# Using Graph Neural Network for gas-liquid interface reconstruction in Volume Of Fluid methods

ML4CFD - DATAIA 2020

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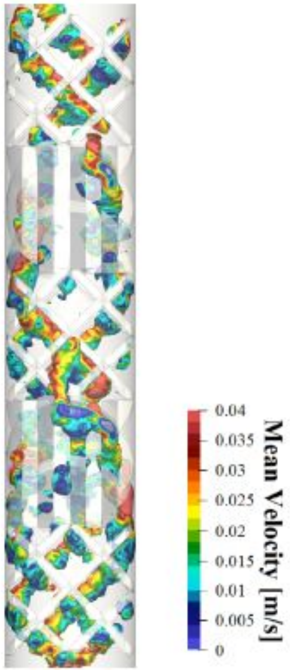
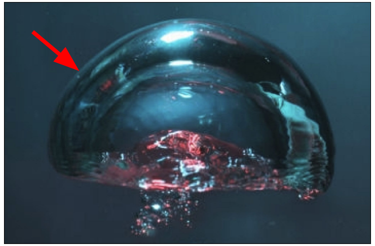
# Background

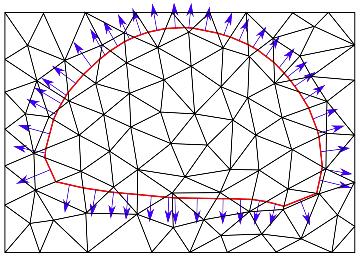



Static mixer*

- Immiscible multiphase flow (ex. gas-liquid phase):
  - cavitation, cooling system, mixer
- Numerical method is an effective approach
- The Volume of Fluid (VoF) method:
  - Consider the dynamics of the surface tension force
  - Reconstructs the interface (i.e., normal, location, curvature)



