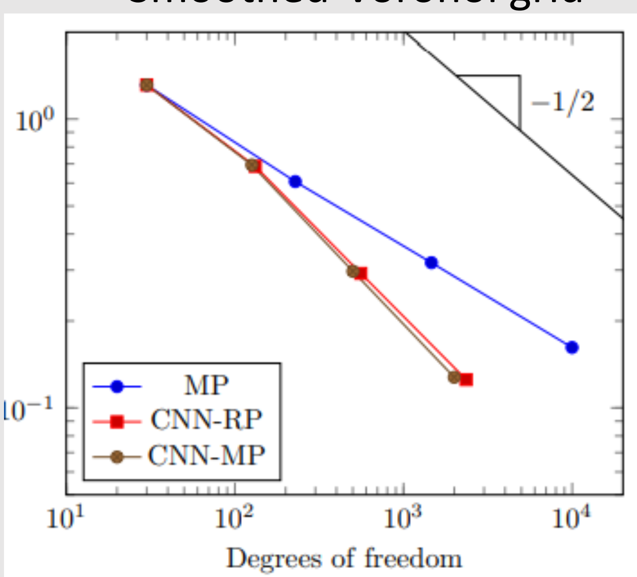
Triangular grid



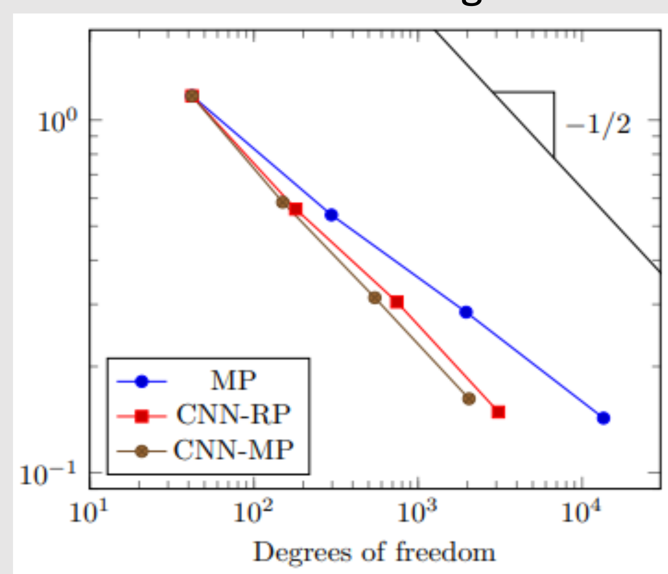
Voronoi grid



Smoothed-Voronoi grid



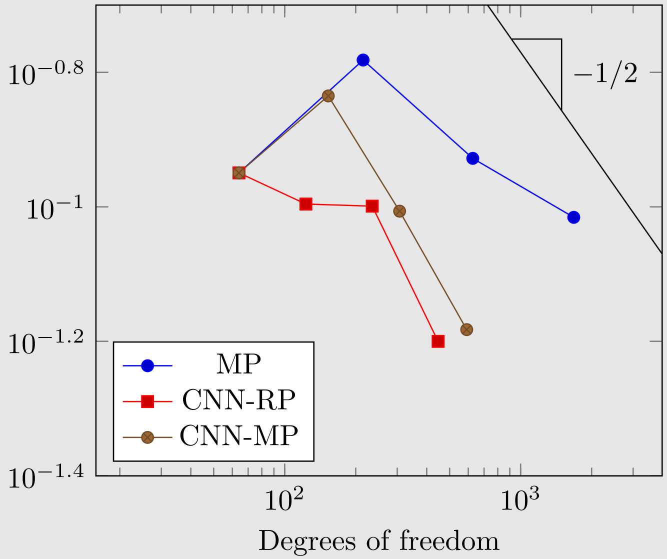
Non-convex grid



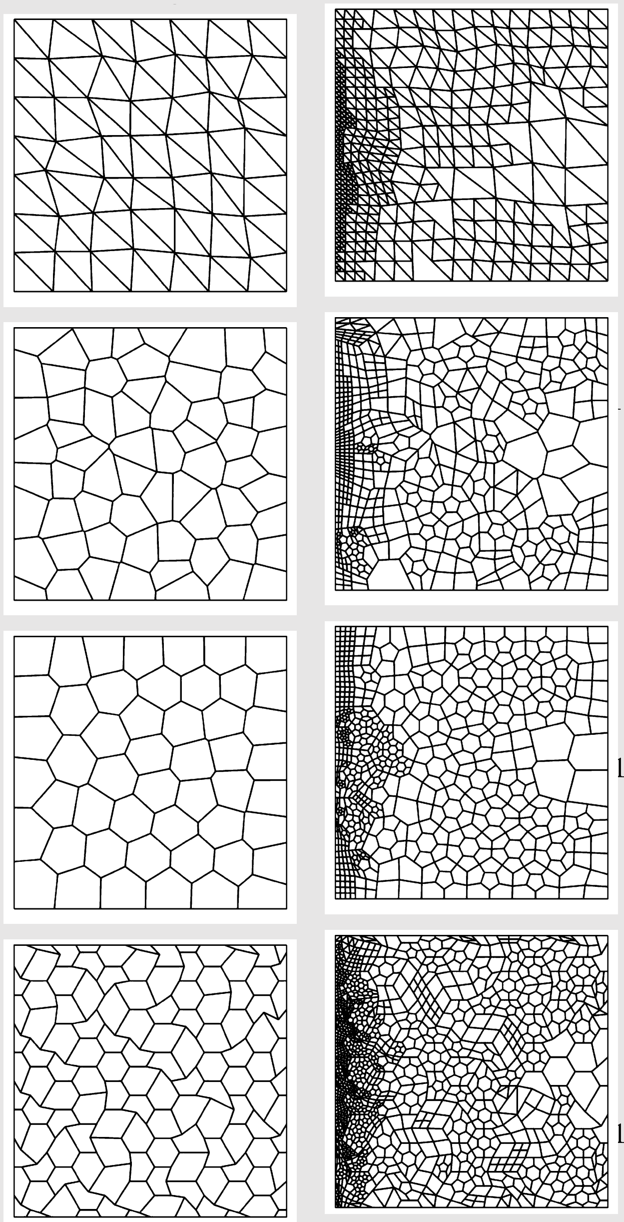
Analogous results for advection-diffusion and Stokes problems.

Solving the Poisson problem using the VEM (adaptive refinement)

