Machine Learning-Enhanced Polytopal Finite Element Methods

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Outline

- Machine Learning-Enhanced Refinement strategies for polygonal/ polyhedral grids

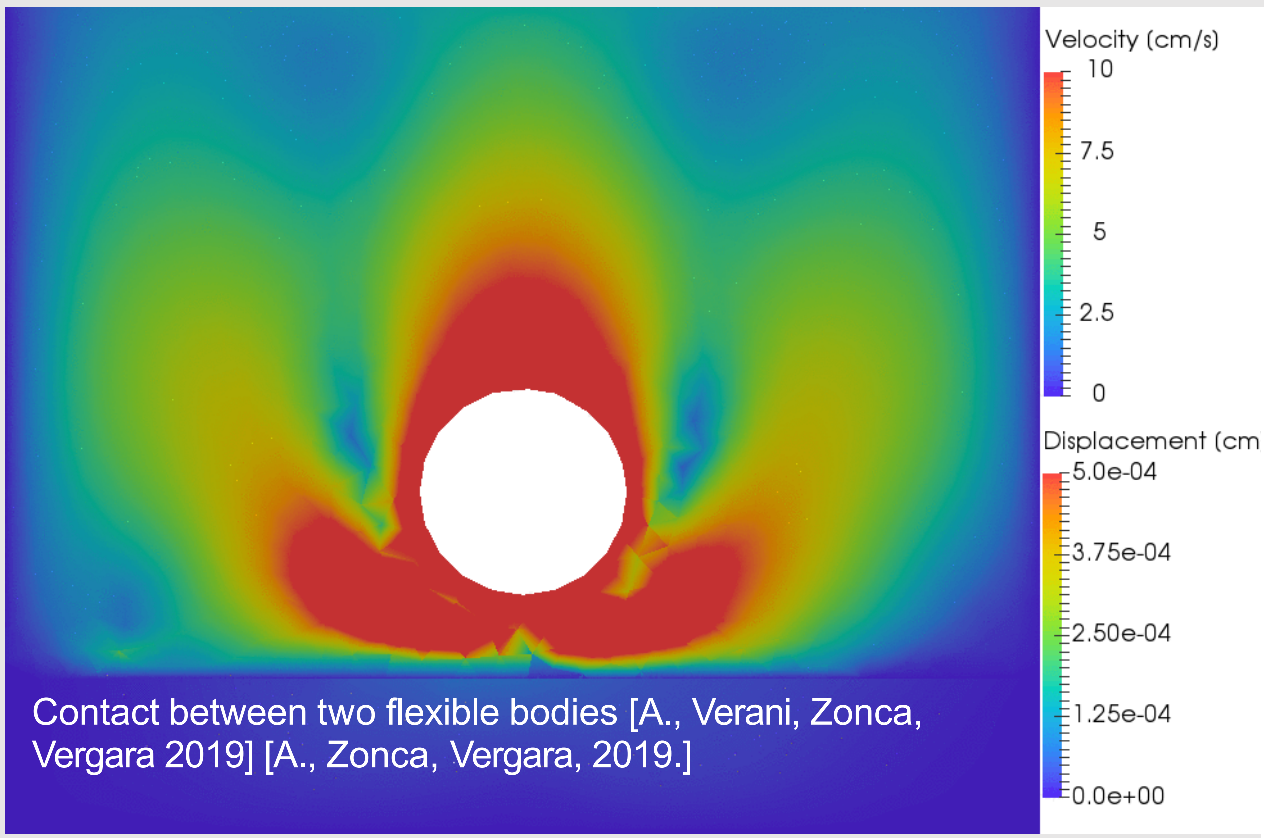
- From Refinement to agglomeration based on Machine Learning-Enhanced techniques

- Applications
    - Modelling brain physiology and neurodegenerative disorders
    - Modelling safety exploitation of subsurface soil

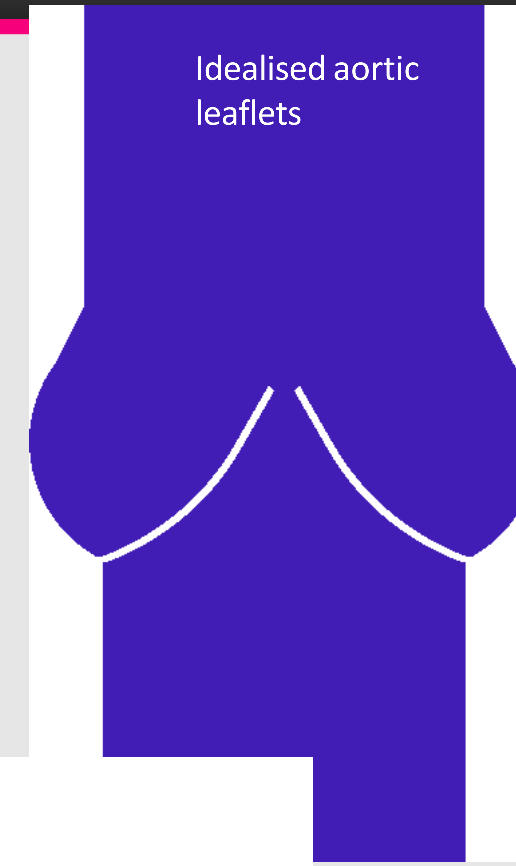
Joint work with: Enrico Manuzzi, Gabriele Martinelli

Motivations

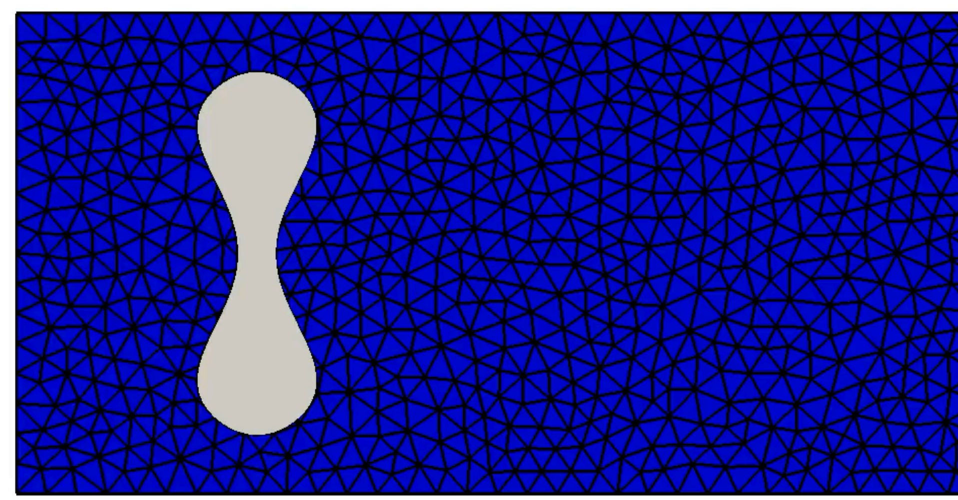
Many engineering and geophysical applications are posed on complex (possibly moving) physical domains (fluid-structure interaction, crack propagation, flow in fractured porous media).



Contact between two flexible bodies [A., Verani, Zonca, Vergara 2019] [A., Zonca, Vergara, 2019.]



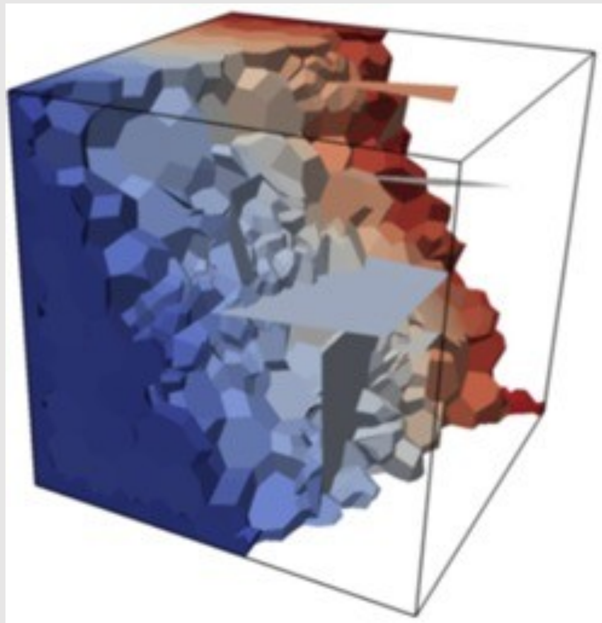
Idealised aortic leaflets

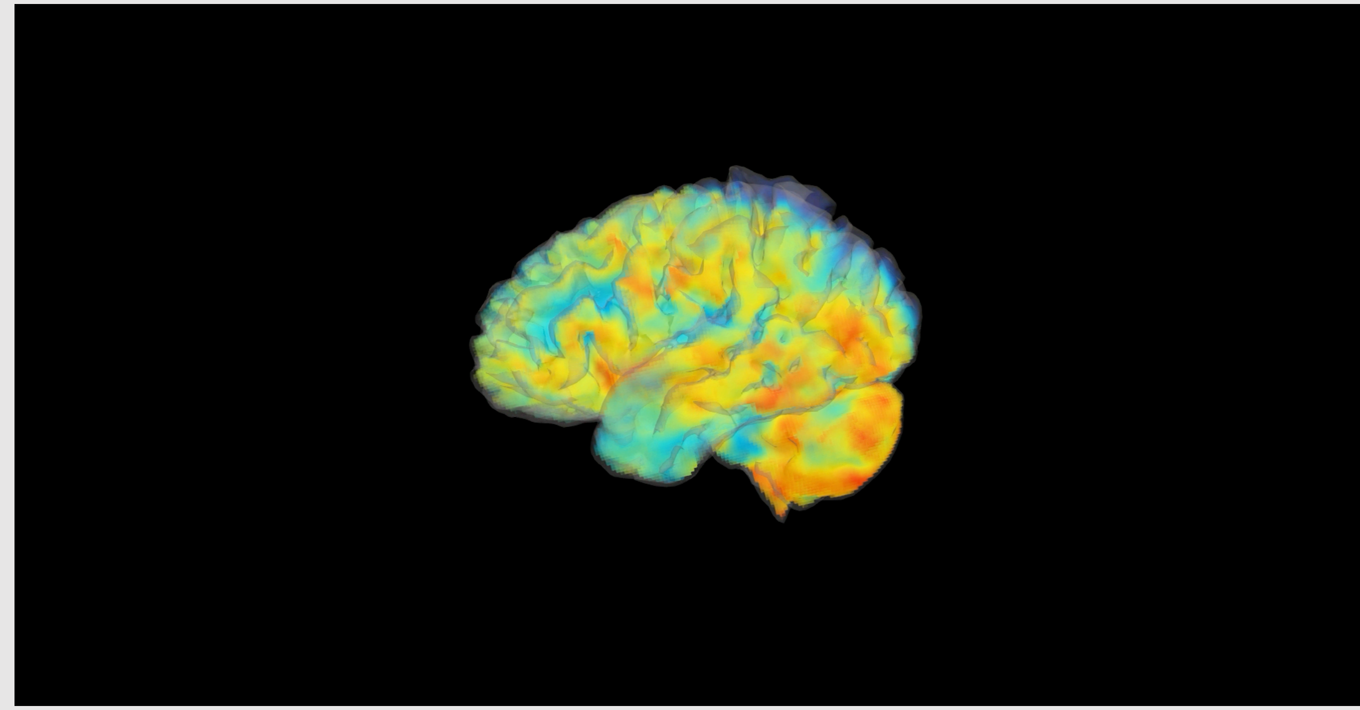


Evolution of an ideal red blood cell experiencing large displacements

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

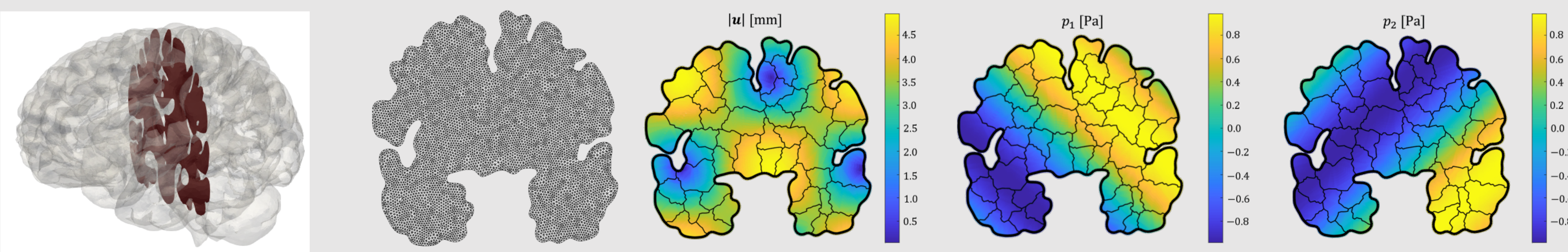
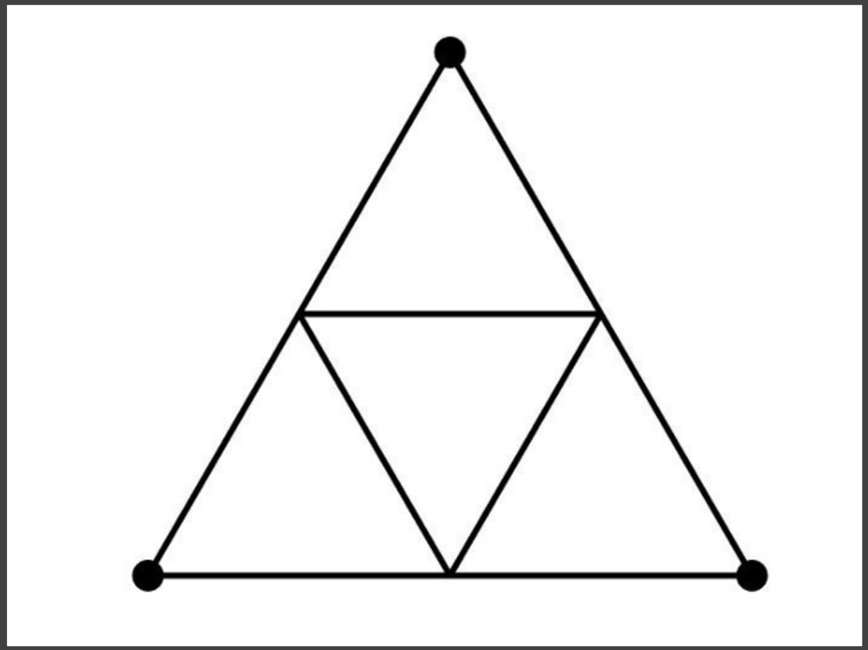
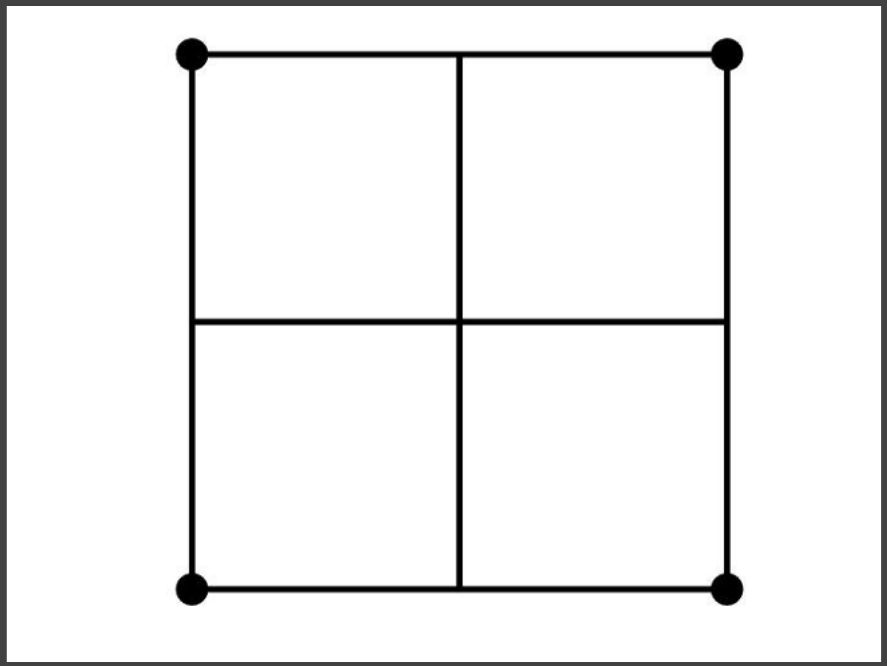


Figure: Agglomerated mesh of brain slice (with GNN)

ML-enhanced mesh refinement (2D)

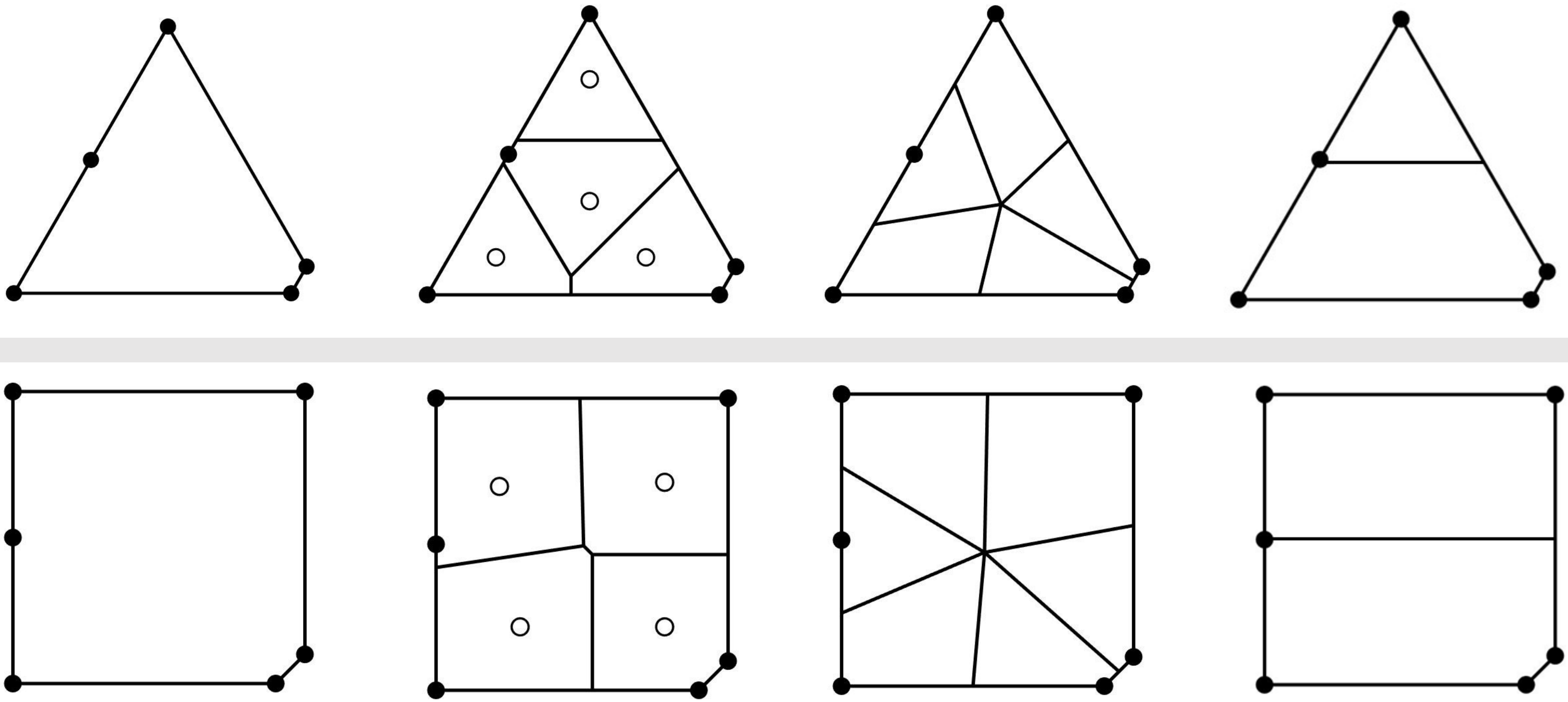




Refinement strategies for triangles and quadrilaterals.