Free surface

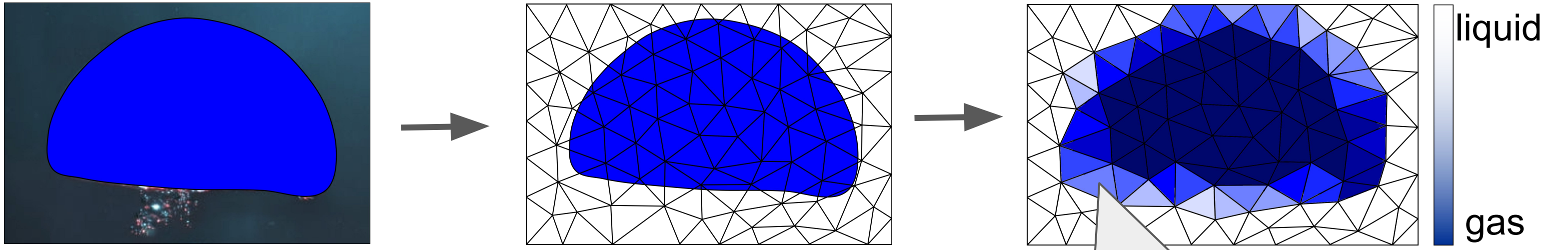


Surface reconstruction

*Picture from Marco Scala's PhD thesis at IFPEN Lyon

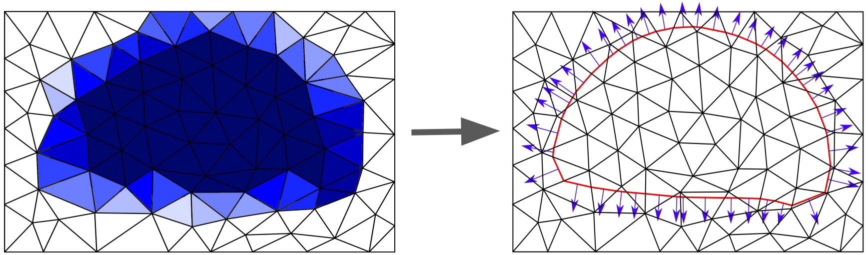
# Discretization & Reconstruction

Discretization



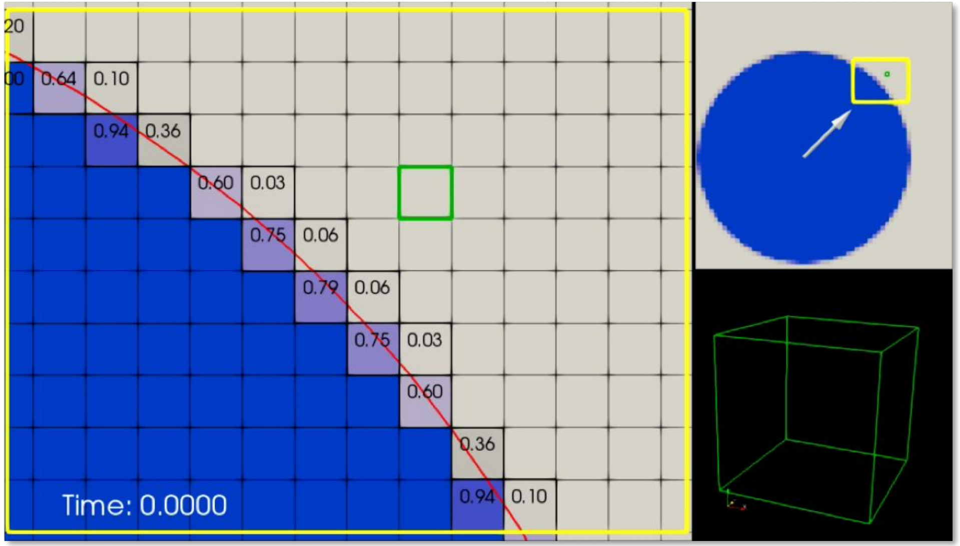

Volume fraction, pressure, velocity are stocked

Reconstruction



- Geometrical information is lost
- In some models geometrical features are required (*i.e.* interface tension force computation)

# Reconstruction by the VoF




Source: OpenFOAM
https://www.youtube.com/watch?v=F2WCsF8Sn84

The VoF is **accurate** (good at mass conservation) and performs well on **structured grids**.

# Navier - Stokes in multiphase flow

**Additional terms** in the Navier-Stokes equations to deal with multiphase flows:

Momentum equation

Pressure Viscosity Surface tension force

$$\frac{\partial \rho \mathbf{U}}{\partial t} + \nabla \cdot (\rho \mathbf{U}\mathbf{U}) = -\nabla p + \rho \mathbf{g} + \nabla \cdot (\mu \nabla \mathbf{U}) + \rho \mathbf{S} + \sigma \kappa \hat{\mathbf{n}}_S \delta(\mathbf{x} - \mathbf{x}_s)$$

Advection Gravity Extra forces

Continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{U}) = 0$$

Density

$$\rho(\mathbf{x}, t) = \begin{cases} \rho_A, & \text{if } \mathbf{x} \text{ in fluid A} \\ \rho_B, & \text{if } \mathbf{x} \text{ in fluid B} \end{cases}$$

Different densities


5

# Surface tension force

The surface tension depends on **local geometrical features** of the interface:

Note that:

$$\kappa = \nabla \cdot \hat{\mathbf{n}}_S$$

$$F_S = \sigma \kappa \hat{\mathbf{n}}_S \delta(\mathbf{x} - \mathbf{x}_s)$$

**Surface tension coefficient**
Constant and depends on the liquid/gas at play

**Mean curvature**
Local curvature of the interface:

$$\frac{1}{2}(\kappa_1 + \kappa_2)$$

**Normal**
Normal direction to the interface in each point of the interface

**kronecker delta**
The surface tension is active only on the interface

# State of art and limitations

- The bottlenecks of the VoF
  - High computation cost
  - Issue with unstructured grids which leads to residual currents
- Neural network approach to reduce the cost
  - Qi et al.(2018): Curvature estimation on 2D surface with Neural Networks (NNs)
  - Patel et al.(2019): Curvature estimation on 3D surface with NNs. Their approach outperformed the conventional methods

# State of art and limitations

- Patel et al.(2019): Multi Layer Perceptron (MLP), emplayable on structured grids with constant discretization.
- Svyetlichnyy et al.(2017): MLP, estimate normal direction on 2D structured grid

| | Structured grid | Unstructured grid | Other remarks |
|---|---|---|---|
| VoF | Good | Instability | Expensive |
| NN | Good | Not available | Less expensive |