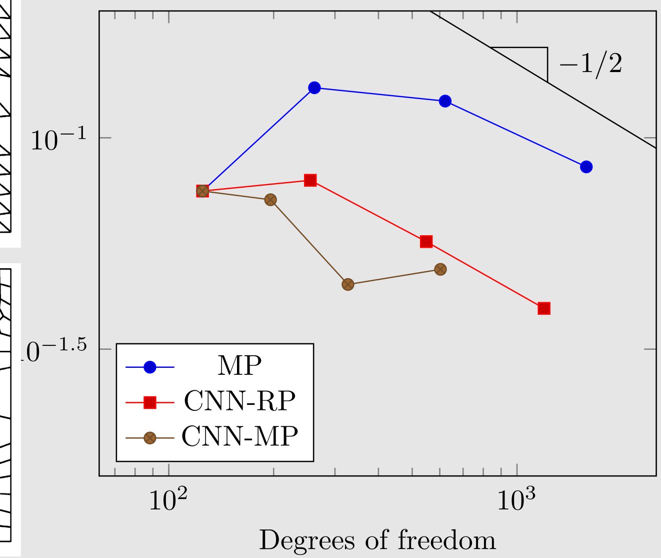
Triangular grid

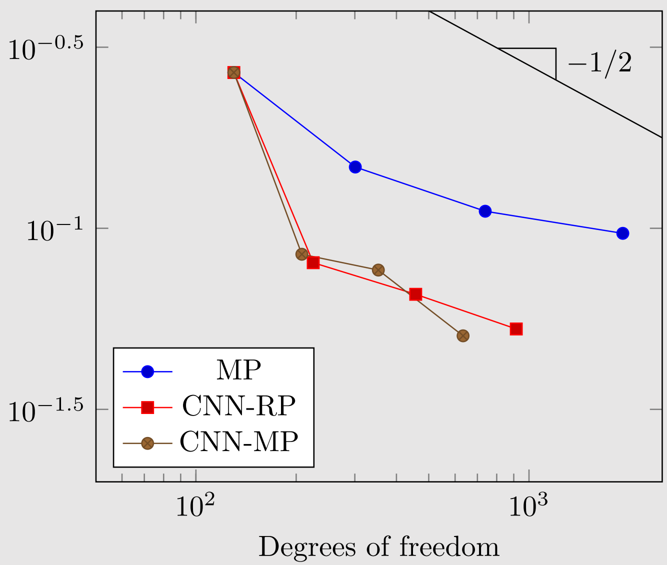


CNN-RP

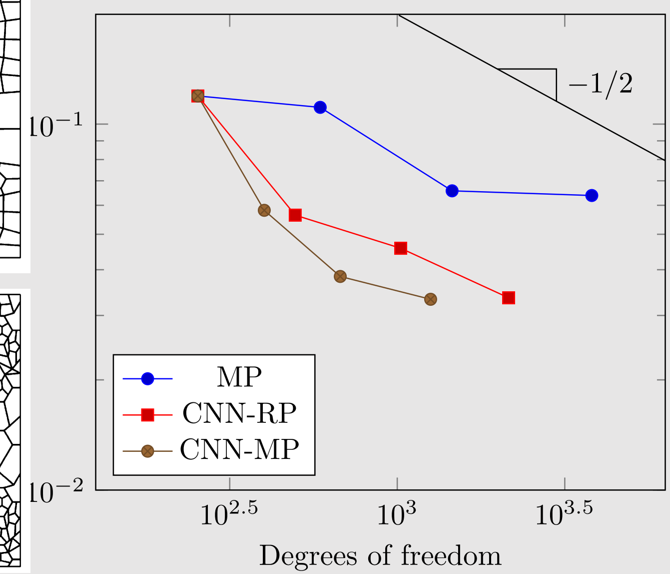


Smoothed-Voronoi grid





Voronoi grid



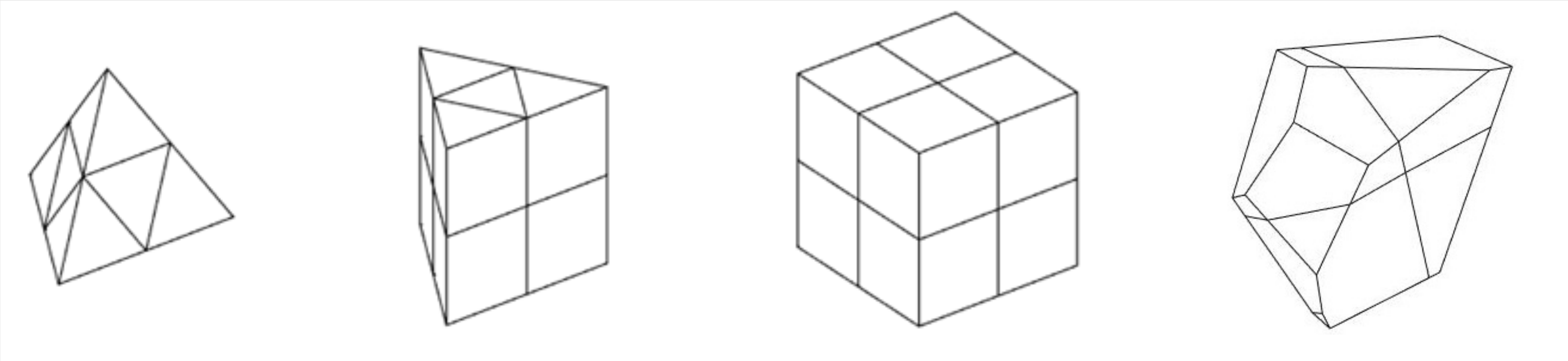
Non-convex grid

ML-enhanced mesh refinement (3D)

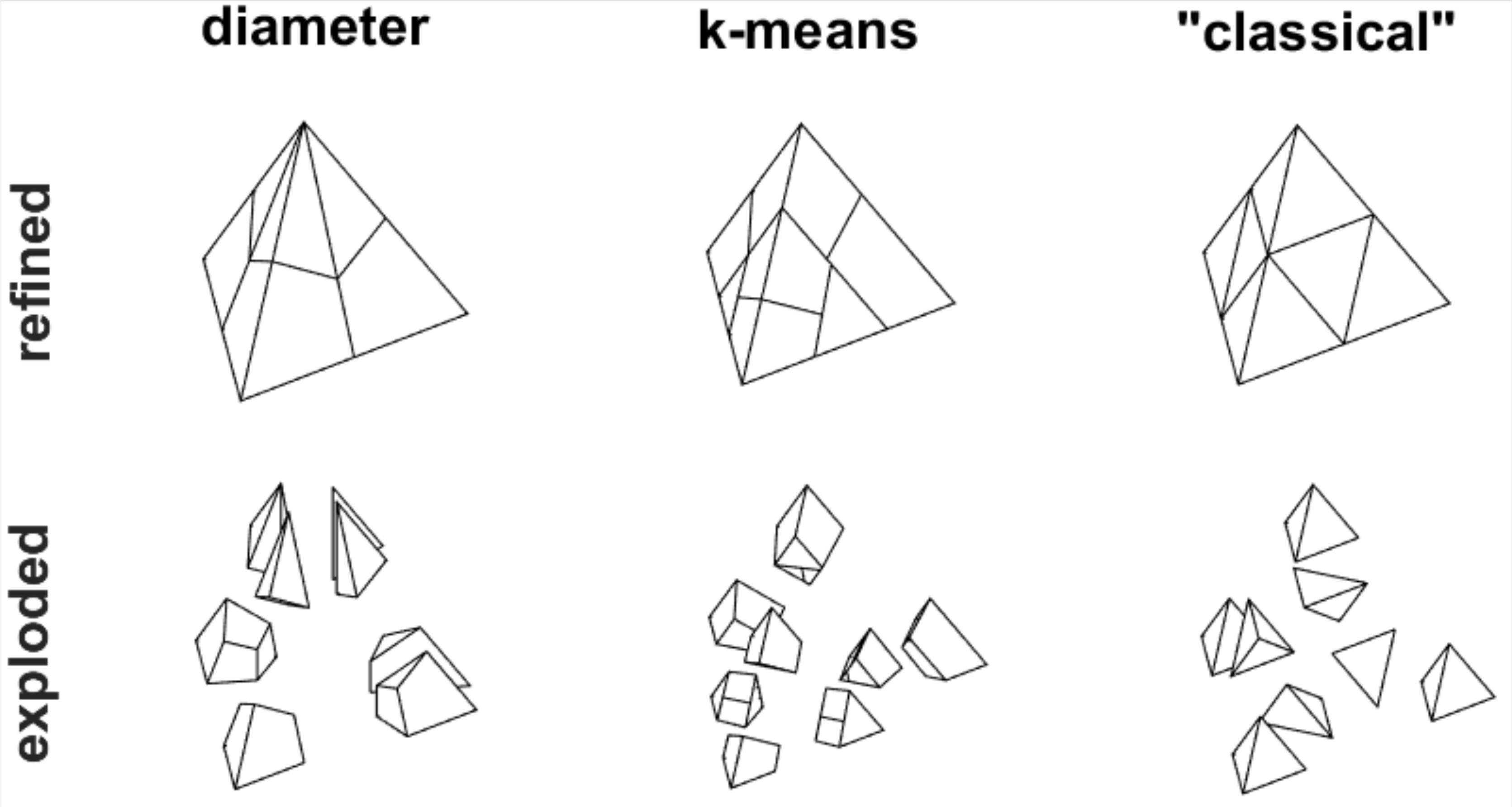
with E. Manuzzi and F. Dassi (U. Milano Bicocca)