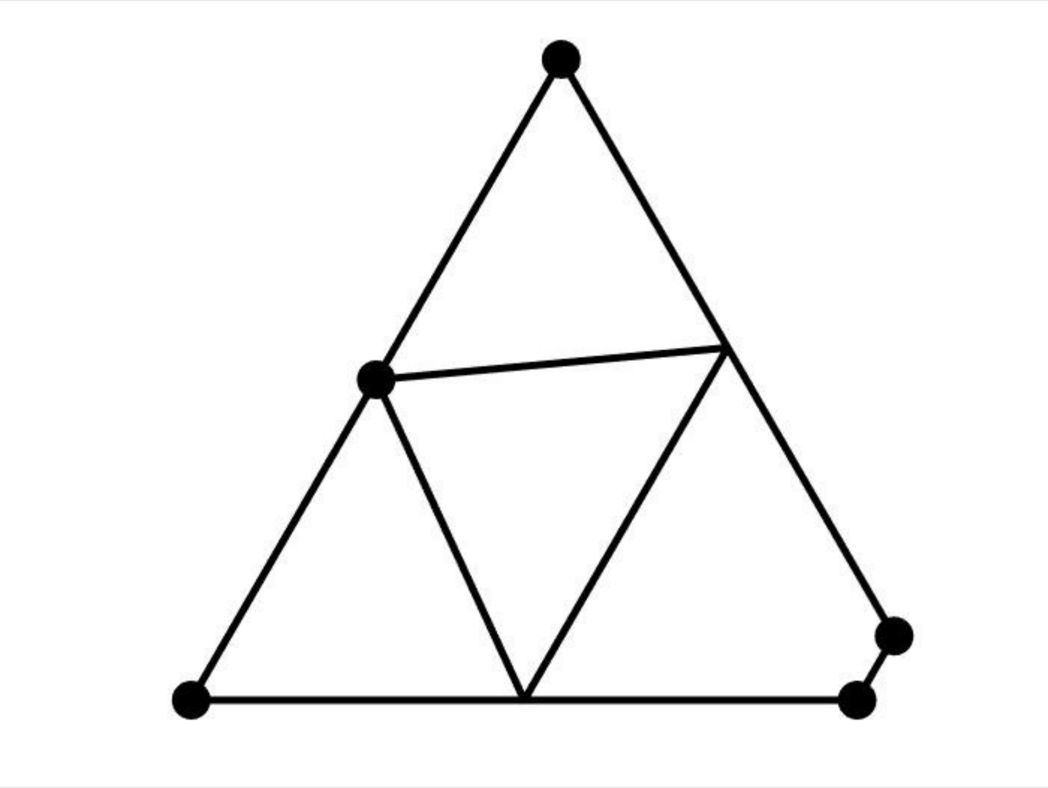
Refinement strategies for general polygons

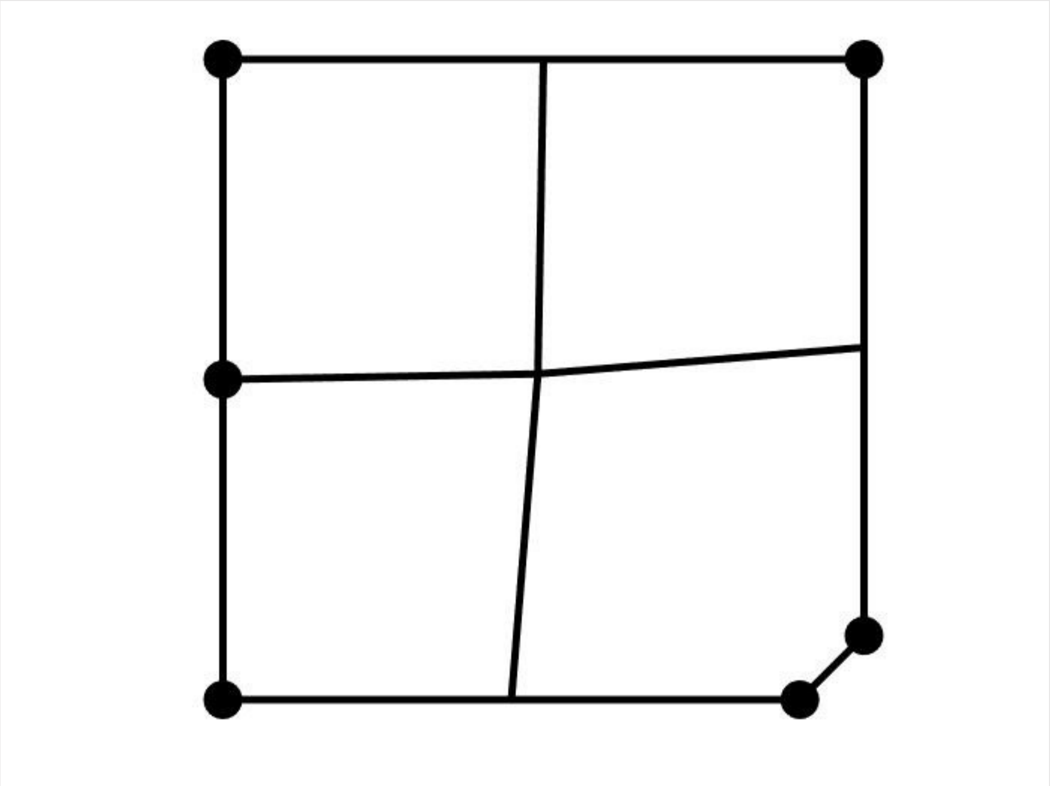
initial polygons	Voronoi	midpoint	preferential direction*



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

“Ideal” strategy



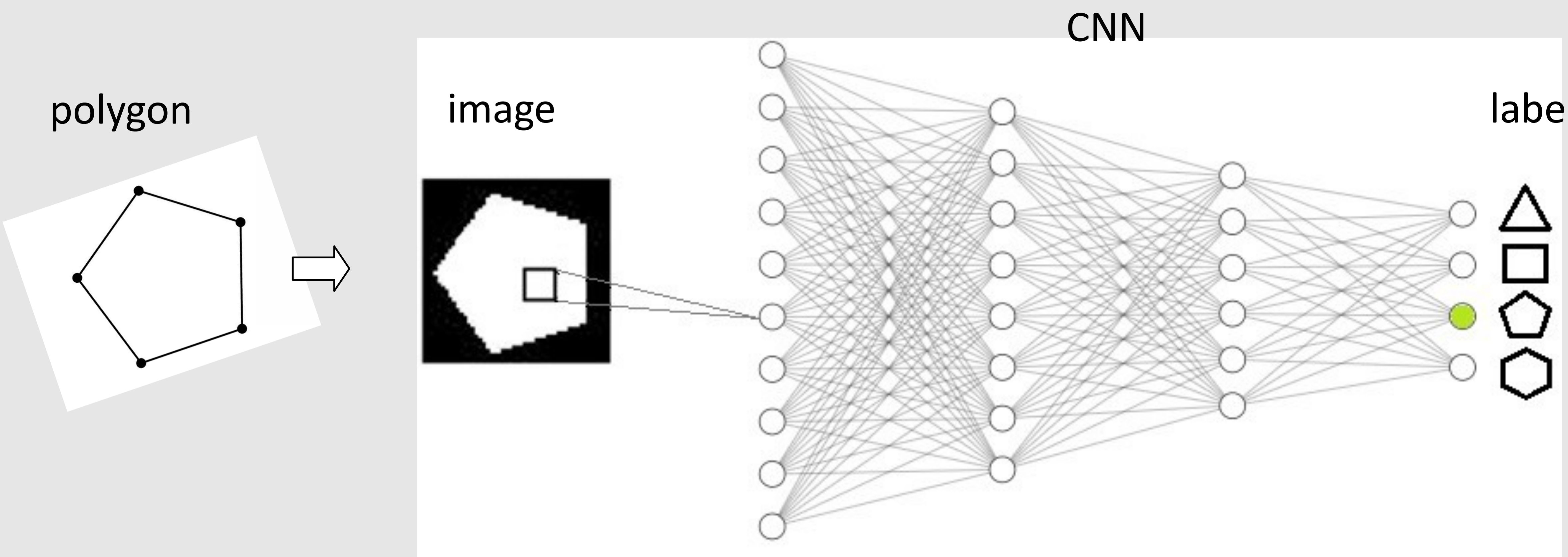


1. Classify the "**shape**" of a polygon.
2. Apply a suitable refinement for that specific shape.

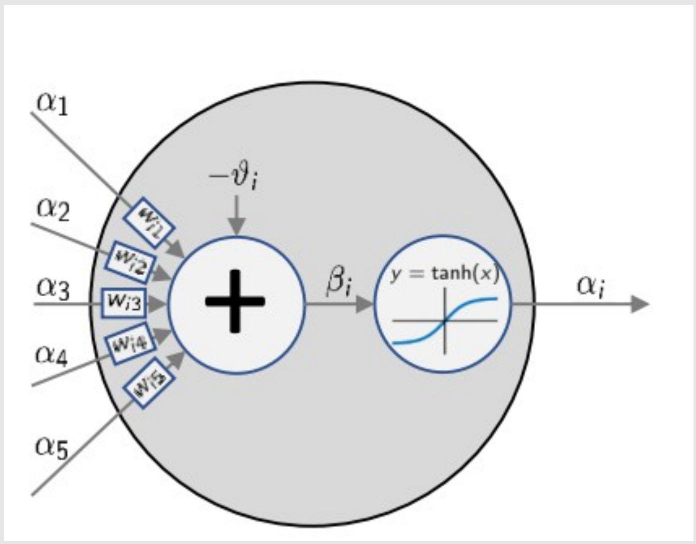
Step 1 can be learned from a database of examples using Machine Learning (ML).

[A., Manuzzi, JCP, 2022]

Image classification using Convolutional Neural Networks (CNNs)



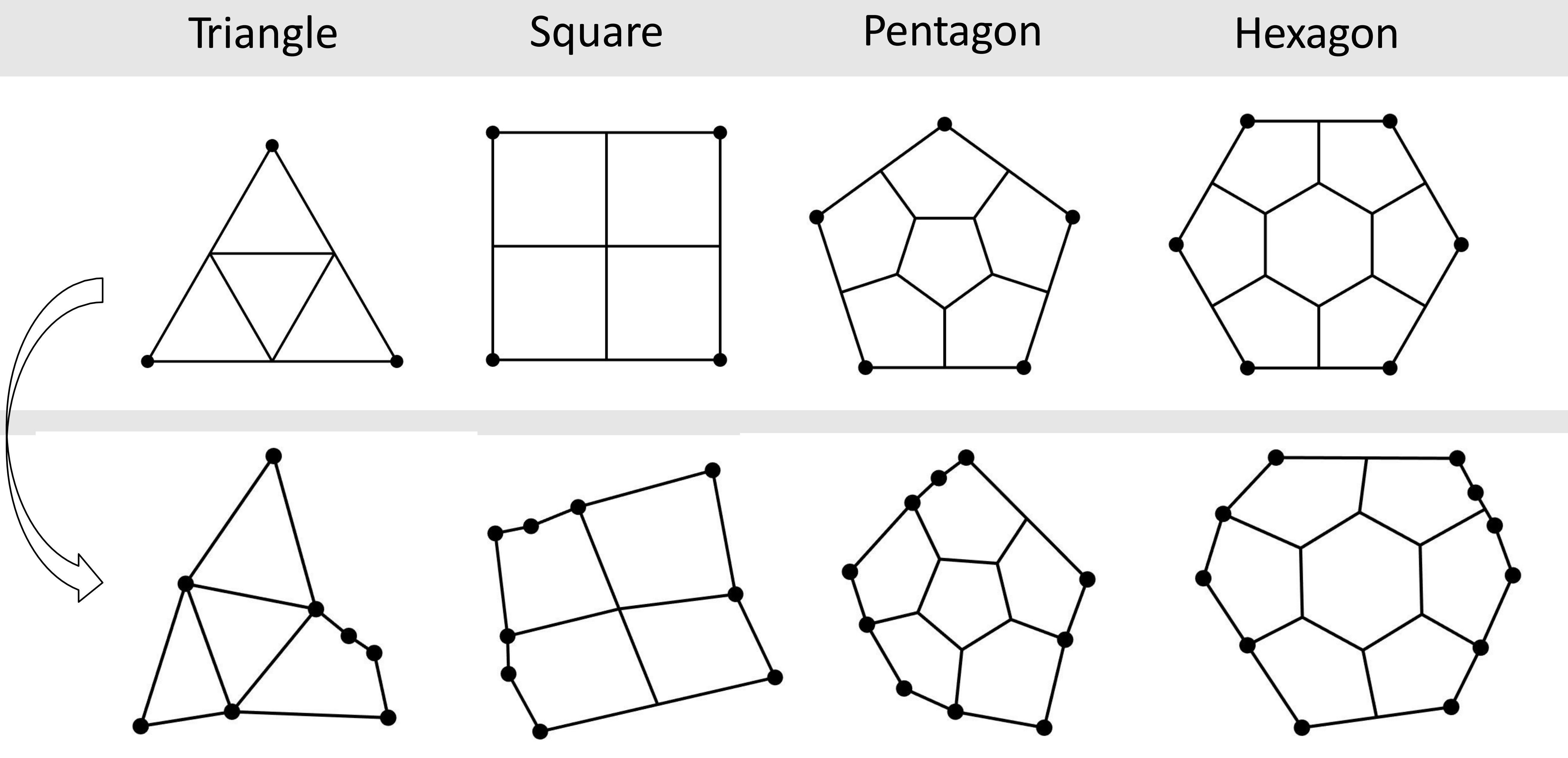
neuron



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

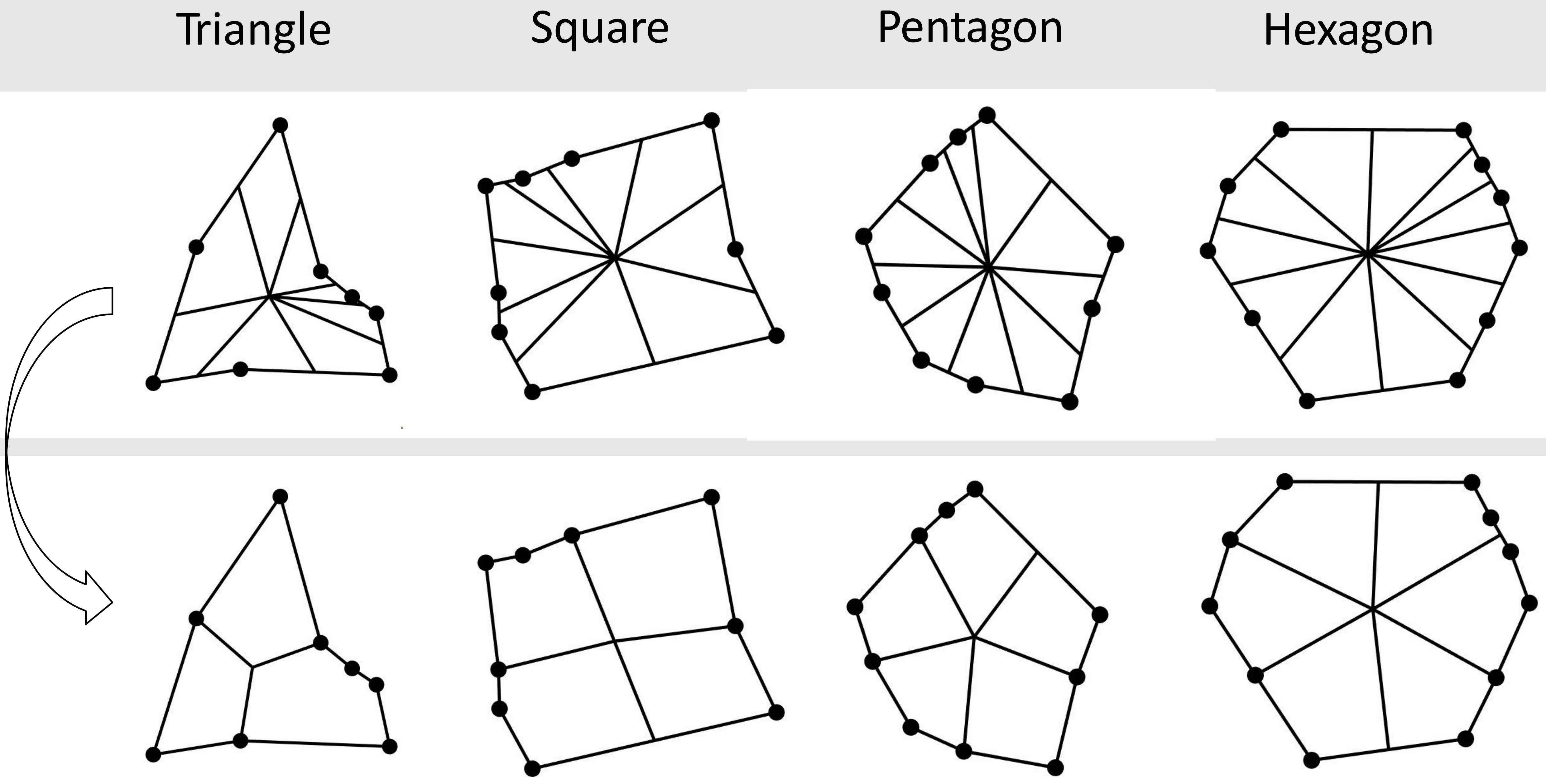
It is expensive but it can be done offline once and for all, while online classification is very fast.