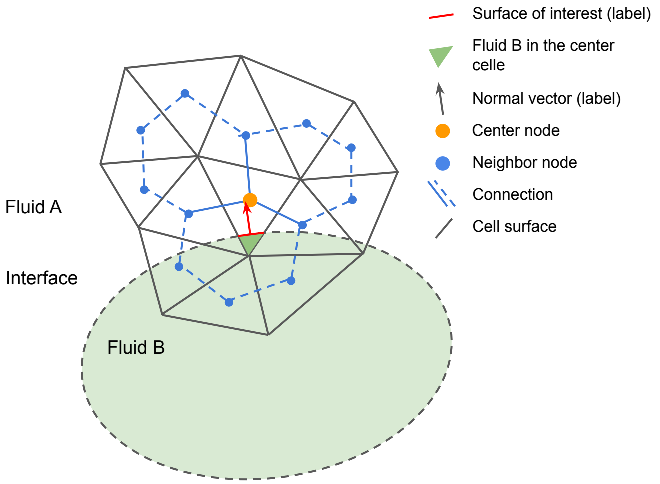
**For industrial cases with complex geometries, unstructured grids are usually employed**

# Objective

- We propose a machine learning-based method:
  - accurate enough to replace conventional reconstruction methods
  - less computational-demanding

- To that end, we study the use of Graph Neural Network architectures to recover interface properties (e.g., normal, curvature, etc.) from the discretized field.

# Graph Neural Networks (GNNs)




Unstructured data are modeled as graph structure

GNNs:

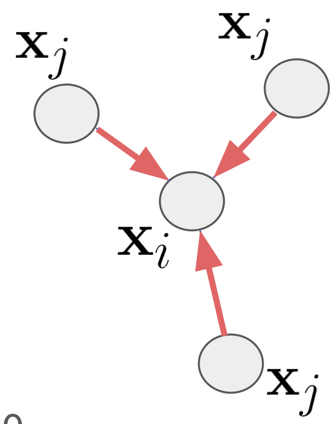
- Geometrically generalized CNNs
- Able to handle a graph-structure (nodes, edges)

For the prediction, GNNs take:

- Node features: volume fraction α, coordinates of vertices
- Edges: element connections

We employ SAGEConv proposed by Hamilton et al.(2017)*

<u>Message passing in SAGEConv</u>




1) $\mathrm{mean}_{j\in\mathcal{N}(i)}\,\mathbf{x}_j$

2) $\mathbf{W}_2\cdot\mathrm{mean}_{j\in\mathcal{N}(i)}\,\mathbf{x}_j$

3) $\mathbf{x}'_i=\mathbf{W}_1\mathbf{x}_i+\mathbf{W}_2\cdot\mathrm{mean}_{j\in\mathcal{N}(i)}\,\mathbf{x}_j$

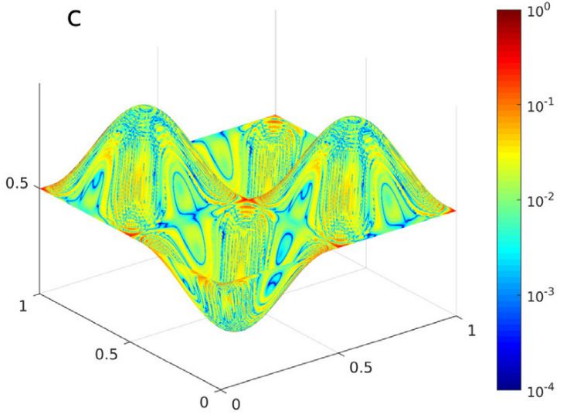
4) $\sigma\left(\mathbf{x}'_i=\mathbf{W}_1\mathbf{x}_i+\mathbf{W}_2\cdot\mathrm{mean}_{j\in\mathcal{N}(i)}\,\mathbf{x}_j\right)$

*Inductive Representation Learning on Large Graphs
William L. Hamilton, Rex Ying, Jure Leskovec

# Synthetic dataset

All previous studies used spherical surfaces

- Larger error at saddle points
- **Biased dataset:** only spherical surfaces are considered in the training