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

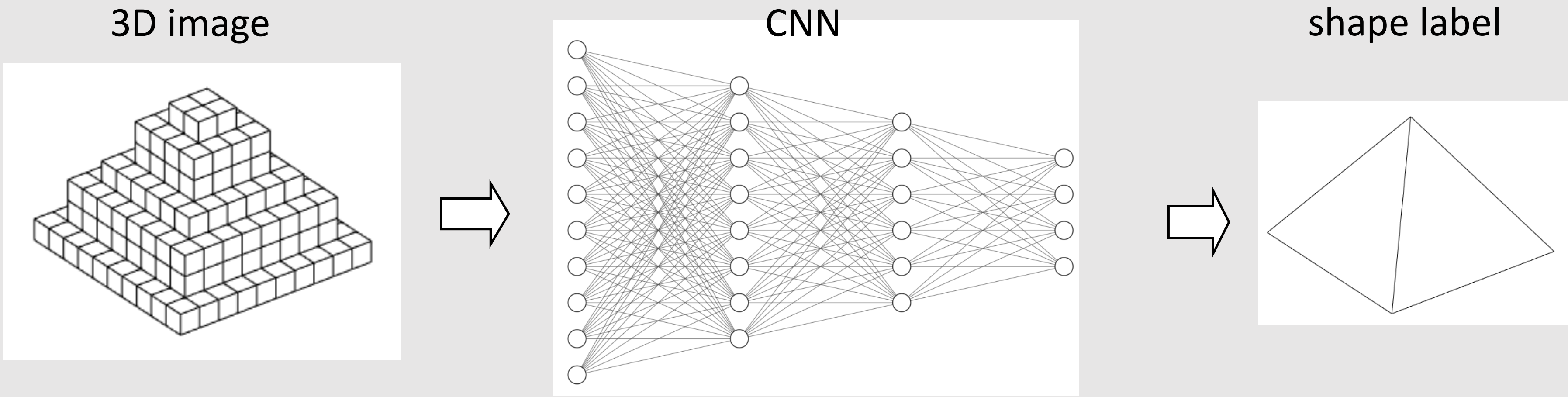


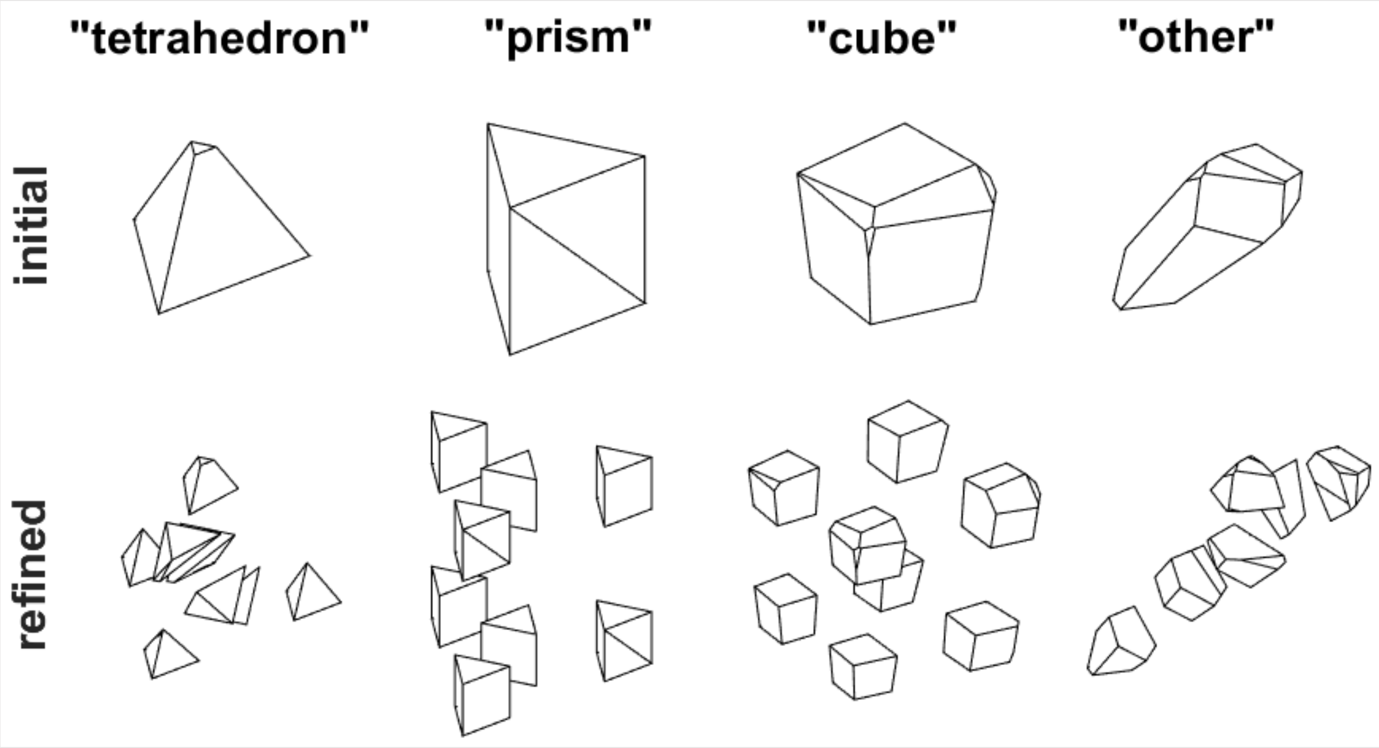
3D refinement strategies for general polyhedra