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".

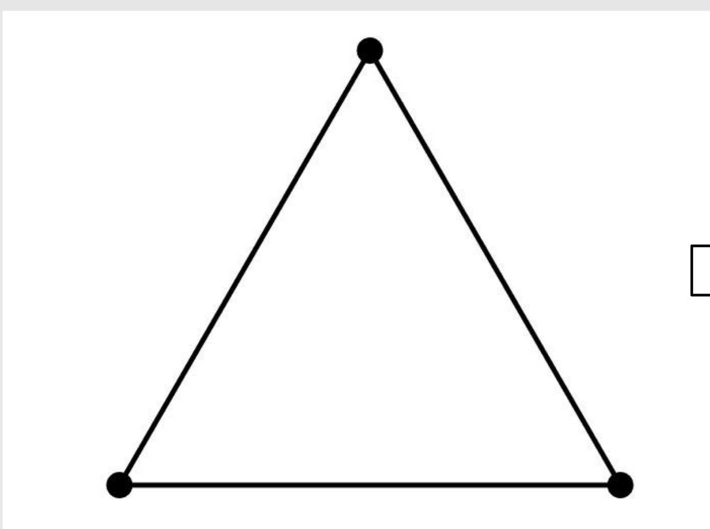
Algorithm 2: CNN-enhanced Mid-Point (CNN-MP) strategy



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

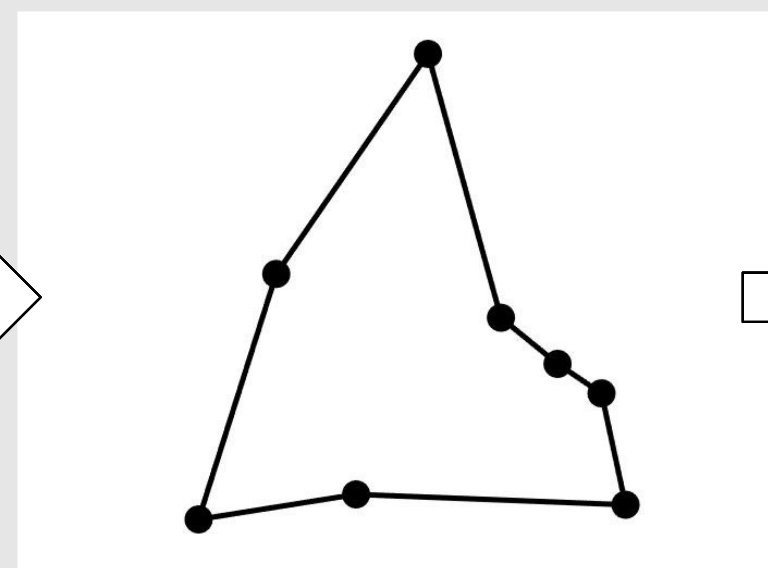
Automatic dataset generation

Reference polygon



Label: "Triangle"

Small distortions applied

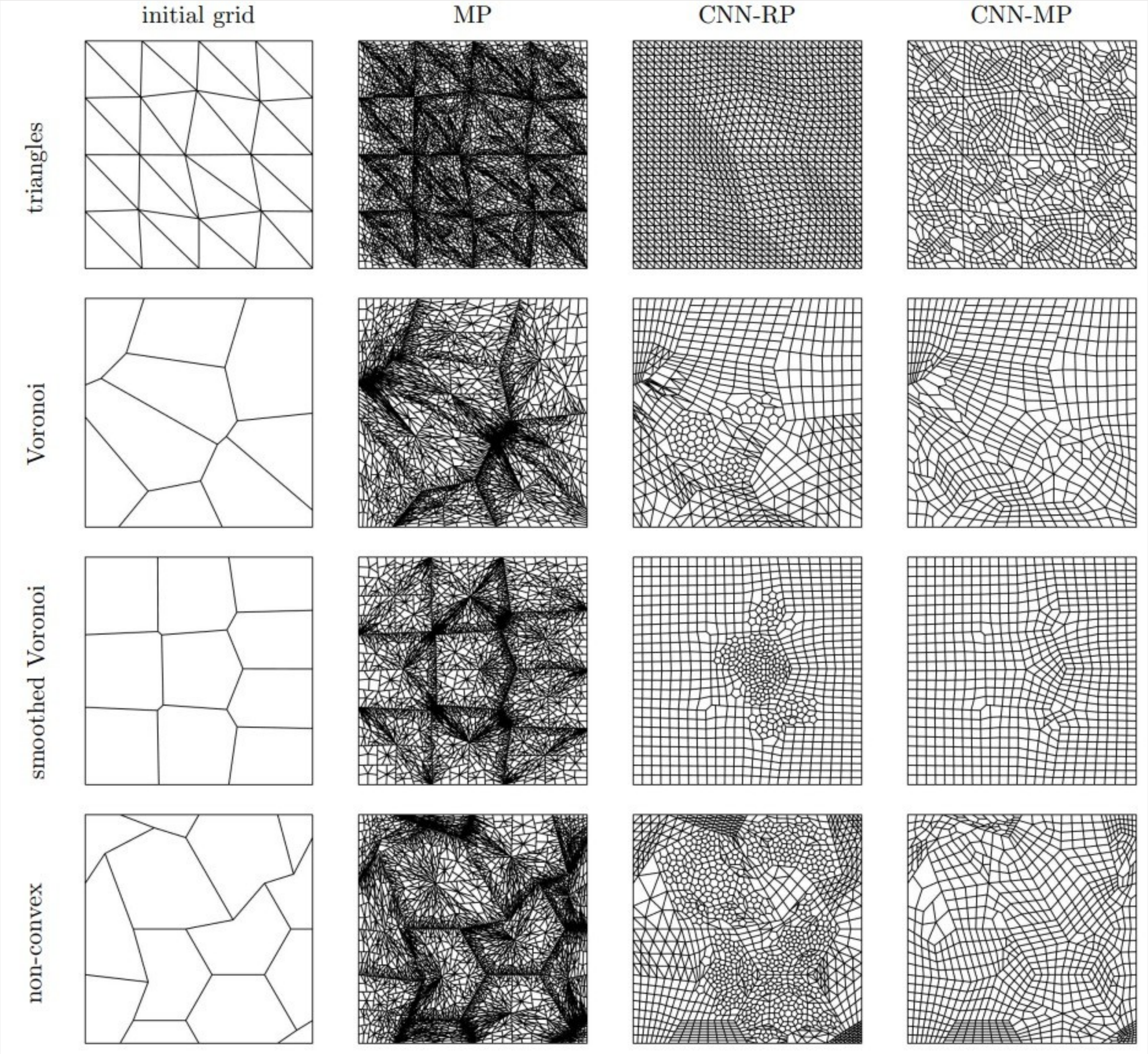


Label: "Triangle"

Binary image 64x64 pixels

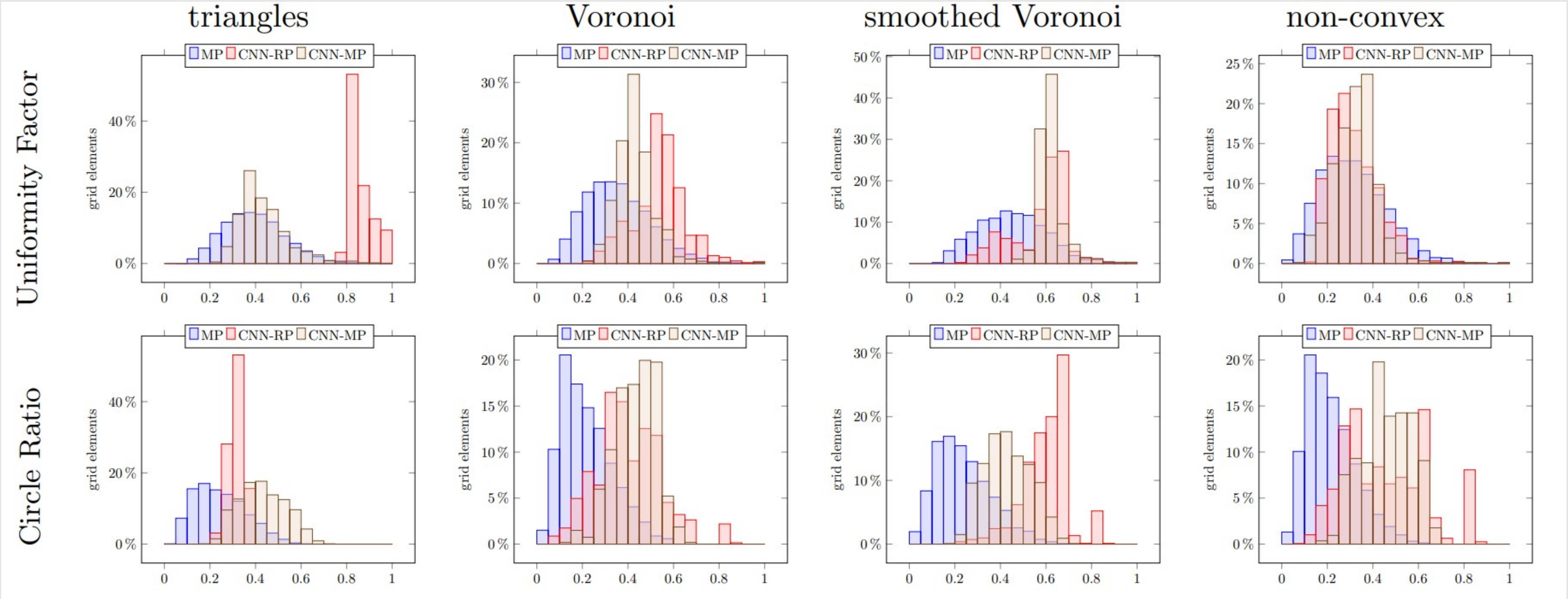
Label: "Triangle"

A preliminary example



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 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 the accuracy

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

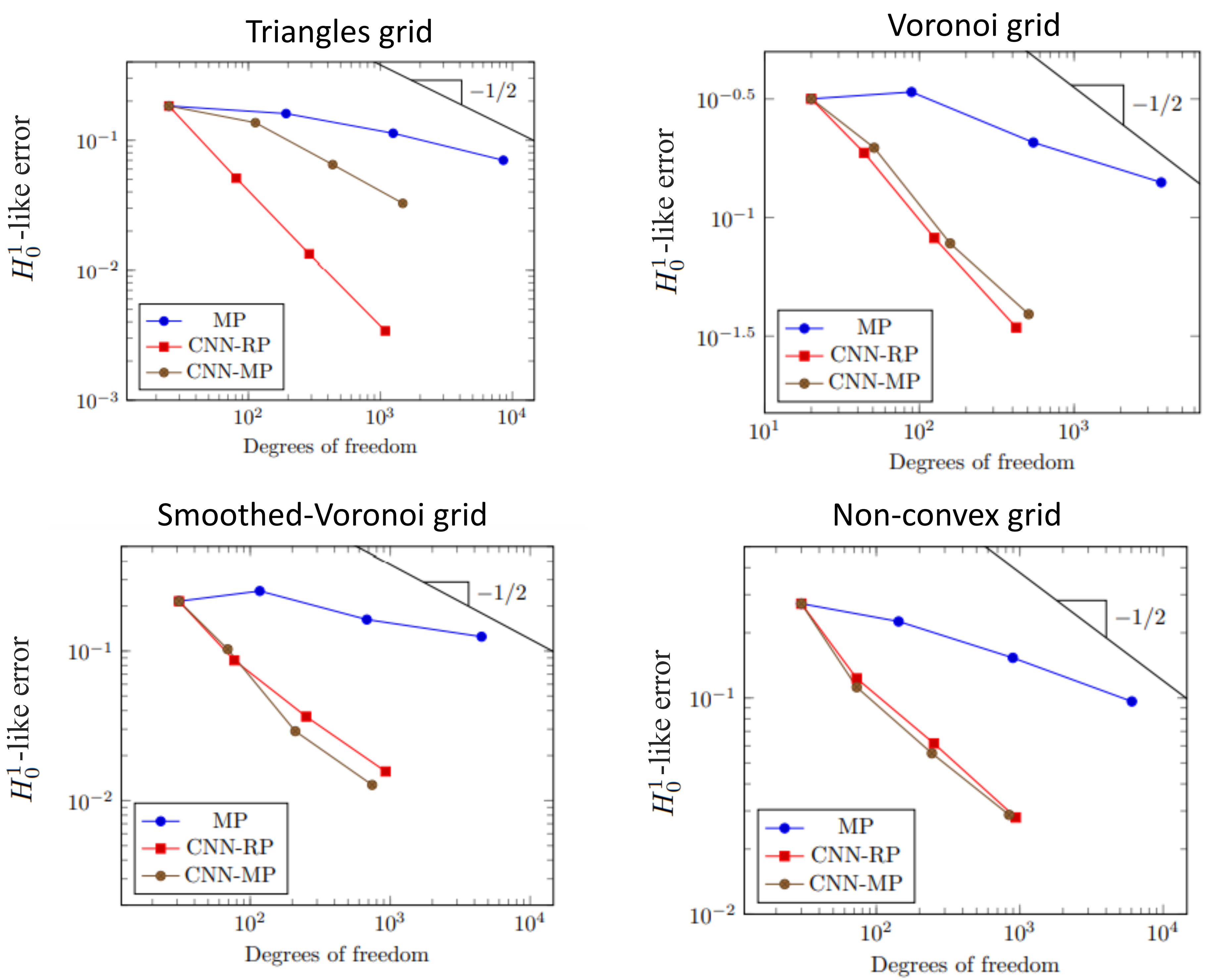
$$-\nabla \cdot (\rho \nabla u) = f \quad \text{in } \Omega, \qquad u = 0 \quad \text{on } \partial\Omega,$$

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],………

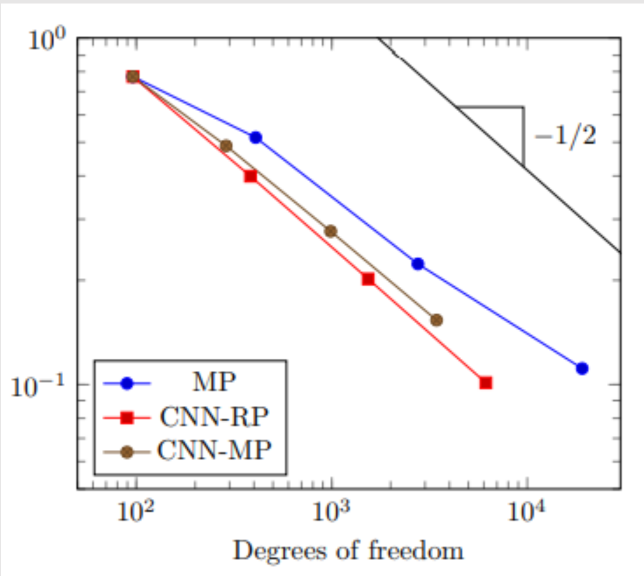
Solving the Poisson problem using the VEM (uniform refinement)



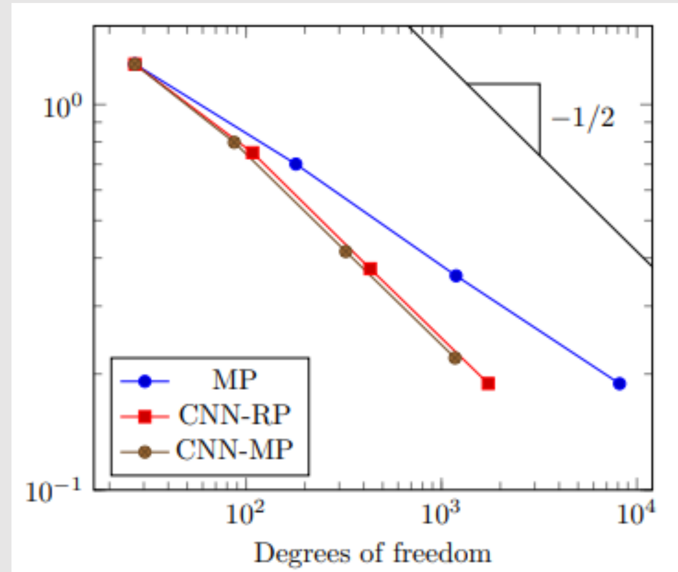
Analogous results for advection-diffusion and Stokes problems and on adaptively refined grids.