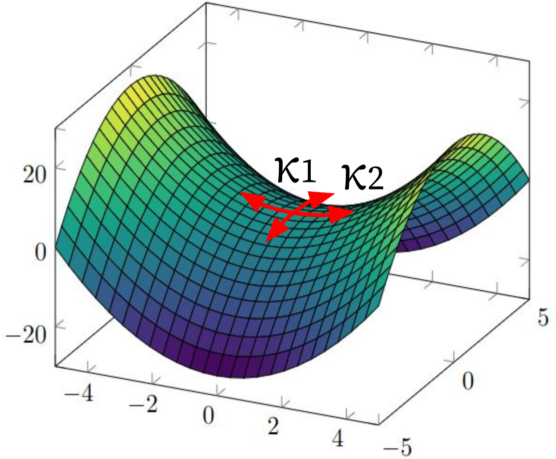



Error on the curvature prediction by ML by Patel et al.(2019)

In our study, we introduce a paraboloid-based dataset

$$\frac{x^2\kappa_1}{2} + \frac{y^2\kappa_2}{2} = z$$

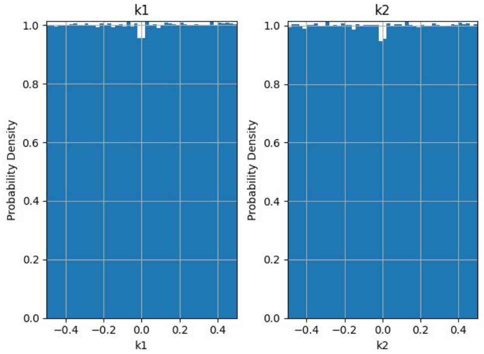
$\kappa_1$, $\kappa_2$ are the curvature on the two parabola at the center which is randomly chosen in space




Paraboloid

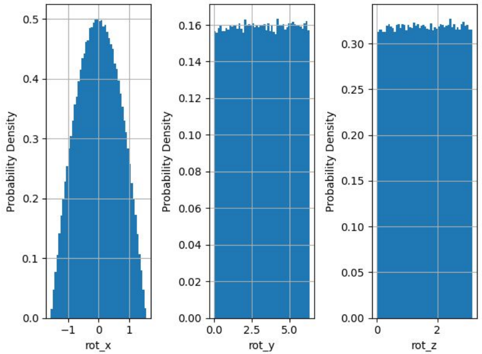
# Distribution in the dataset

PDF

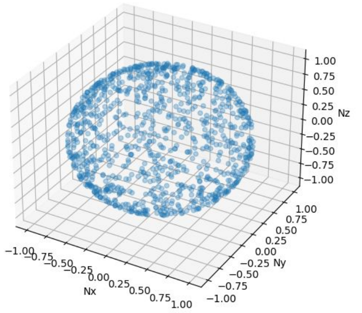



Normalized histogram of
$\kappa 1, \kappa 2$

PDF




Normalized histogram of $rot_{x,y,z}$




Normal (1k graphs displayed for the simplicity)

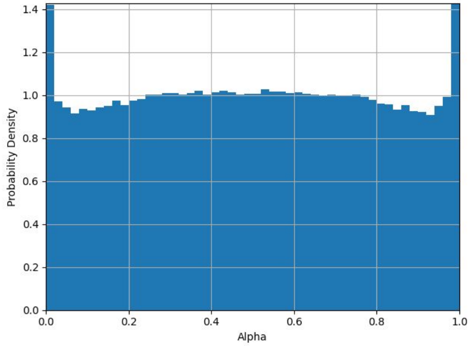
Uniforme distribution:

- Curvature $\kappa 1, \kappa 2$
- 3D-rotation
- Volume fraction α
- Center point of the surface