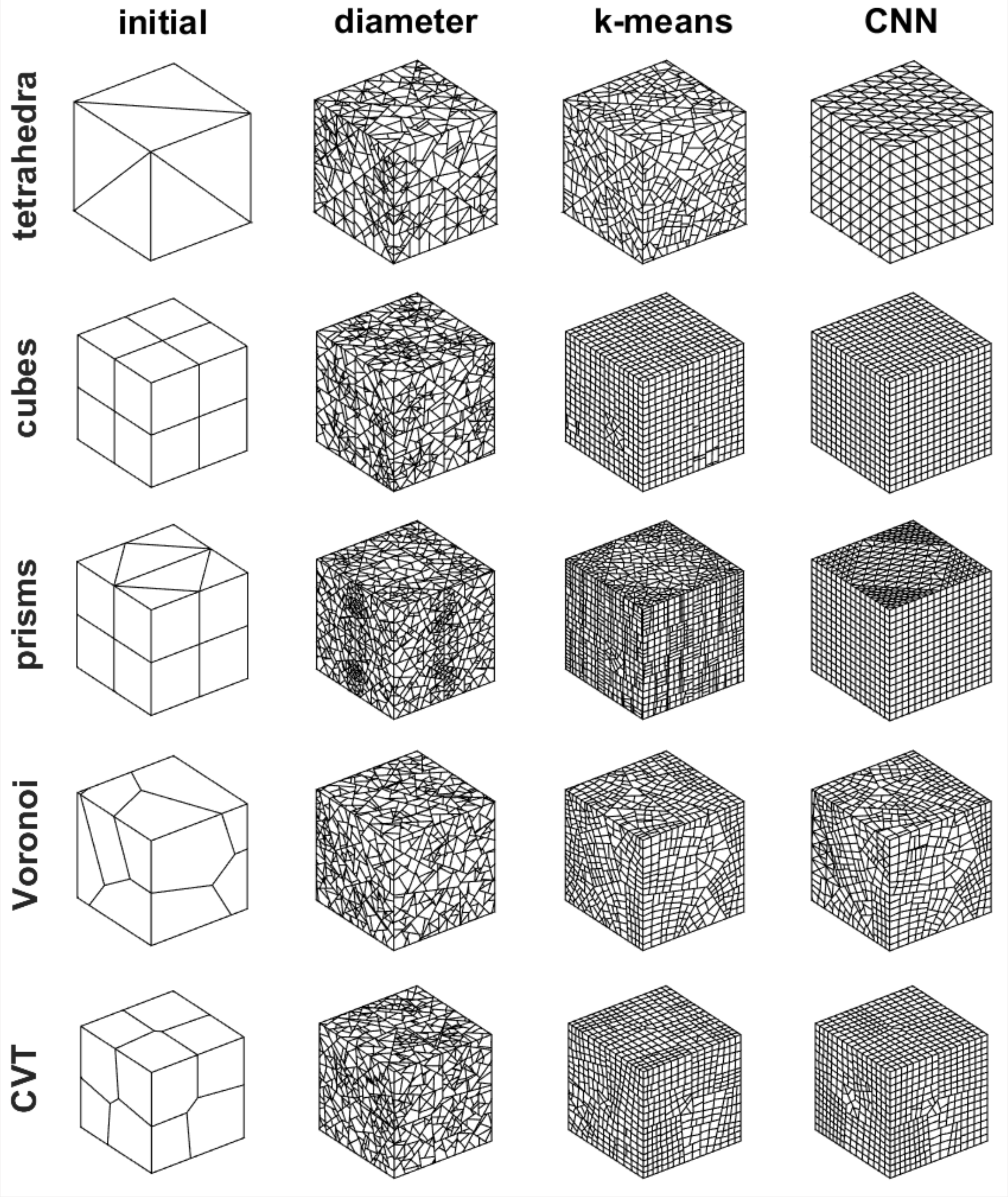
- Diameter strategy: cut the element perpendicular to its diameter.
- K-means strategy: cut the element balancing the volume distribution.
- "Classical" strategies: if the element has a specific shape refine it using a predefined strategy.

3D CNN-enhanced refinement strategies



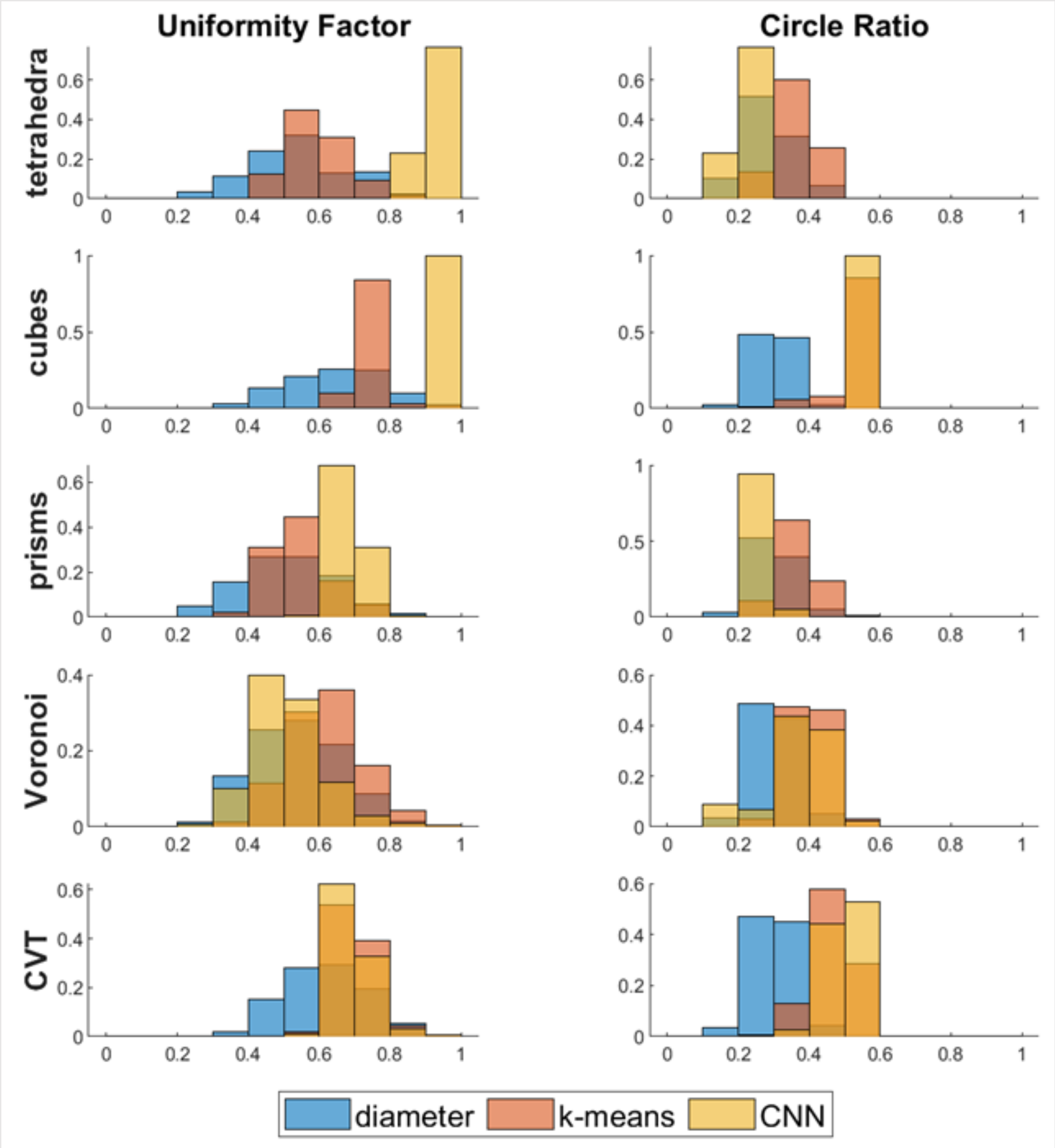


The CNN classifies the 3D image of the input polyhedron according to its shape, in order to apply suitable refinement strategies. Elements in class "other" are refined using the k-means strategy.