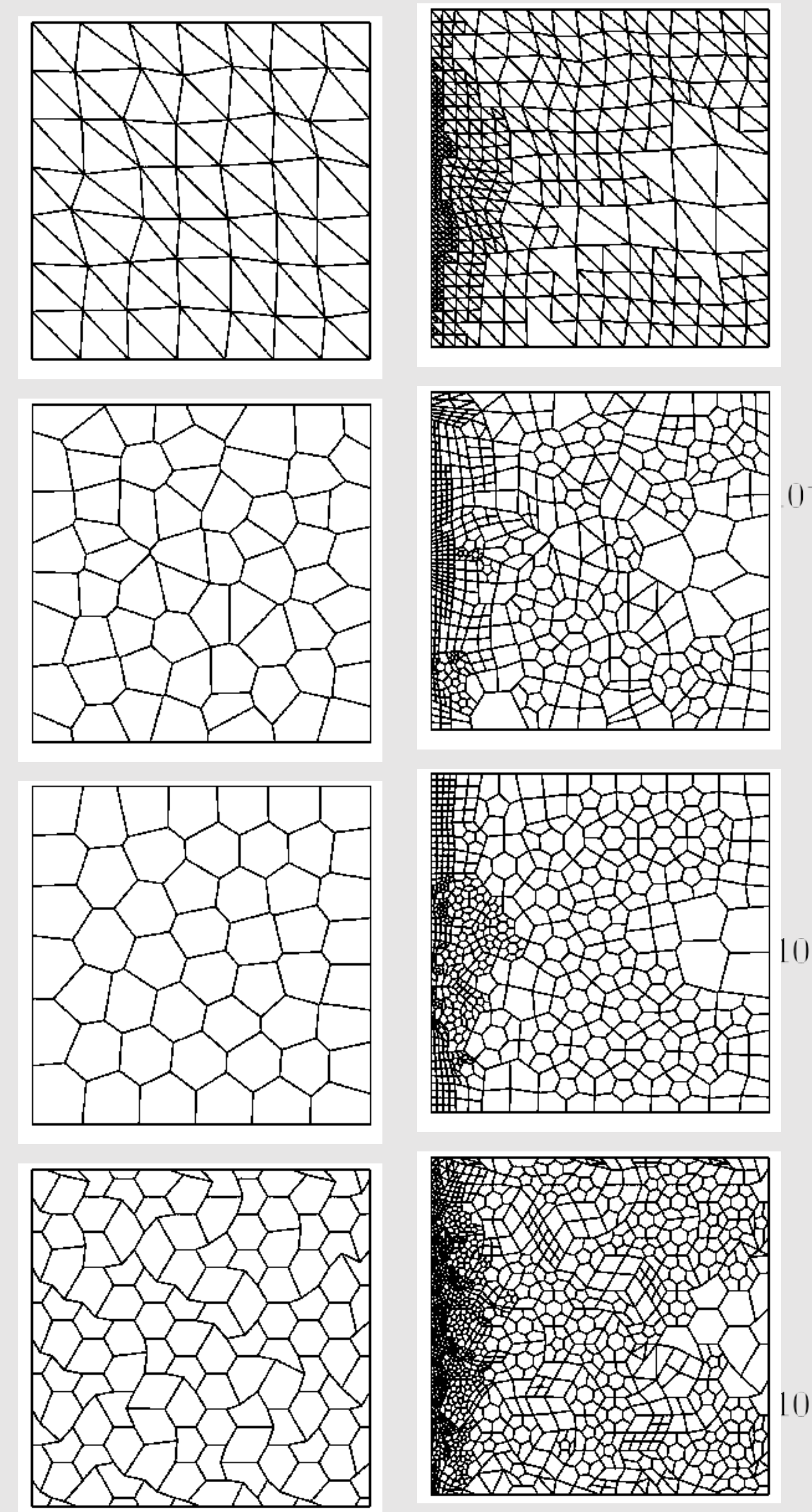
Solving the Poisson problem using the PolyDG method (uniform refinement)

Triangular grid

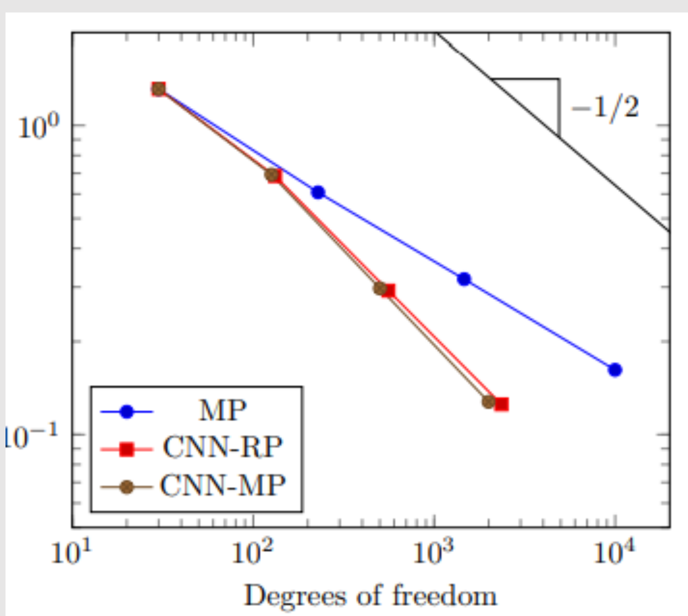


Voronoi grid

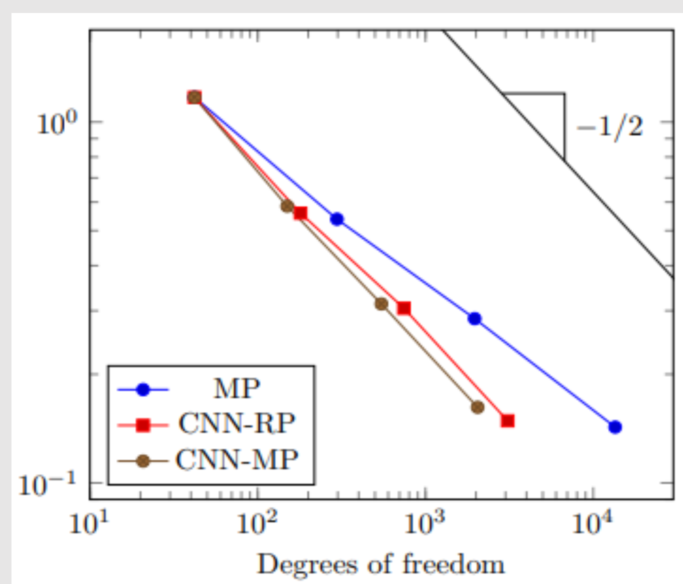




Smoothed-Voronoi grid



Non-convex grid



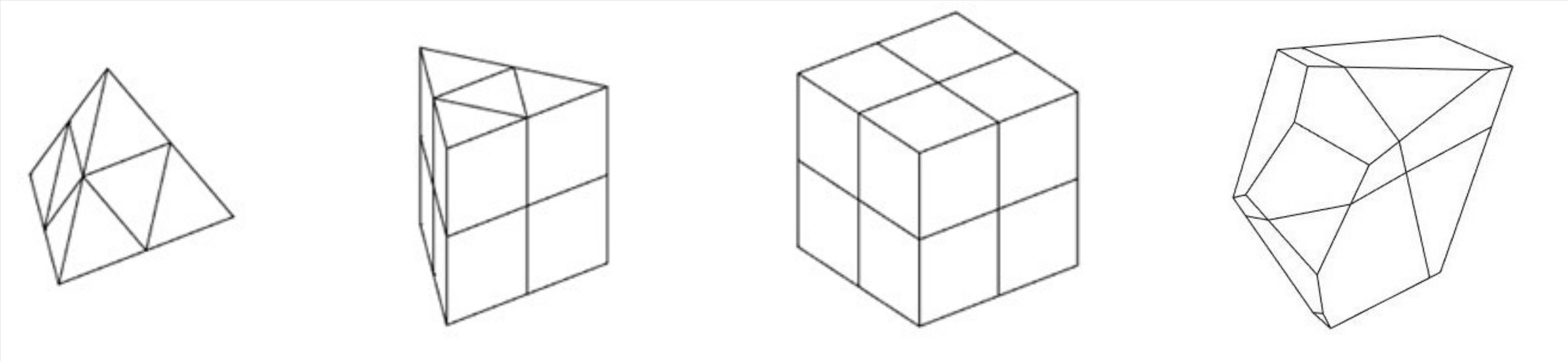
Analogous results for advection-diffusion and Stokes problems and on adaptively refined grids.

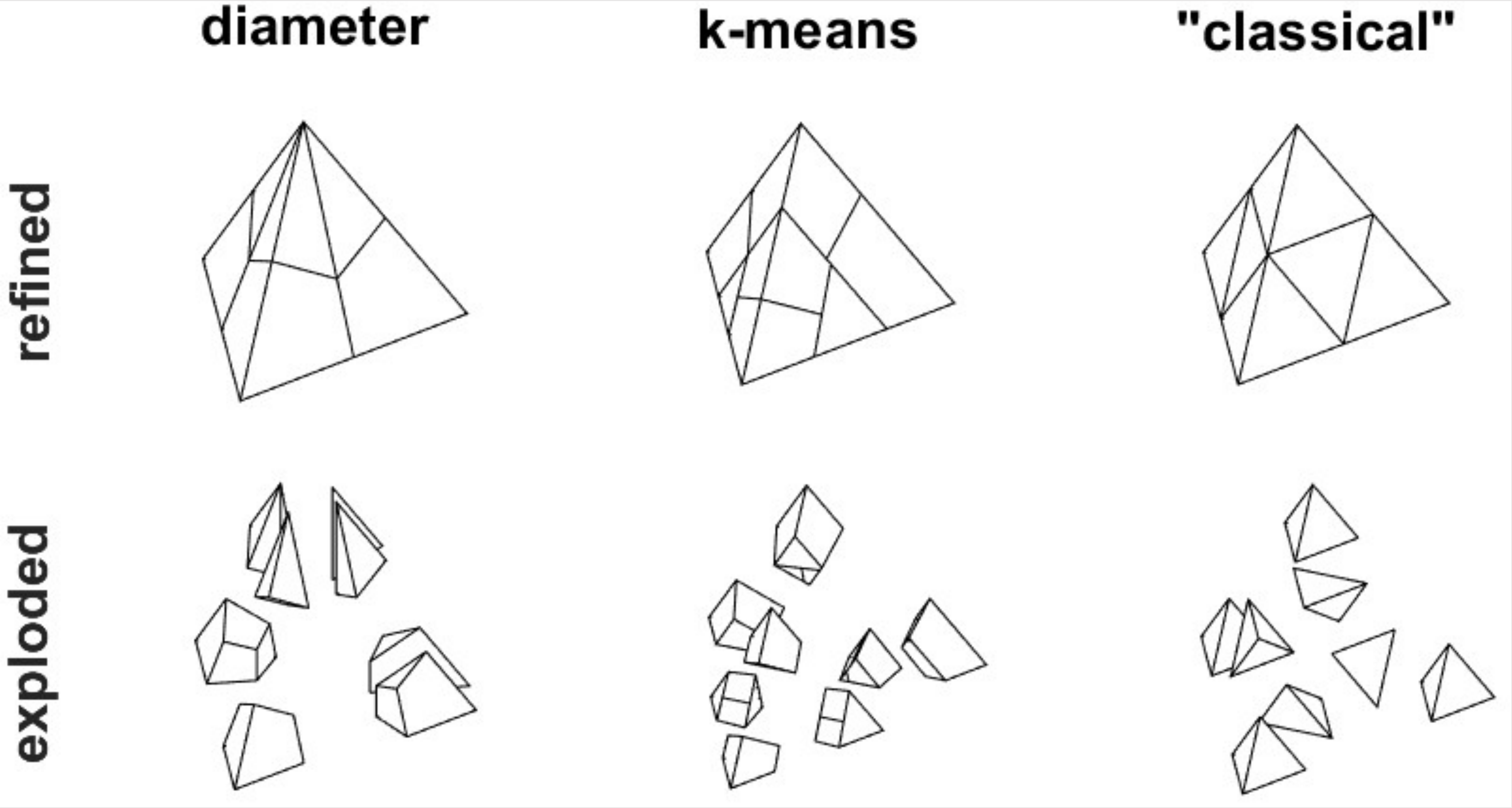
ML-enhanced mesh refinement (3D)

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

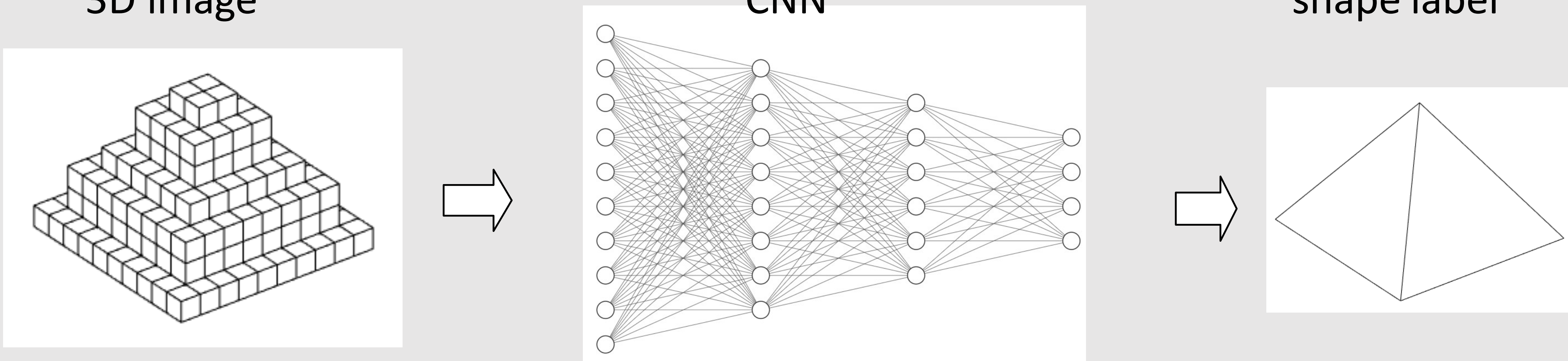


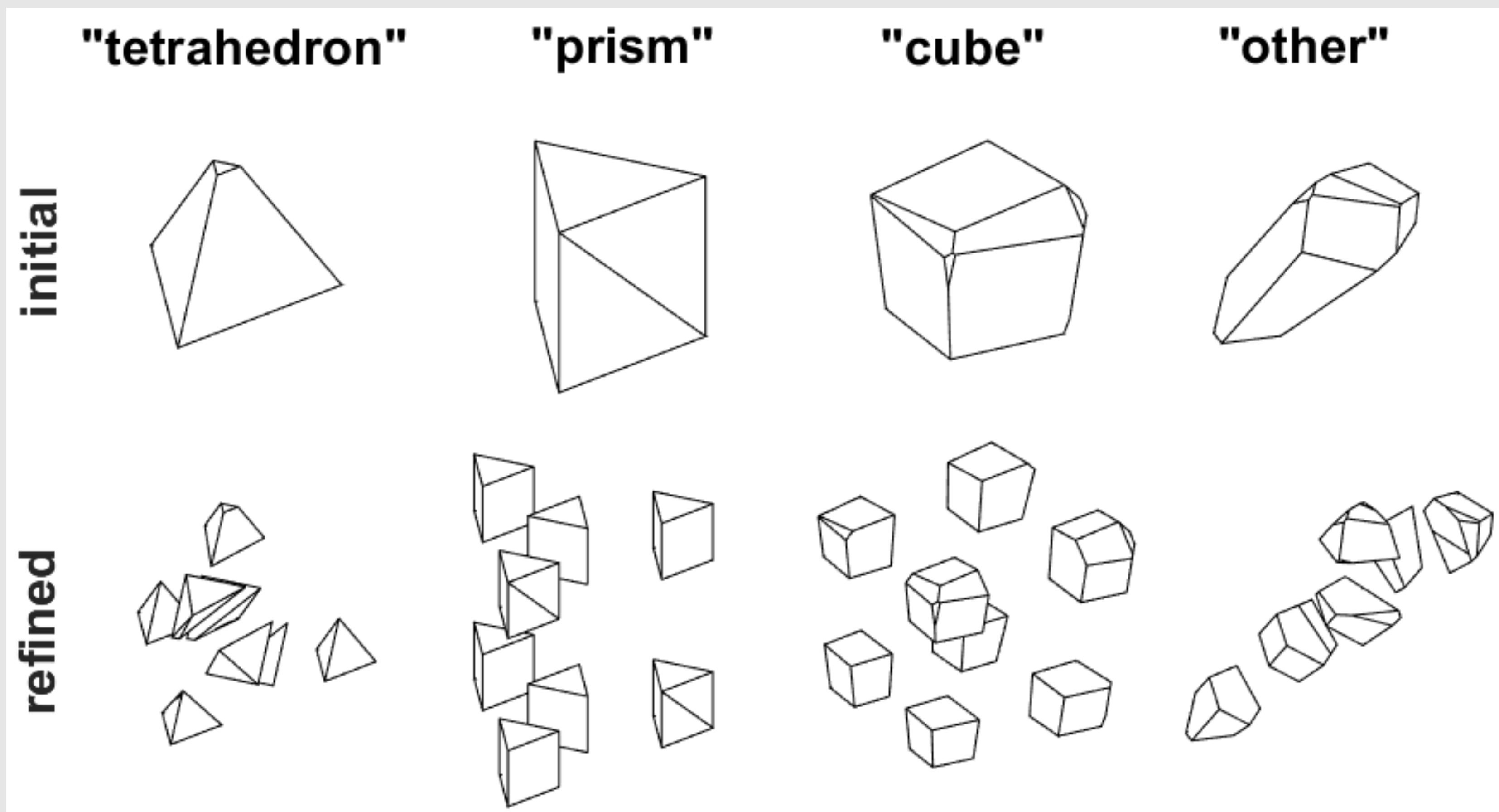


- Diameter strategy: cut the element perpendicular to its diameter.
- K-means strategy: cut the element balancing the volume distribution.
- "Classical" strategies: if the element has a specific shape refine it using a predefined strategy.