of each paraboloid surface

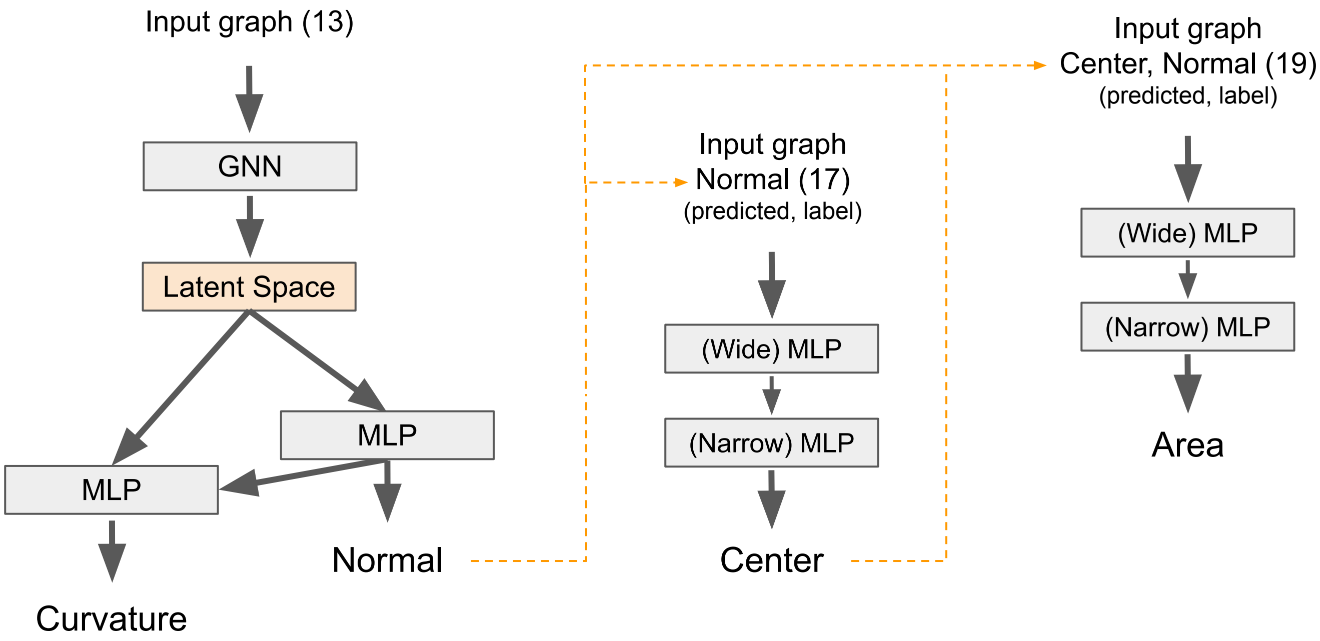
=> **A non-biased dataset has been then generated**

PDF




Alpha

# Architecture

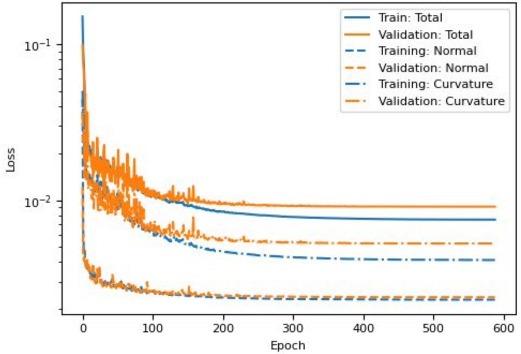


# Training

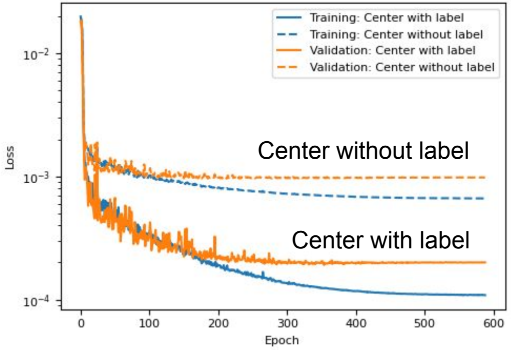
- 500k graphs: 1 graph = 1 normal, 1 curvature
- Train/Validation/Test ratio: 7:2:1
- Variable learning rate (min.1e-6)
- Adam optimizer
- Input: node features, edges
- Predict: normal, curvature, etc.
- Loss: L2
    - Total = Normal + Curvature + Center(w/o label) + Area(w/o label)

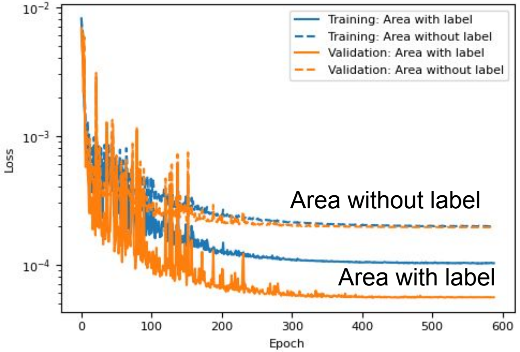
- All the variables converge
- No improvement after 508th epoch
- No overfitting