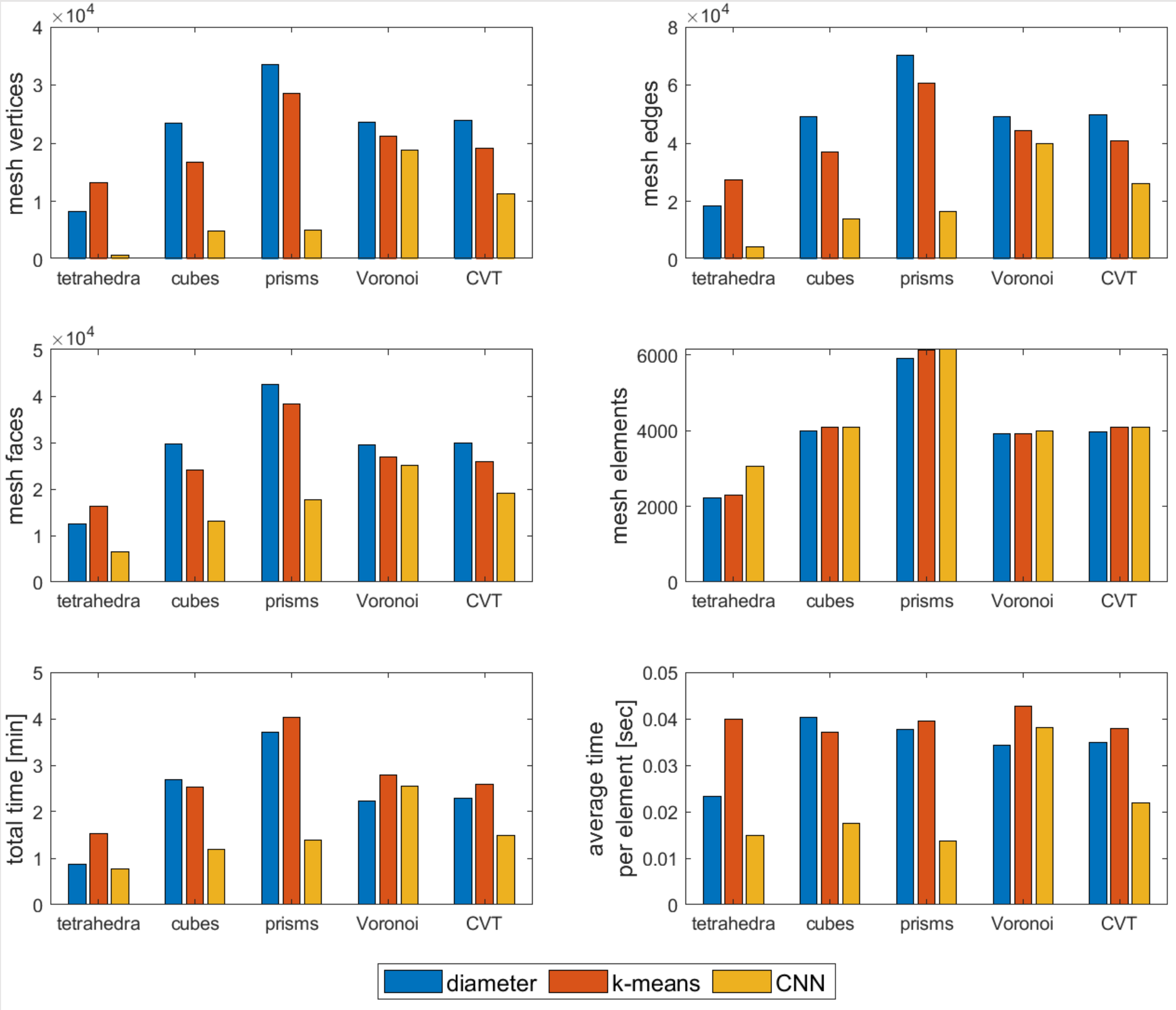
Refined grids obtained after three steps of uniform refinement based on employing the diameter, the k-means and the CNN strategies.

Quality Metrics



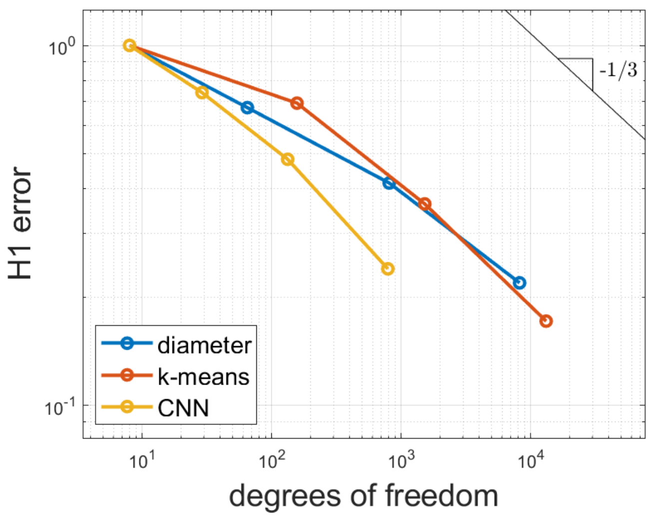
$$\text{Uniformity Factor} = \frac{\text{element size}}{\text{mesh size}} \qquad \text{Circle Ratio} = \frac{\text{inscribed circle radius}}{\text{circumscribed circle radius}}$$

Effects of ML-based refinement strategies on statistics of computational complexity

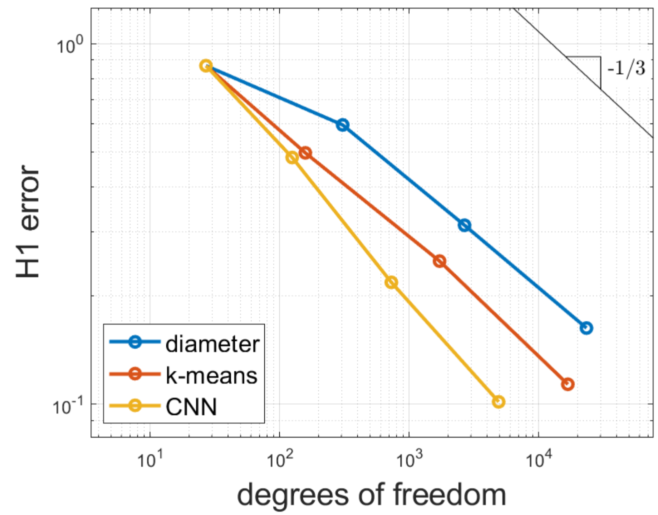


Solving the Poisson problem with the VEM (3D)