3D refinement strategies for general polyhedra

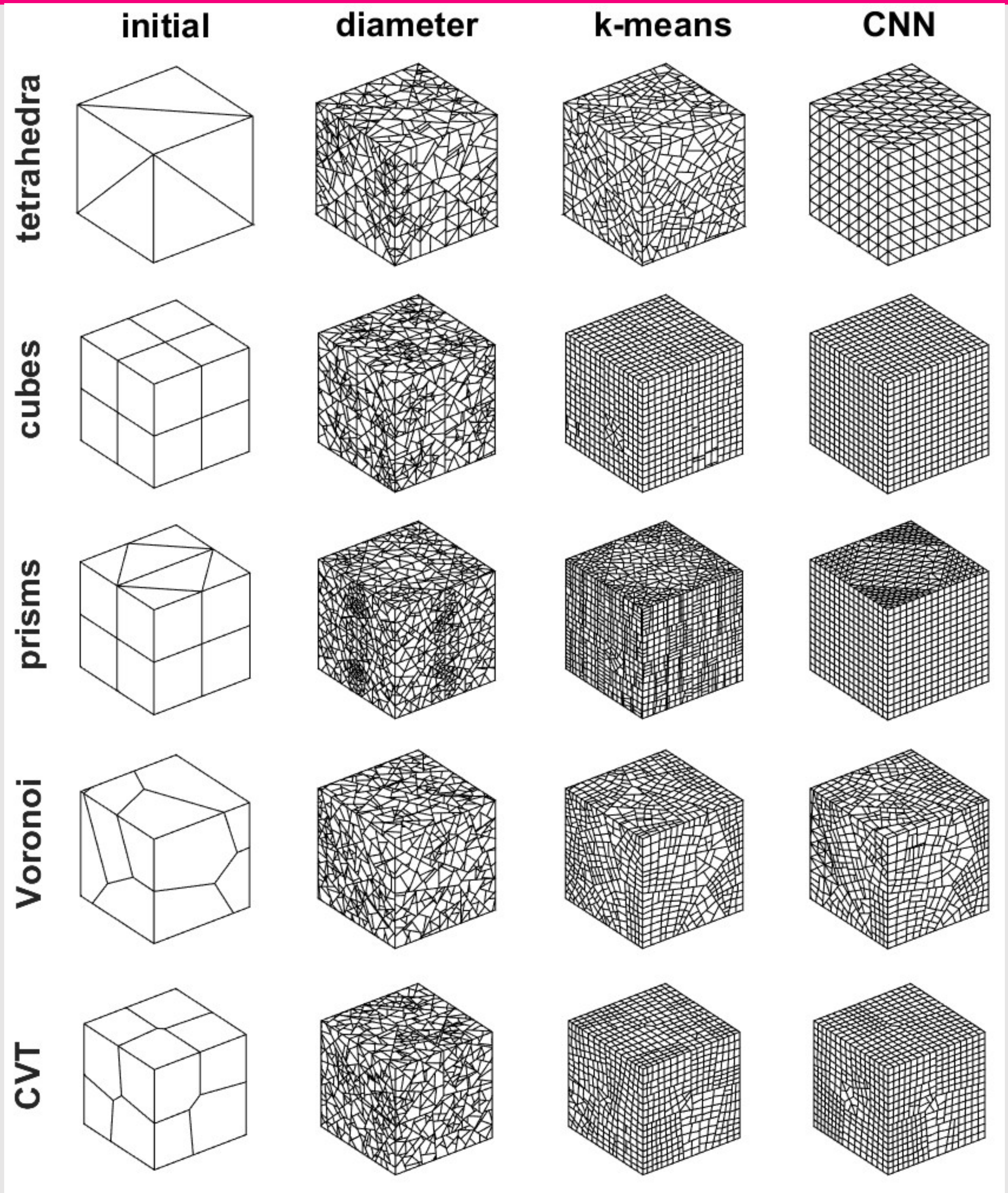
3D image CNN shape label





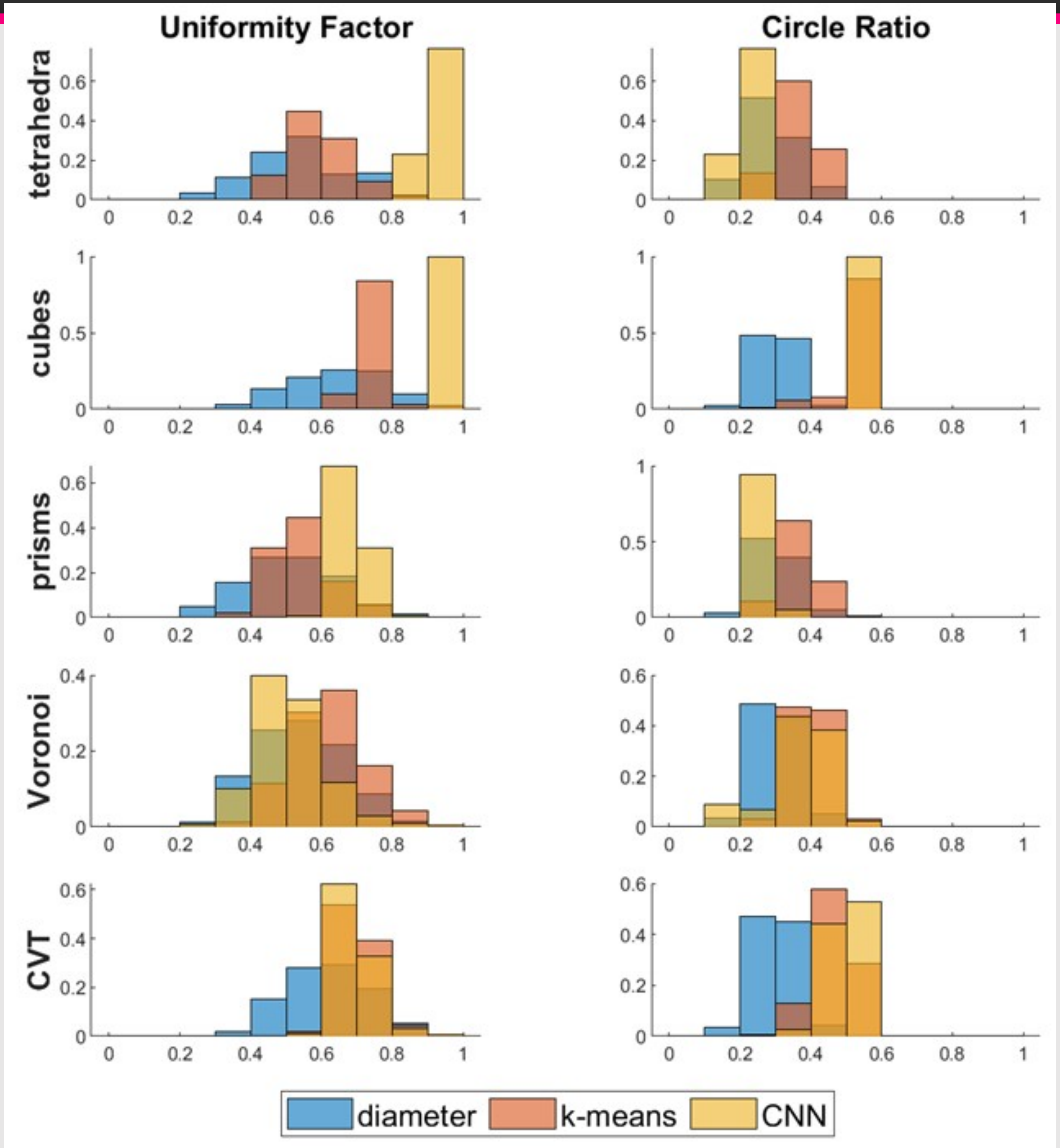
The CNN classifies the 3D image of the input polyhedron according to its shape, in order to apply suitable refinement strategies. Elements in class "other" are refined using the k-means strategy.

Some examples



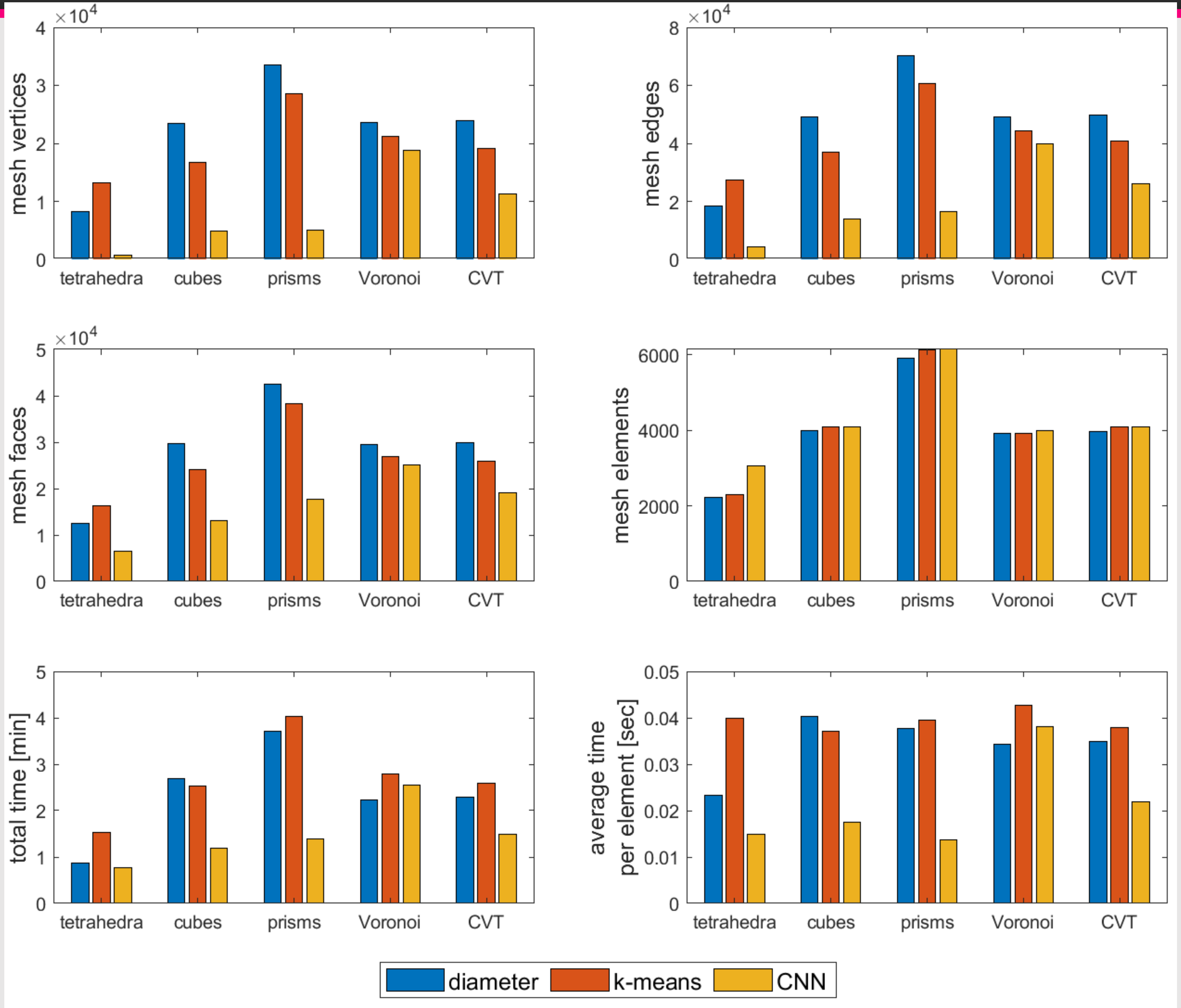
Refined grids obtained after three steps of uniform refinement based on employing the diameter, the k-means and the CNN strategies.

Quality Metrics



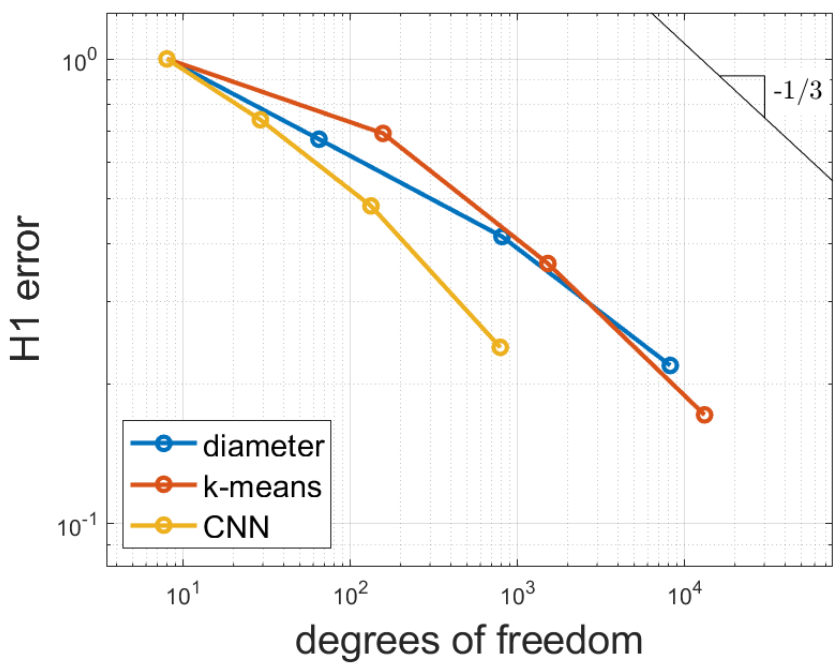
Uniformity Factor = $\frac{\text{element size}}{\text{mesh size}}$ Circle Ratio = $\frac{\text{inscribed circle radius}}{\text{circumscribed circle radius}}$

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

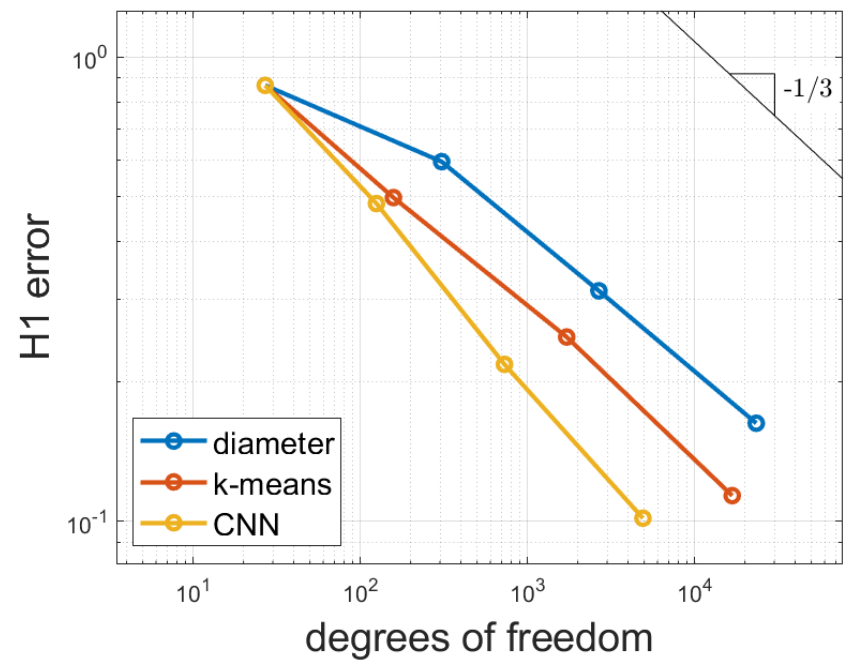


Solving the Poisson problem with the VEM (3D)