Blue: training
Orange: validation




Total
Curvature
Normal



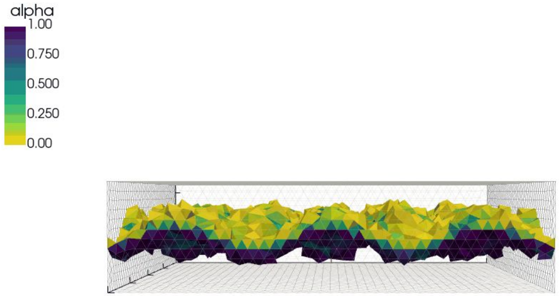
# Generalization

Prediction on a **new surface** different from the paraboloid for the training:

$$f(x) = 0.1 \sin 9x \cos 9y$$

$$|H|_{\max} = 0.703$$

$$H_{\text{training}} \approx [-0.75, 0.75]$$

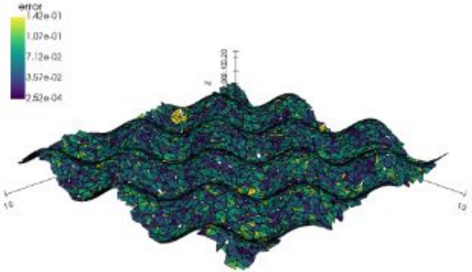


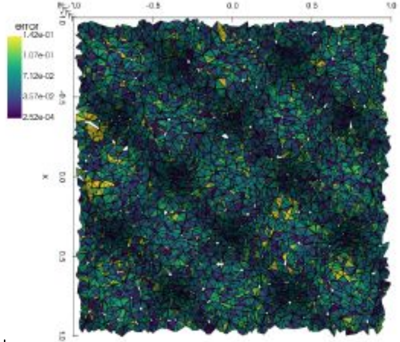
# Prediction error

- 0.01< α < 0.99
- Uniform and no dependence on the geometry
- Smooth distribution, no outlier in the histograms

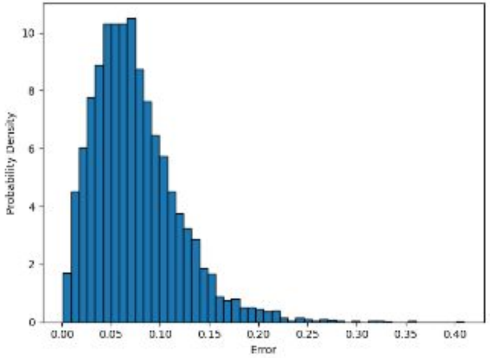
Normal: $N_{error} = \|\mathbf{N}_{label} - \mathbf{N}_{pred}\|$