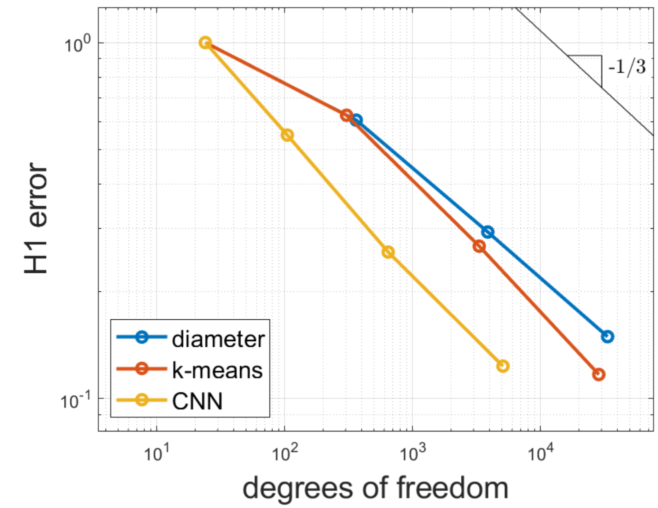
Tetrahedra grid



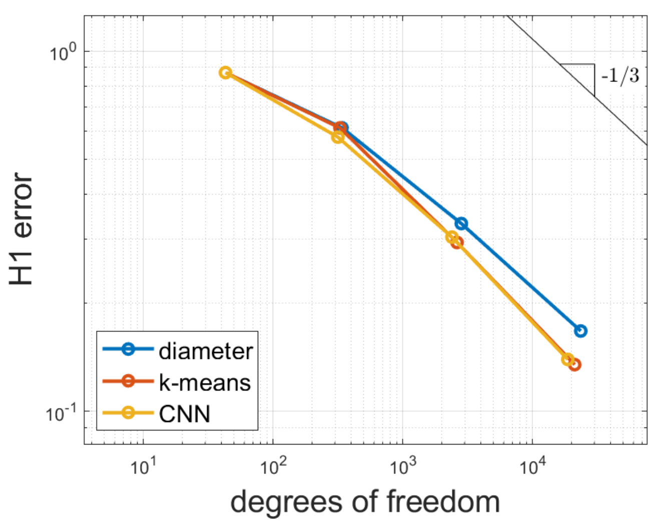
Cubes grid



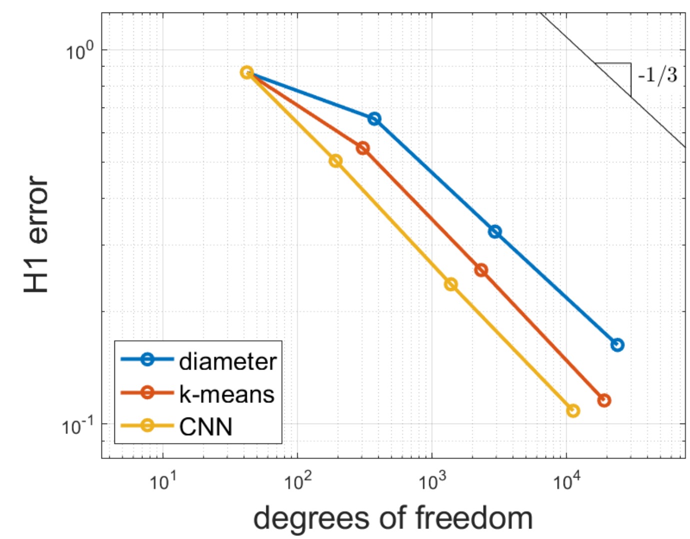
Prisms grid



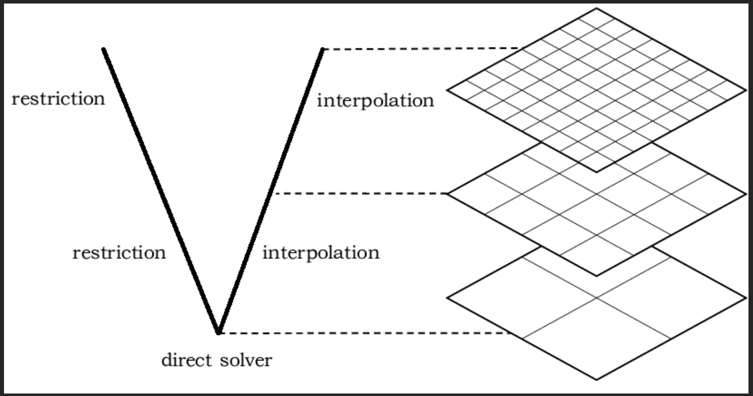
Voronoi grid

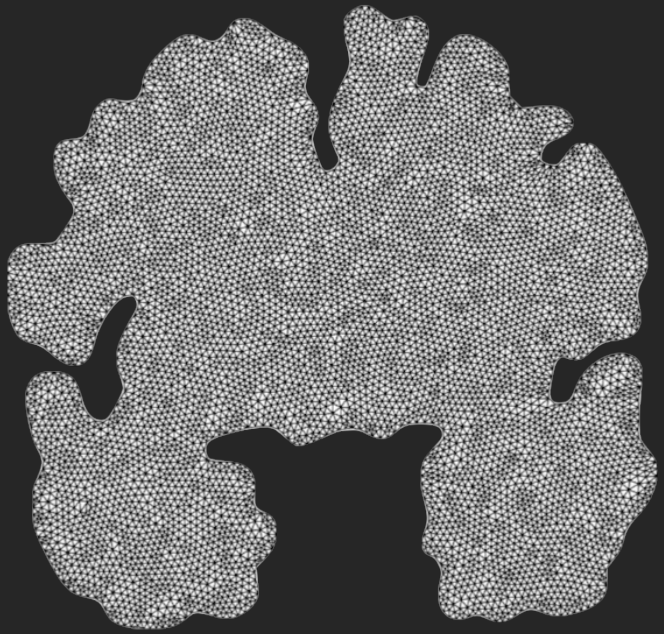


CVT grid



Analogous results for the VEM of order higher than 1.





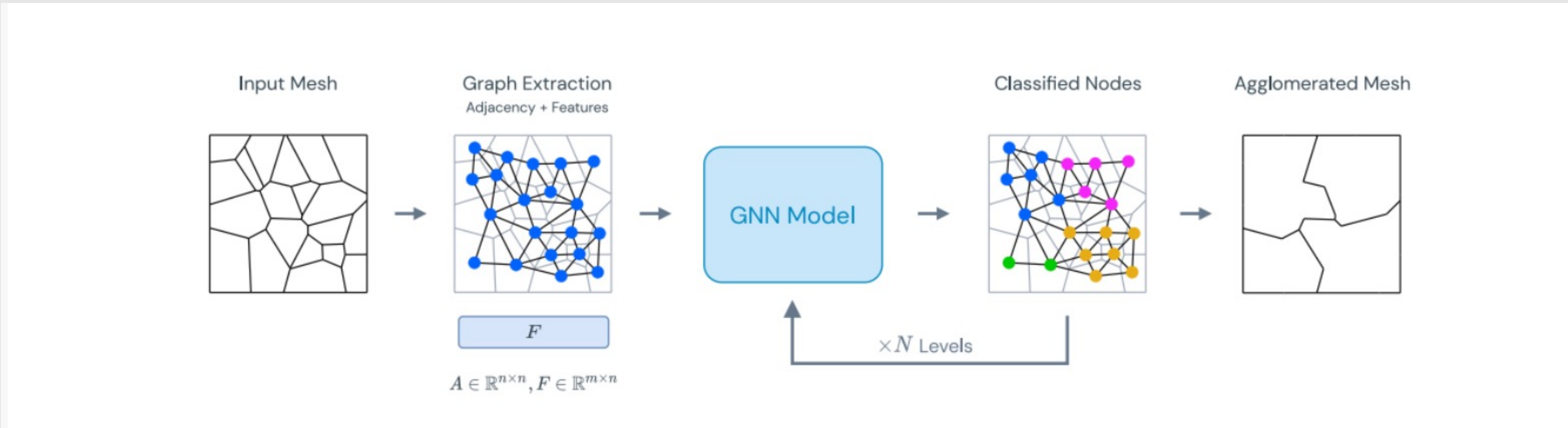
ML-enhanced agglomeration strategies

Merging neighboring mesh elements to obtain a coarser grid.