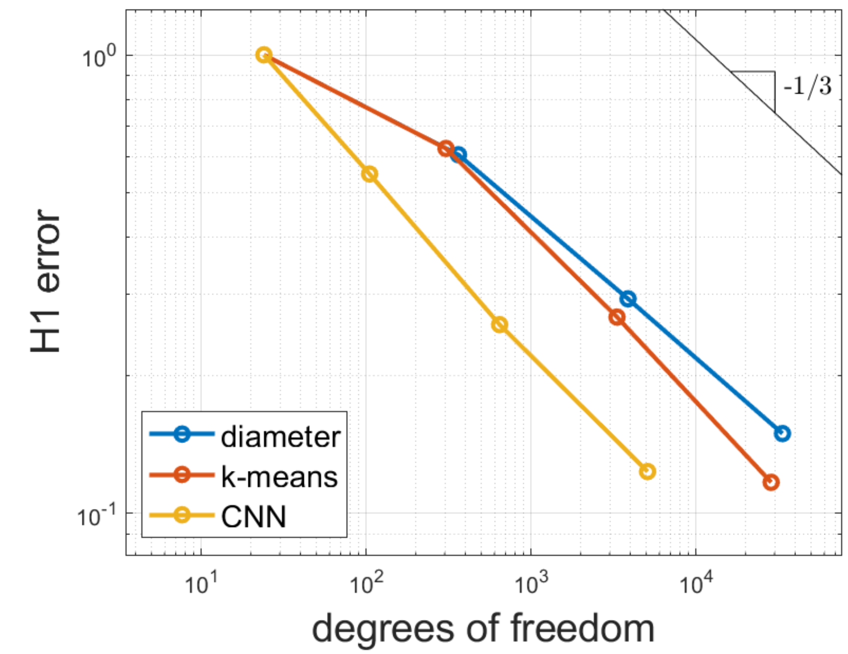
Tetrahedra



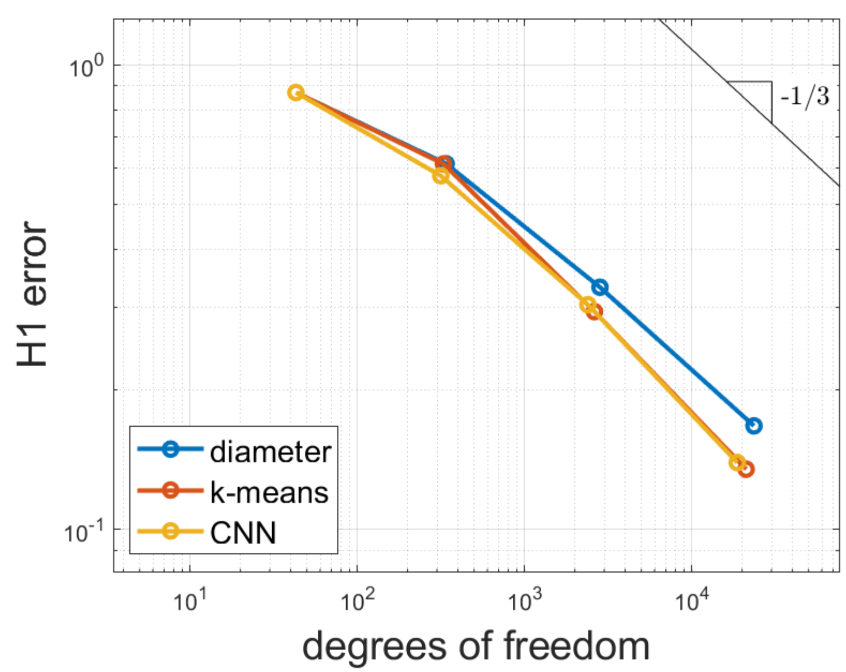
Cubes



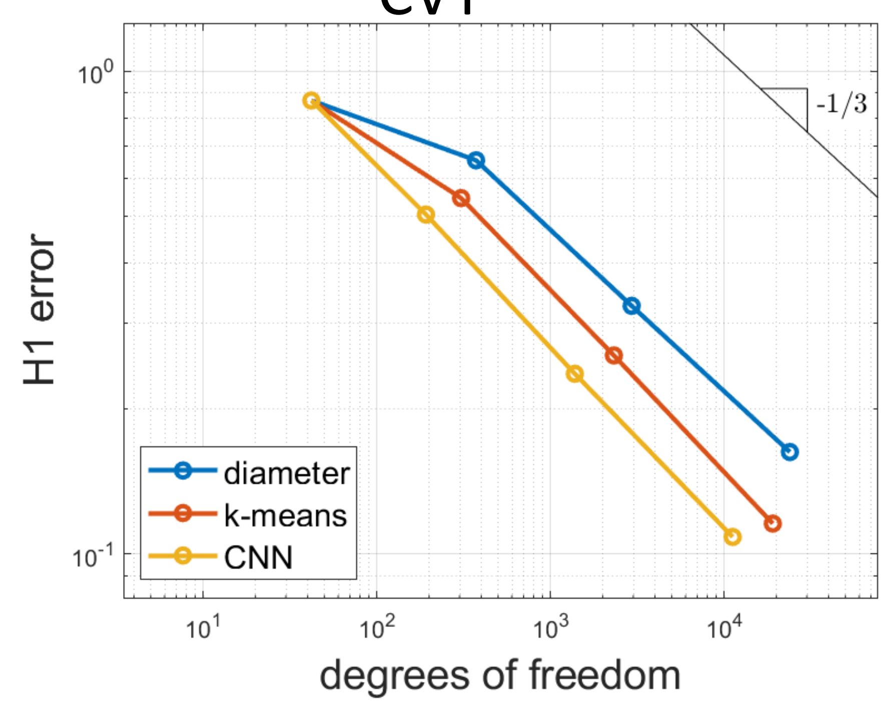
Prisms



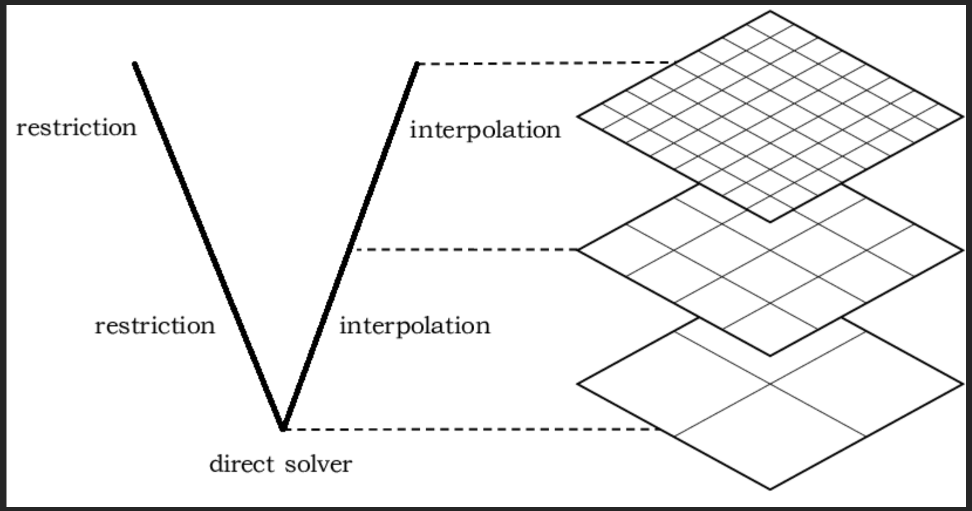
Voronoi

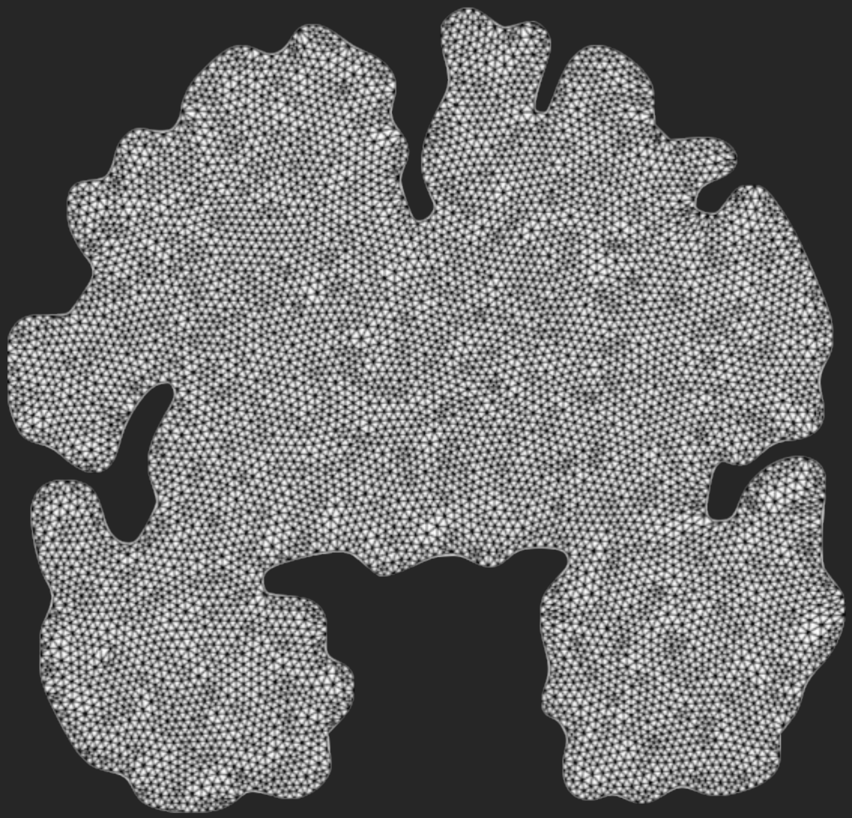


CVT



Analogous results for the VEM of order higher than 1.



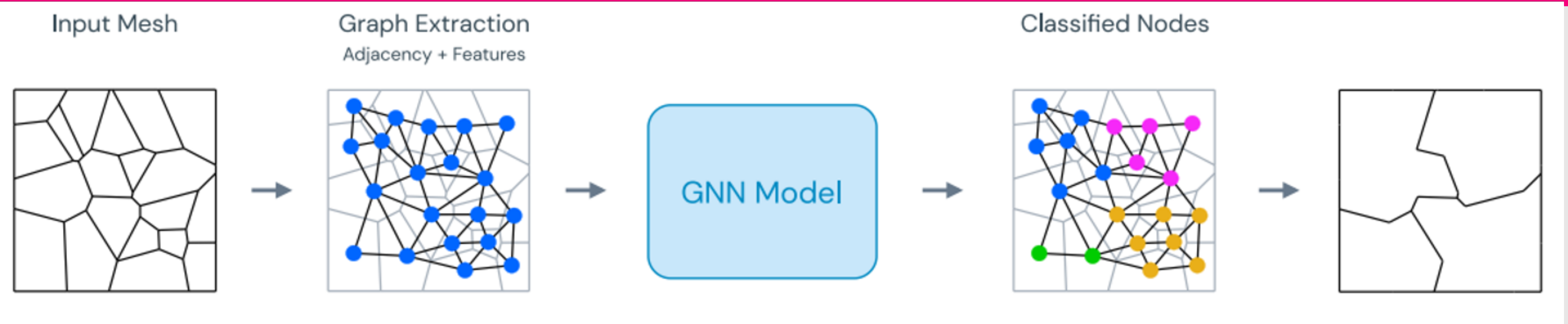


ML-enhanced agglomeration strategies

Merging neighboring mesh elements to obtain a coarser grid.

- Design of multilevel solvers
- Defeaturing of complex geometries
- Reduction of the number of degrees of freedom

Agglomeration using Graph Neural Networks (so far)



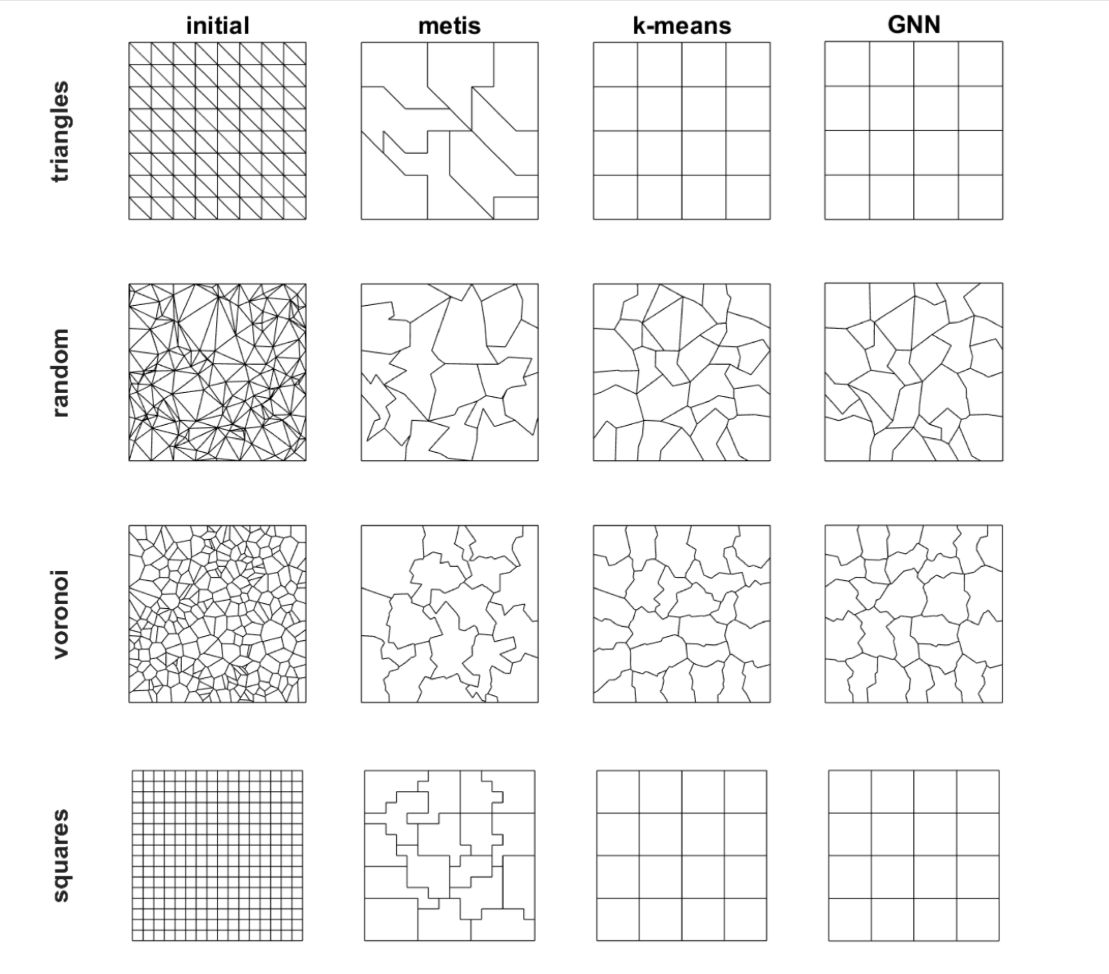
Objective:
Find a partition with minimal interconnections between sets, while keeping errors (volumes) balanced.

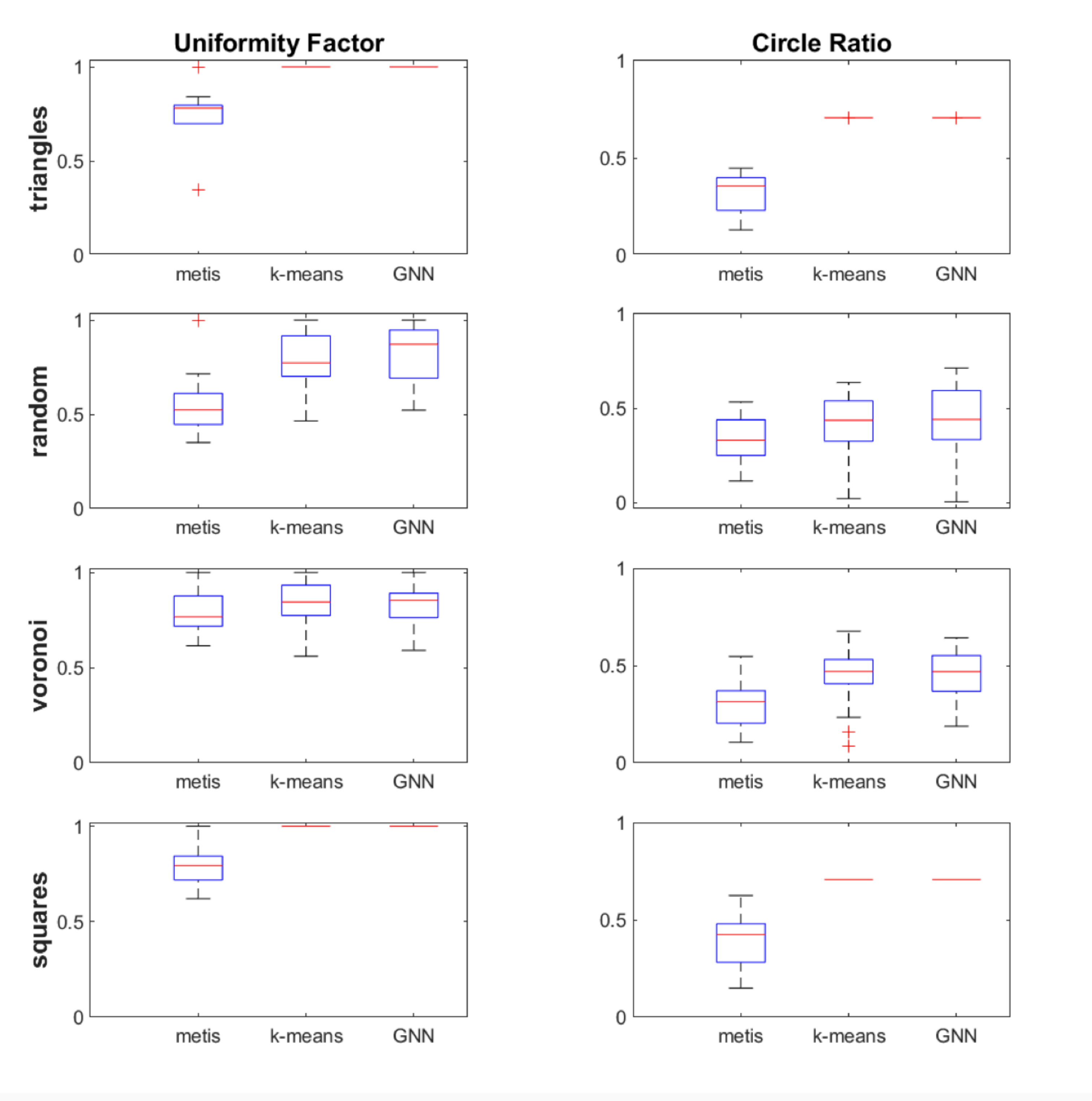
Advantages:
Fast inference and full exploitation of both graph and geometrical features.
Process naturally and simultaneously both the graph structure of mesh and the geometrical information(areas of the elements or their barycentric coordinates)

Training is performed by minimizing the expected normalized cut of the graph

[P.F. Antonietti, N. Farenga, E. Manuzzi, G. Martinelli, L. Saverio, 2024.]

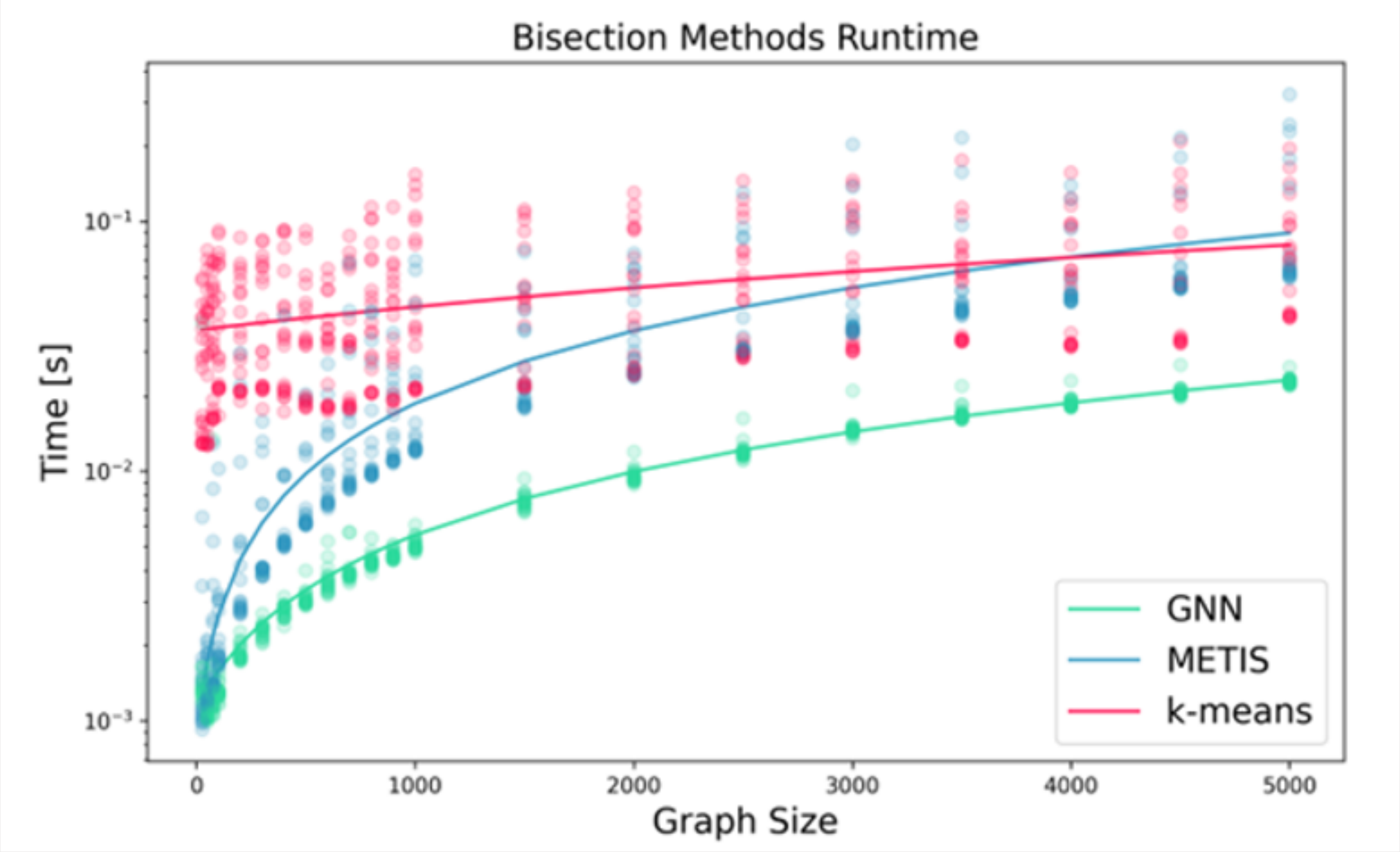
Effects of ML-based agglomeration strategies on Quality Metrics





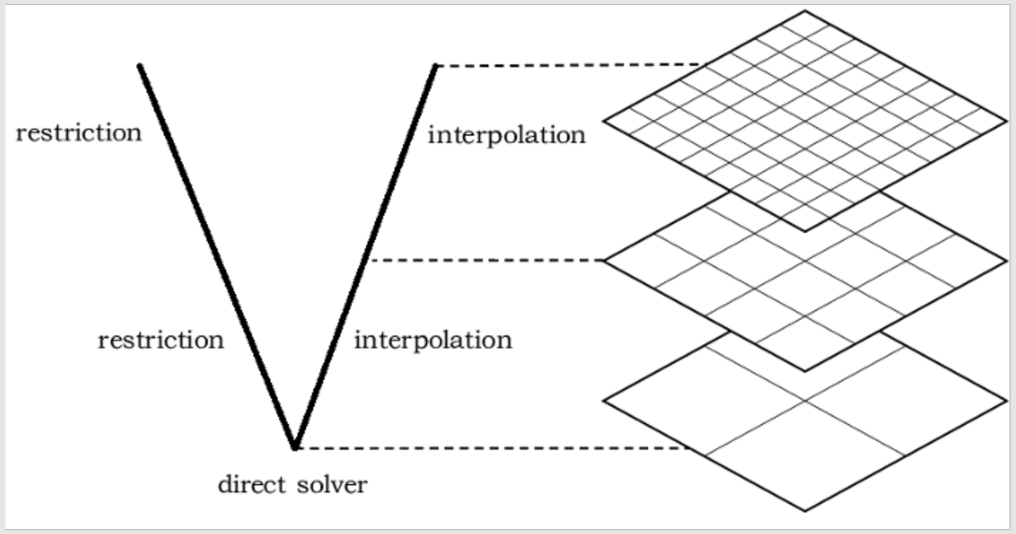
Agglomerated grids based on employing metis. Metis is «standard» for graph partitioning.

Computational times



Runtime performance for different graph bisection models (METIS, k-means, GNN) as a function of the number of nodes in the connectivity graph of Voronoi meshes. The y-axis is in logarithmic scale

Applications of ML-based agglomeration strategies: MG solvers

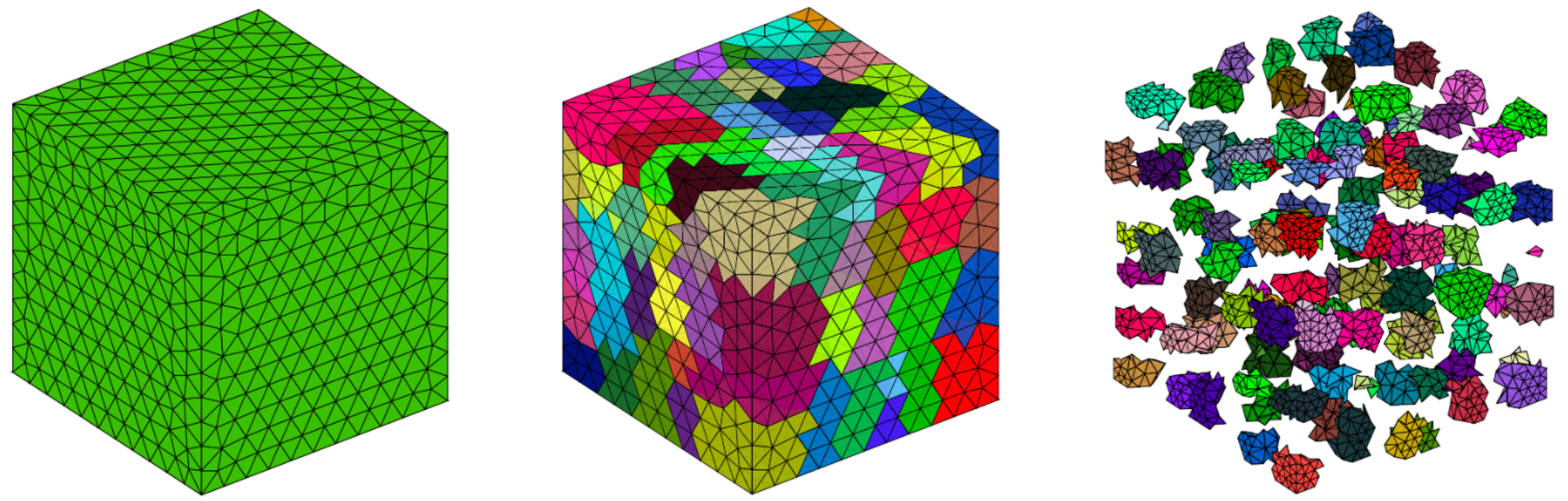


Iteration count of the MG algorithm. Different initial grids agglomerated with different strategies (METIS, k-means, GNN) and different levels. As a comparison, the iteration count of the Conjugate Gradient (CG) method are reported in the last column.

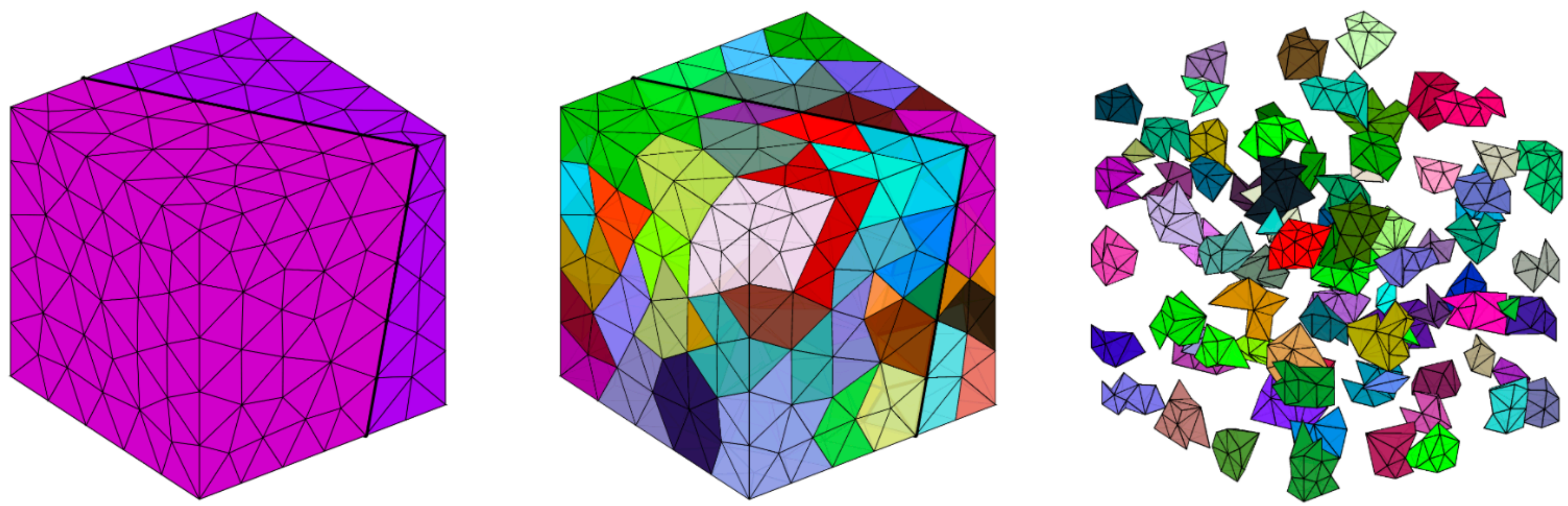
grids	ℓ	Agglomeration-based MG			CG
		metis	k-means	GNN	
triangles	2	21	9	9	114
	3	21	9	9	
	4	21	9	9	
random	2	46	41	32	655
	3	46	41	32	
	4	46	41	32	

Agglomeration in 3D

The agglomeration in 3D is much more complicated, suitable modification the 2D algorithm.

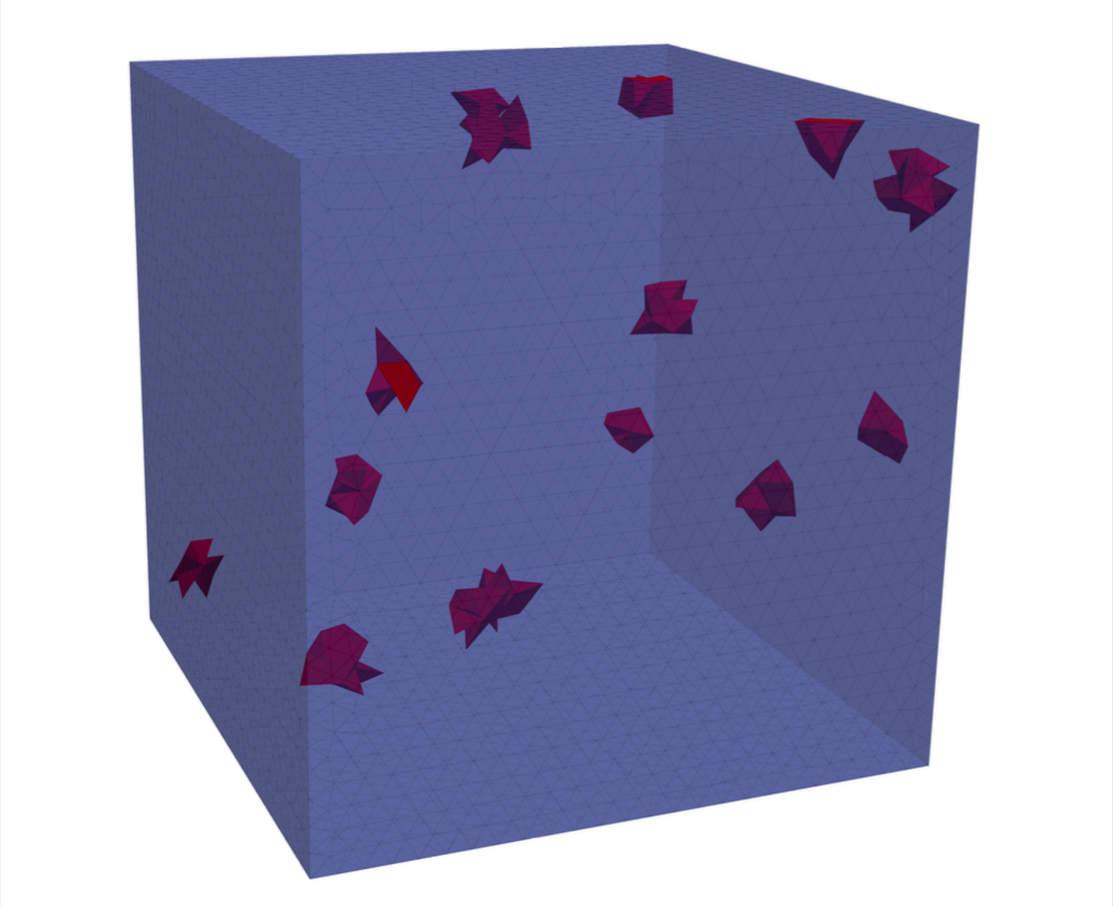


(a) original mesh **(b)** agglomerated mesh **(c)** agglomerated mesh (exploded)

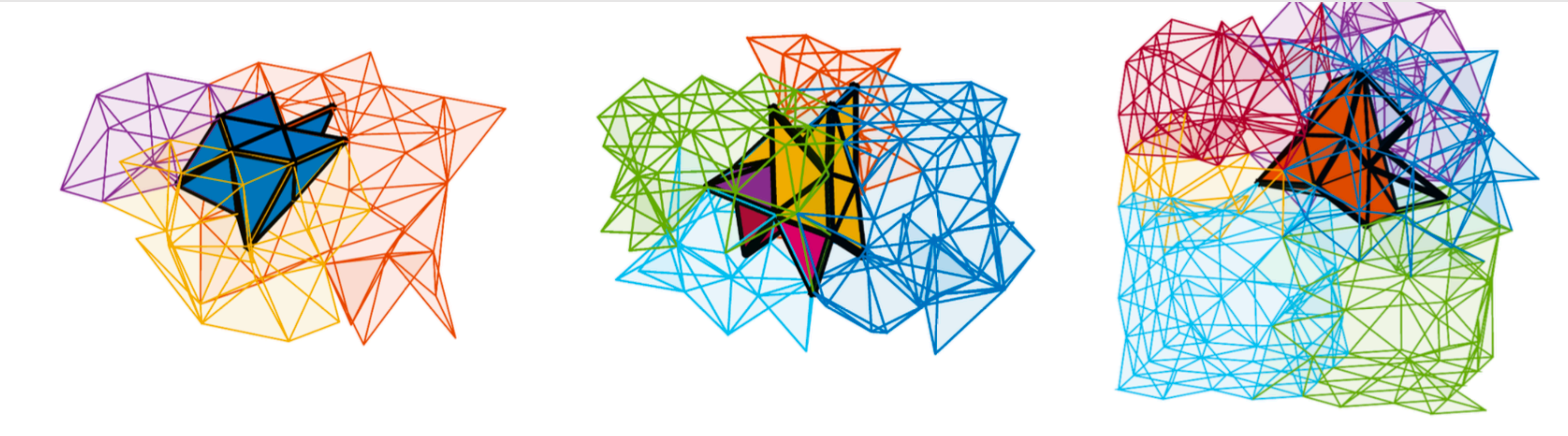


(a) original mesh **(b)** agglomerated mesh **(c)** agglomerated mesh (exploded)

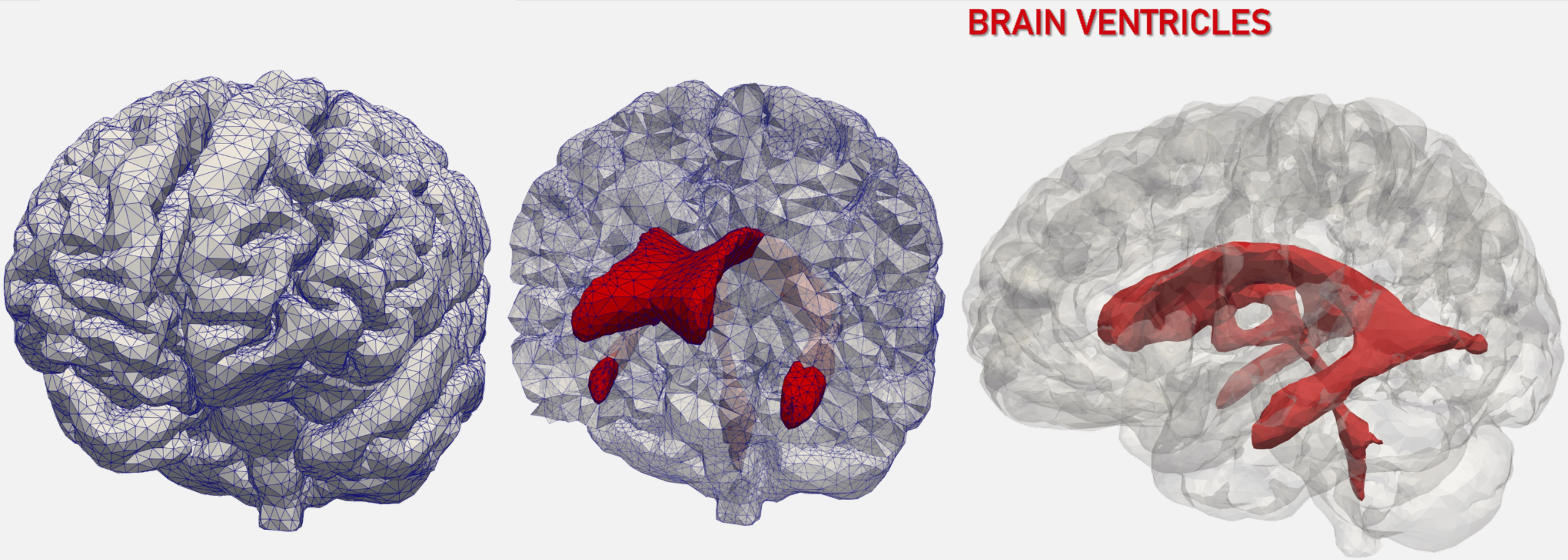
Agglomeration in 3D



Domain with inclusions



3D - real domains



The brain MRI images were provided by **OASIS-3: Longitudinal Multimodal Neuroimaging**: Principal Investigators: T. Benzinger, D. Marcus, J. Morris; NIH P30 AG066444, P50 AG00561, P30 NS09857781, P01 AG026276, P01 AG003991, R01 AG043434, UL1 TR000448, R01 EB009352. AV-45 doses were provided by Avid Radiopharmaceuticals, a wholly owned subsidiary of Eli Lilly.