- Design of multilevel solvers

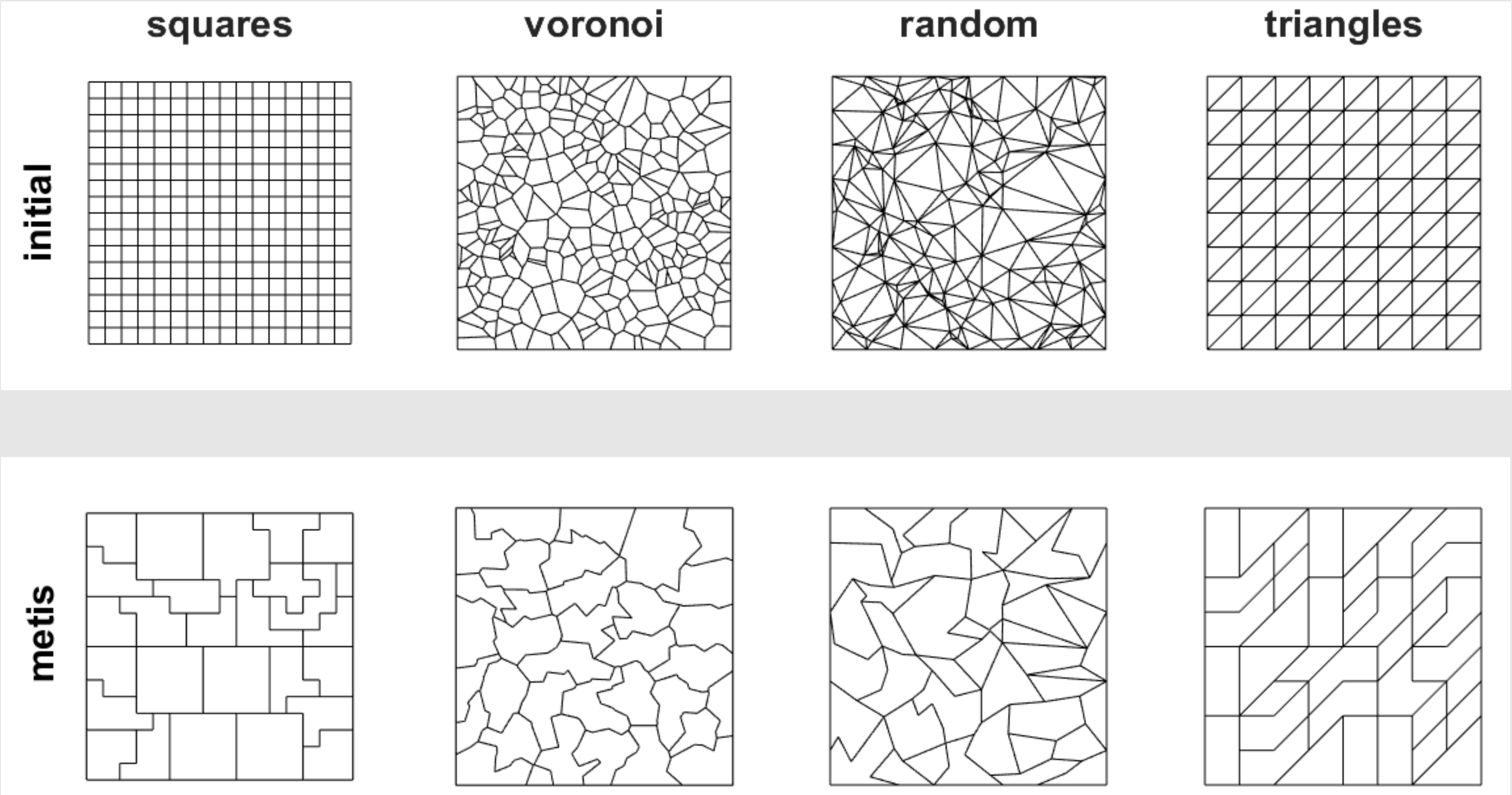
- Defeaturing of complex geometries

Agglomeration using Graph Neural Networks (so far)



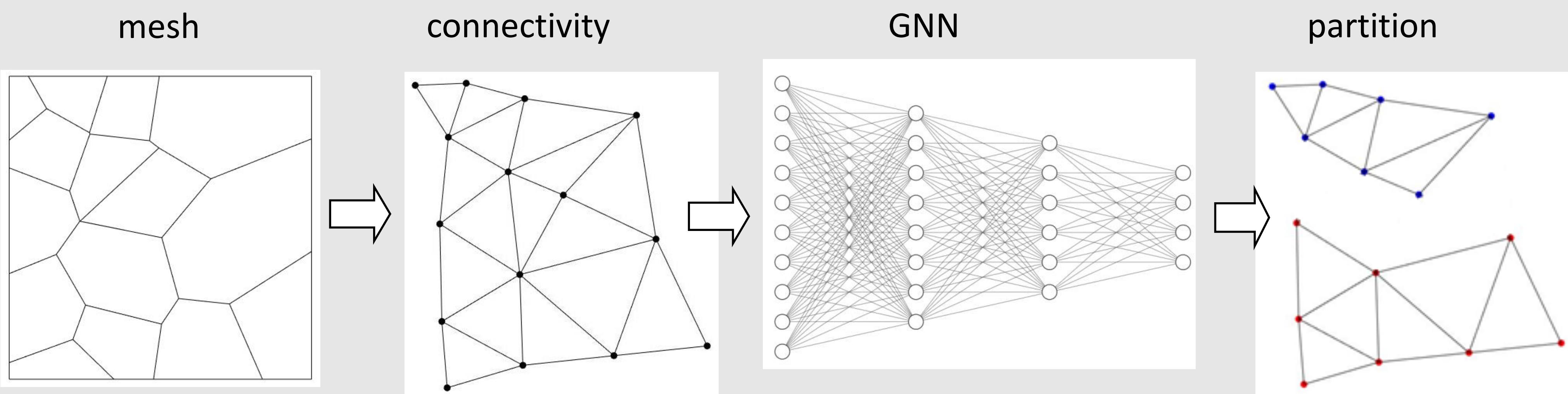
Objective:
Find a partition with minimal interconnections between sets, while keeping errors (volumes) balanced.

Advantages:
Fast inference and full exploitation of both graph and geometrical features.



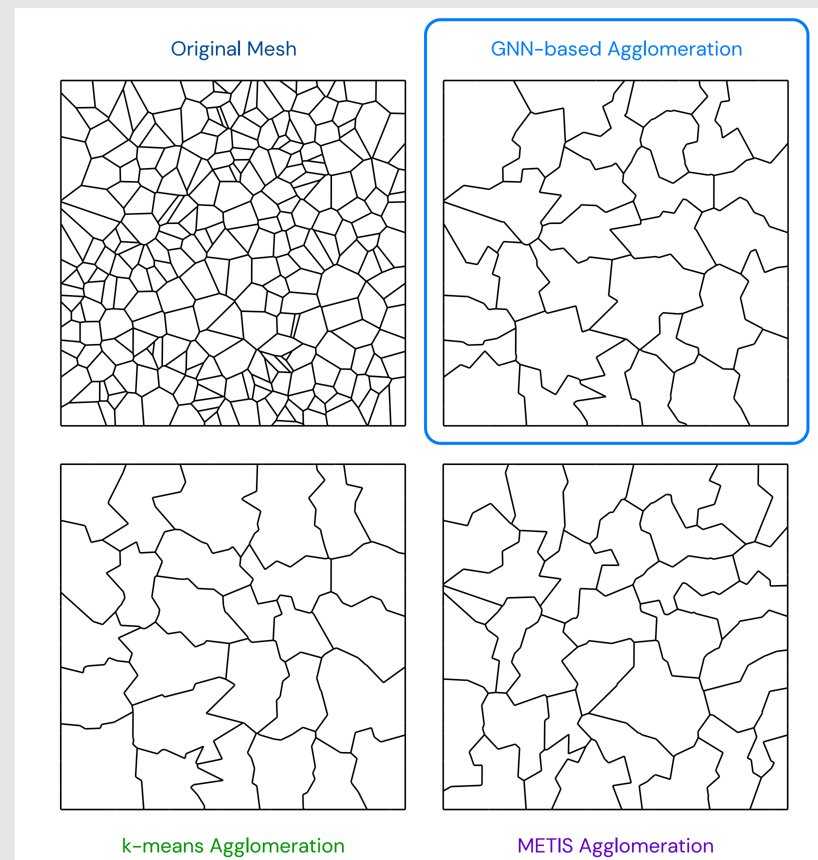
Agglomerated grids based on employing metis. Metis is «standard» for graph partitioning.