OASIS
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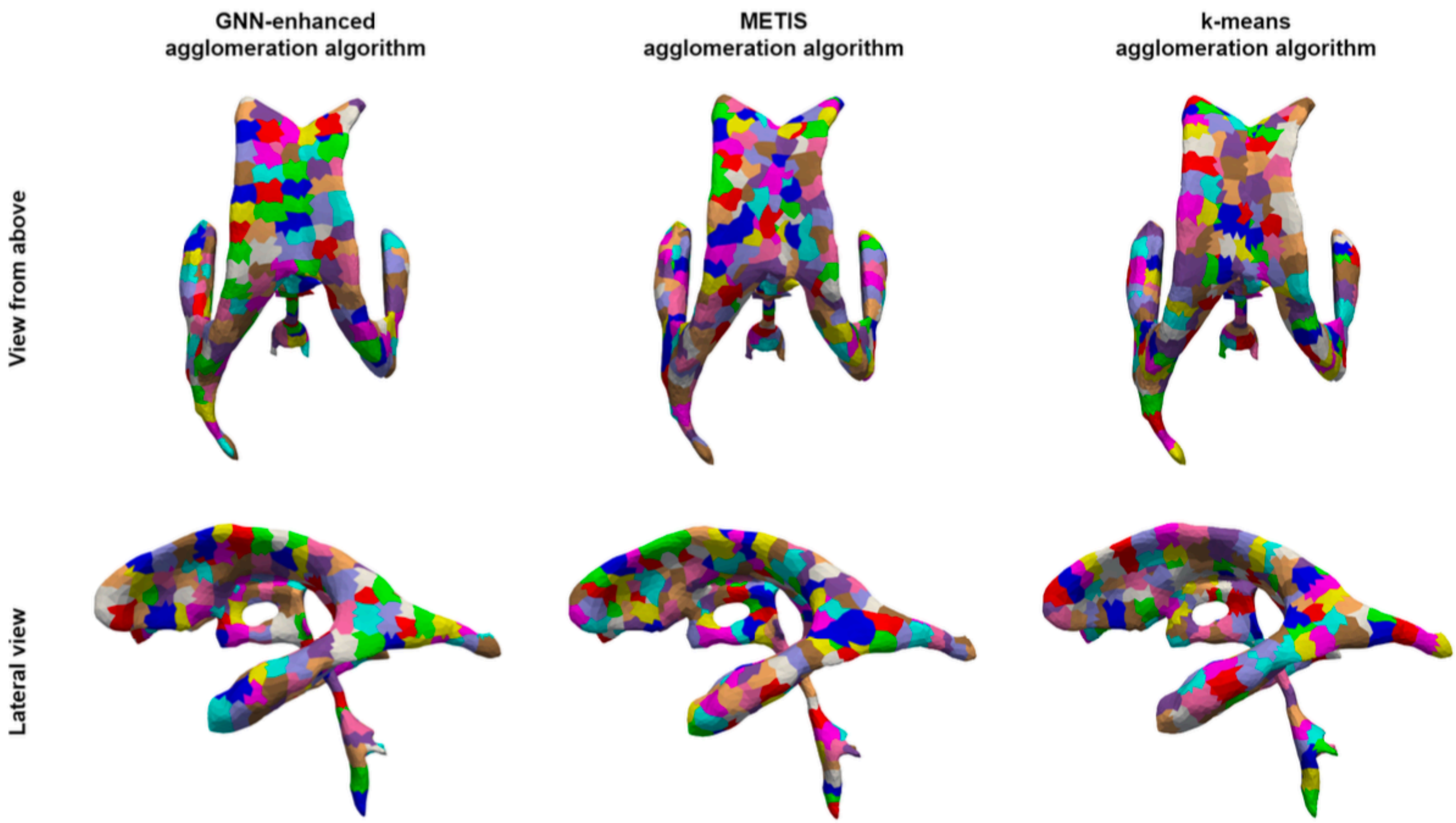
3D - real domains

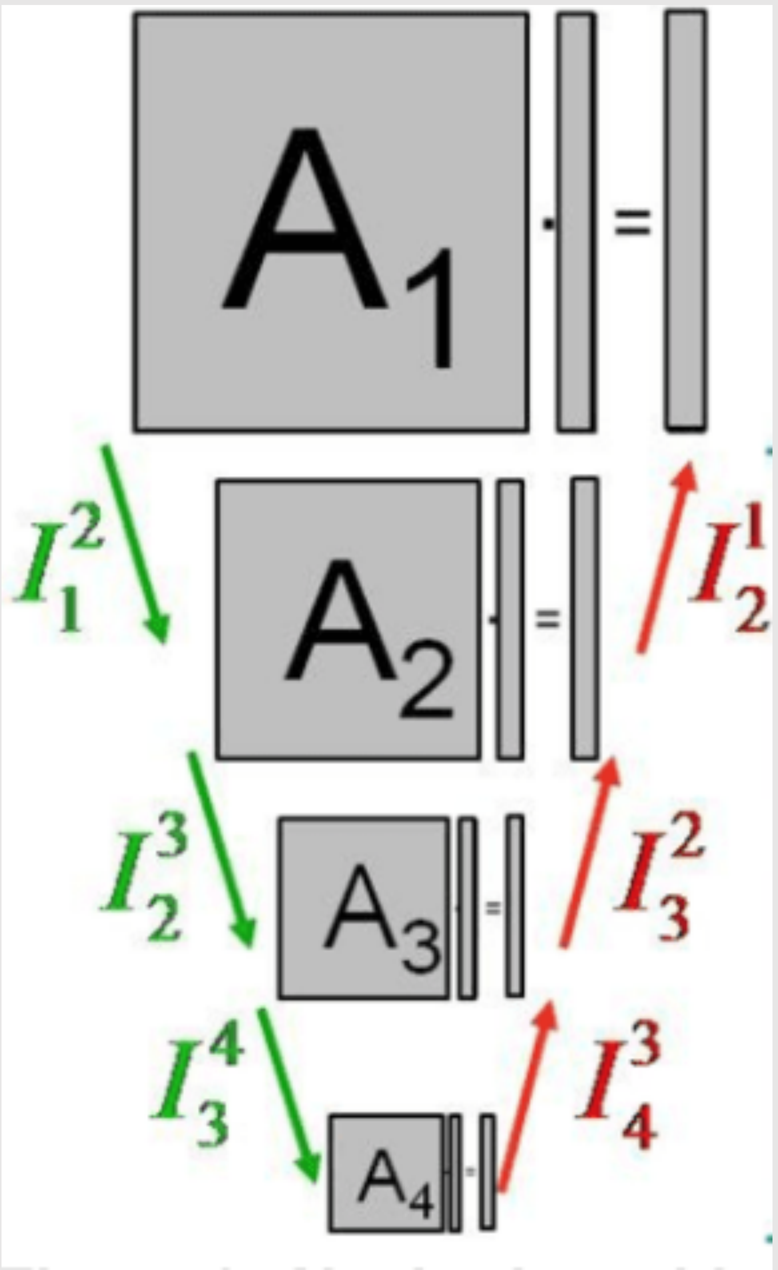


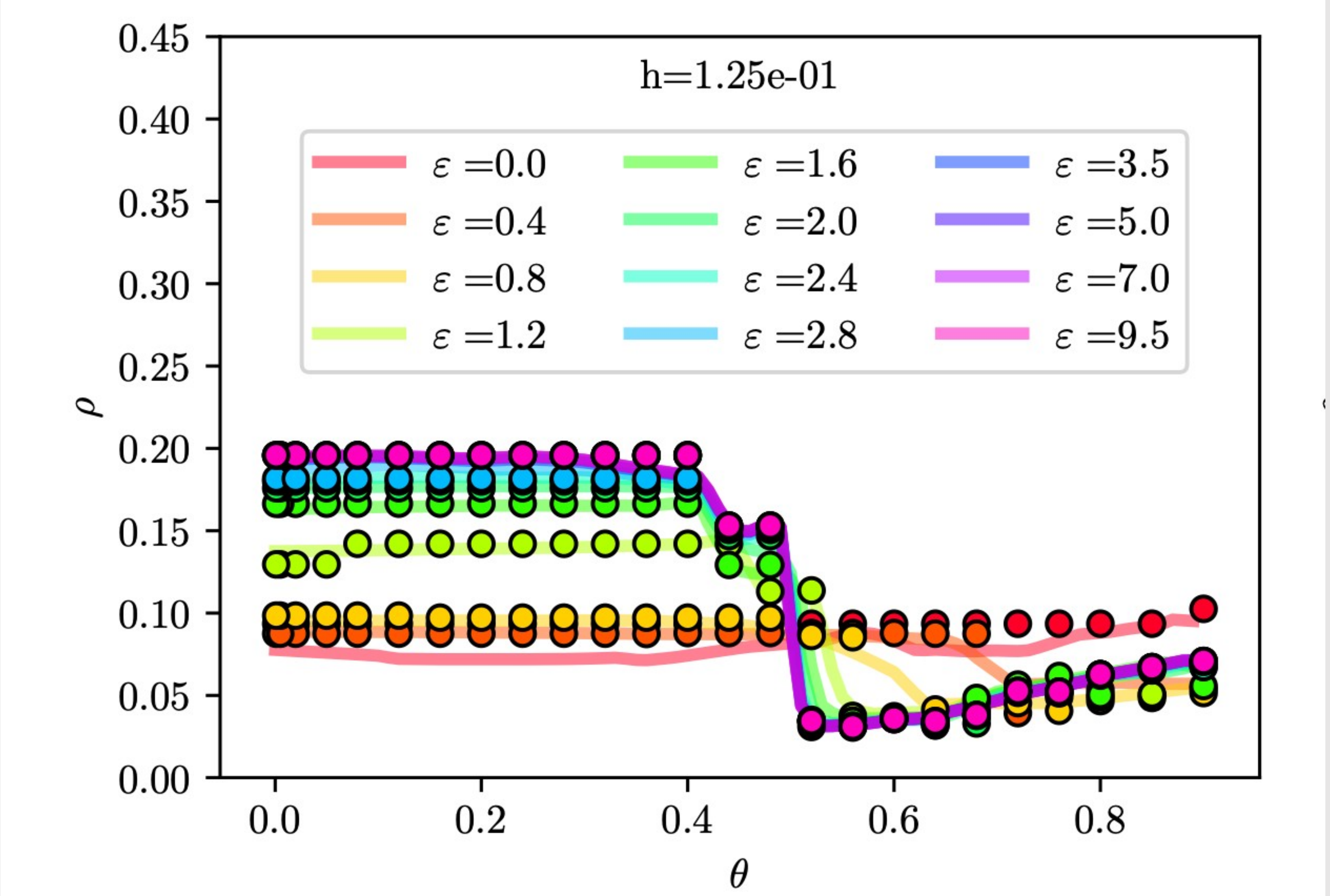
ML-enhanced Algebraic Multigrid Methods

Learn the best AMG parameters via Deep Learning

ML-enhanced AMG Methods

[P.F. Antonietti, L. Dede', M. Caldana, 2023 & 2024]

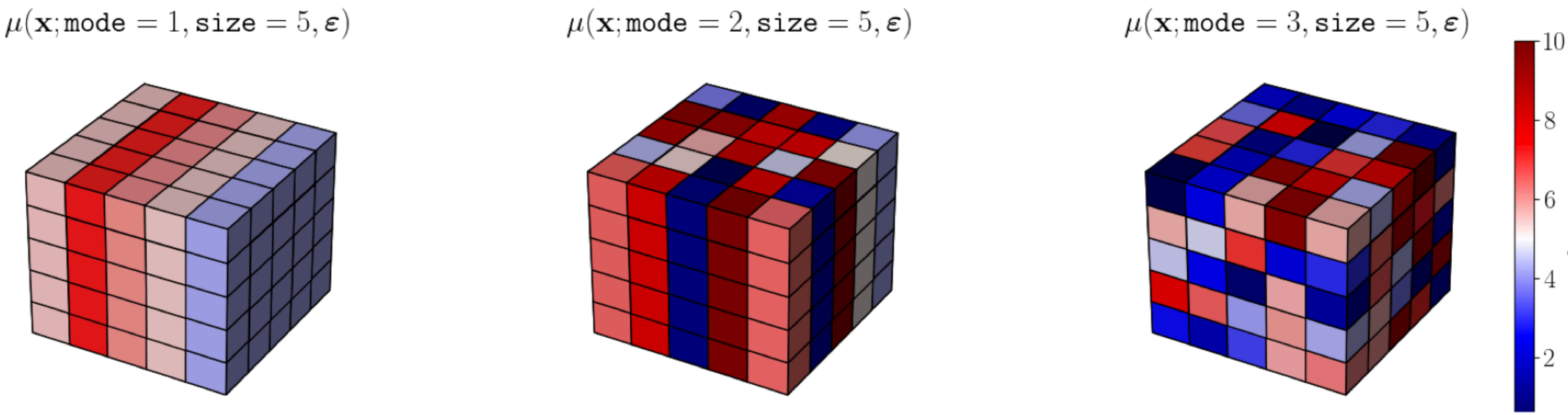


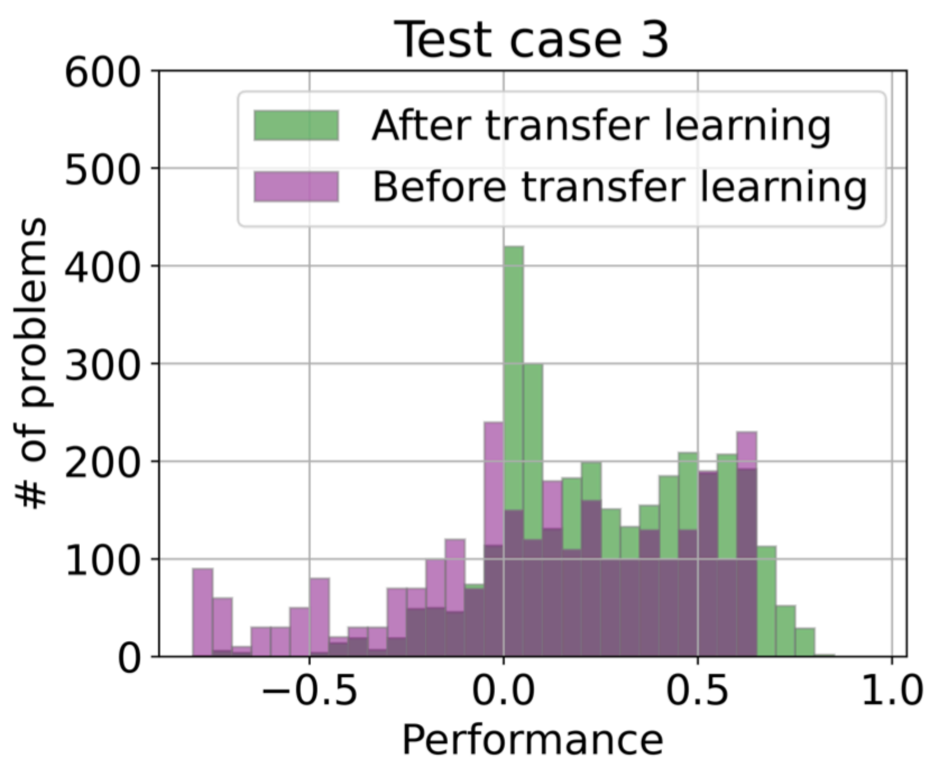


Improving efficiency of algebraic multigrid methods through artificial neural networks: choosing the strong threshold parameter θ as the one the ANN predicts to give the best performance ($\approx 30\,\%$ gain)

Ongoing: Modelling neurodegenerative diseases

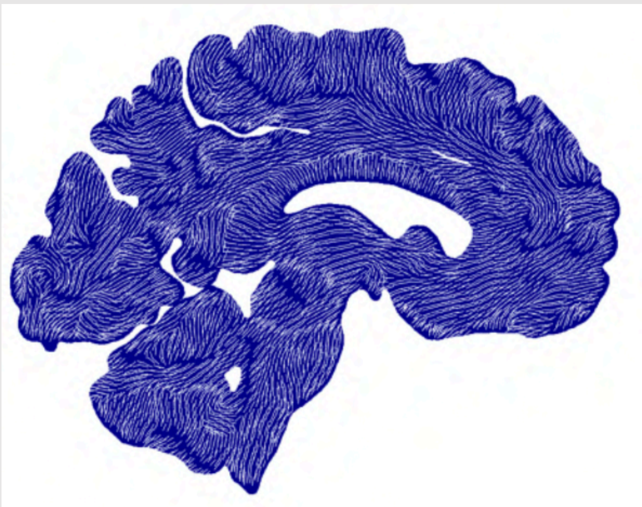
[P.F. Antonietti, L. Dede', M. Caldana, 2023 & 2024]

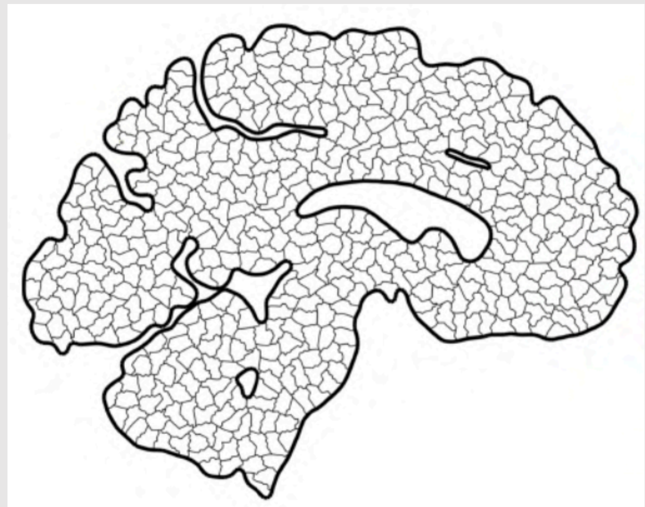




Improving efficiency of algebraic multigrid methods through artificial neural networks: choosing the strong threshold parameter θ as the one the ANN predicts to give the best performance.

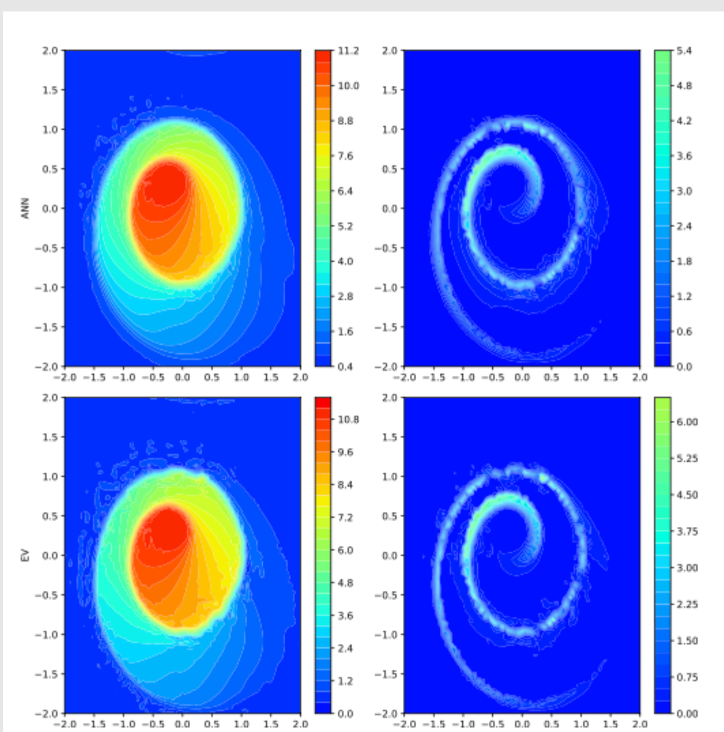
Modelling neurodegenerative diseases





PolyDG method for FK equation with applications α-Synuclein Spreading in Parkinson’s

Joint work with: Mattia Corti



Learning artificial viscosity models with DG methods

Joint work with: Luca Dedè, Matteo Caldana

Conclusions

➡ 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.

➡GNN can be employed to drive agglomeration procedures

- Design of multilevel solvers
- Defeaturing of complex geometries

➡GNN can be employed to accelerate Algebraic Solvers

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