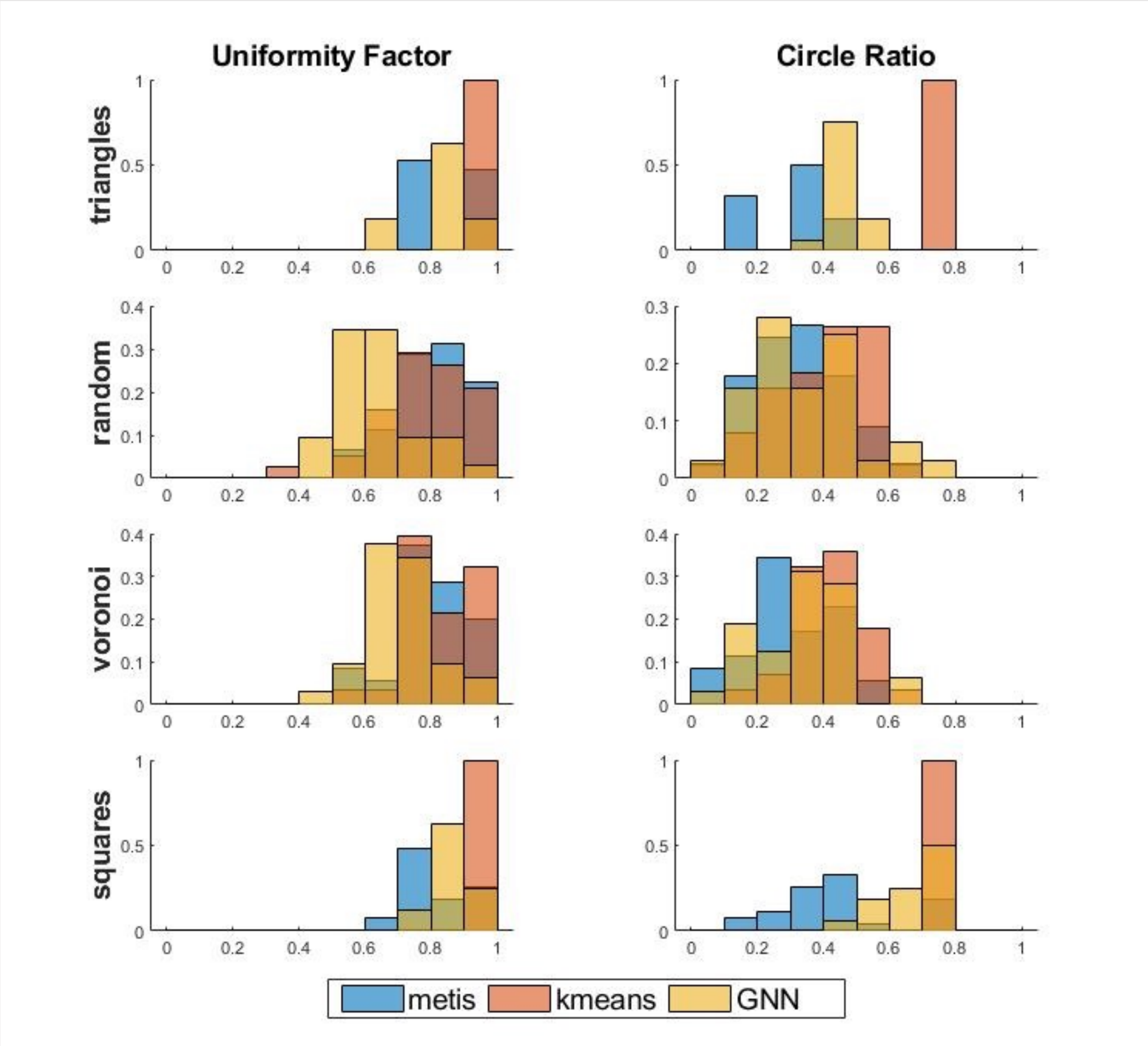
Agglomeration using Graph Neural Networks (so far)



GNN-based method can be competitive wrt SotA methods (Metis, Kmeans, …)?

- Implement different model architectures
- Optimize model's runtime





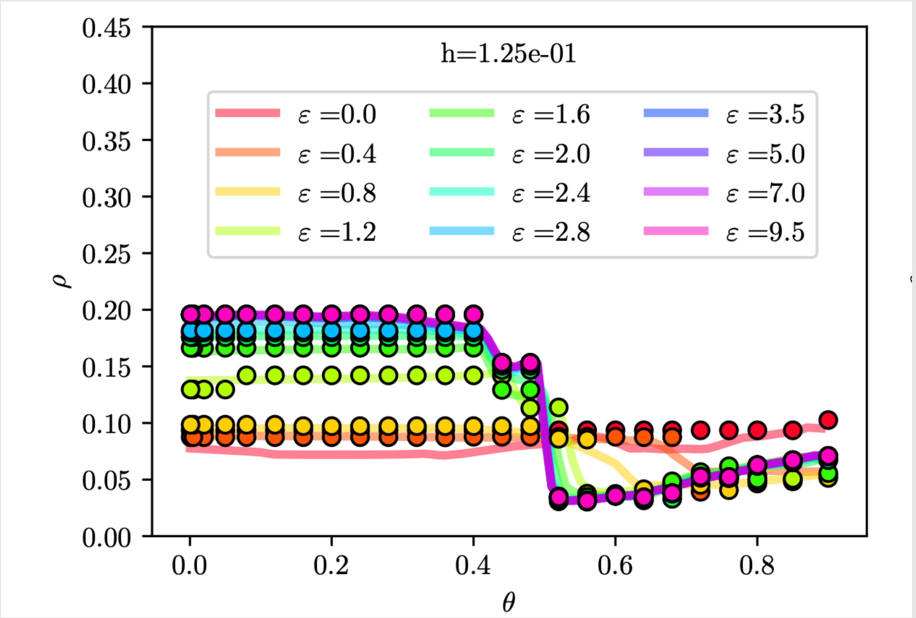
Quality factors

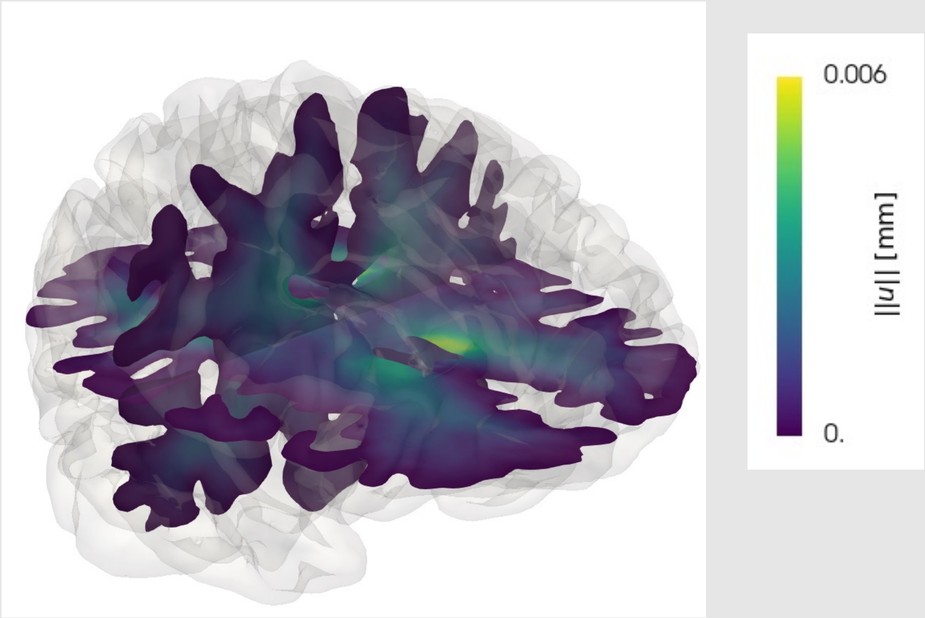
Conclusions

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

Ongoing

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 θ as the one the ANN predicts to give the best performance.
4. Application of the described algorithms in the context of
   - Modelling neurodegenerative deseases
   - Geophysical applications, including fluid-structure interaction with complex and moving geometries.





Thank you for your attention !!

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