Median: 6.05e-2



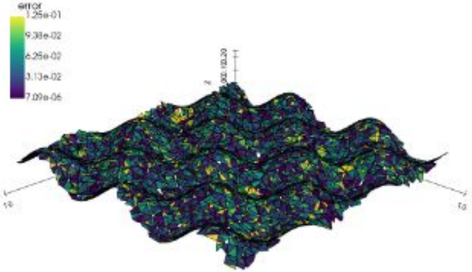


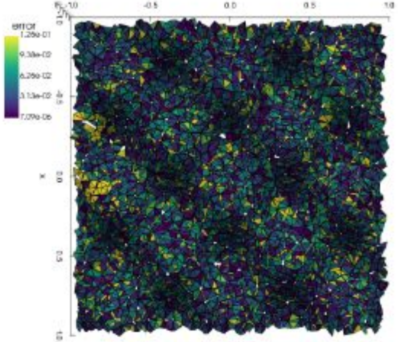
Normalized histogram

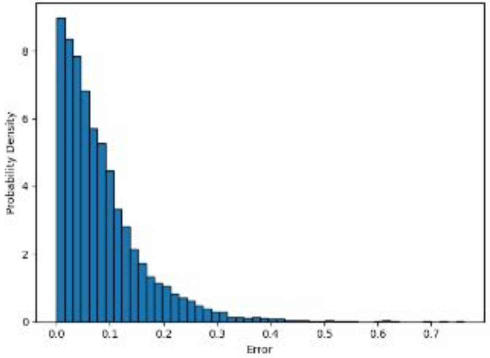



Curvature: $H_{error} = |H_{label} - H_{pred}|$

Median: 4.32e-2







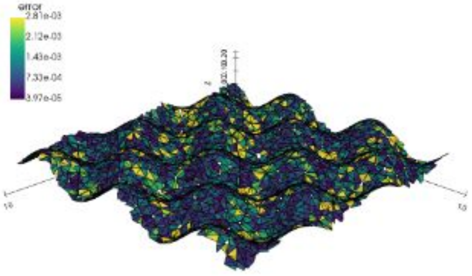
# Prediction error

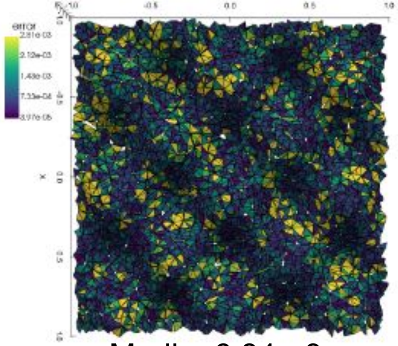
- 0.01< α < 0.99
- Uniform and no dependence on the geometry
- Smooth distribution, no outlier in the histograms

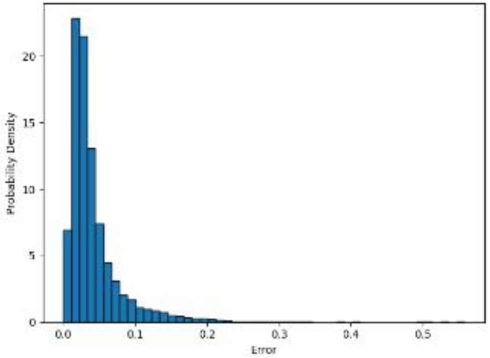
Center: $M_{error} = \|\mathbf{M}_{label} - \mathbf{M}_{pred}\|$

Media: 1.84e-2

Normalized histogram

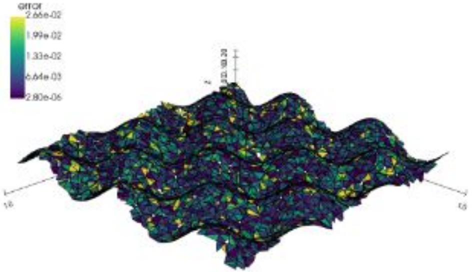


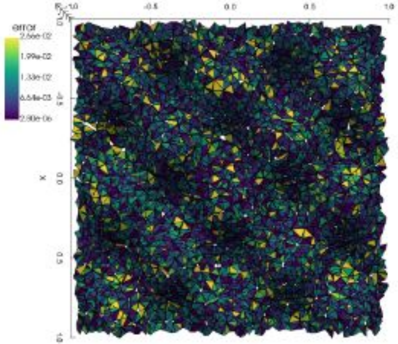



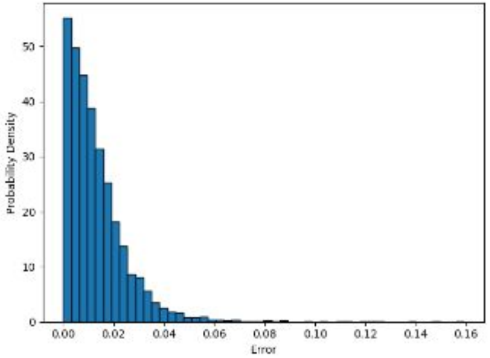




Area: $A_{error} = |A_{label} - A_{pred}|$

Media: 6.84e-3

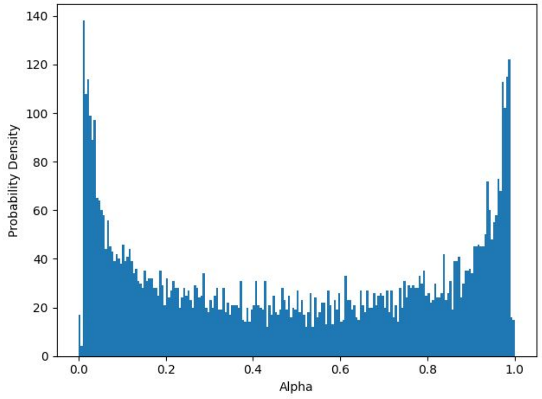


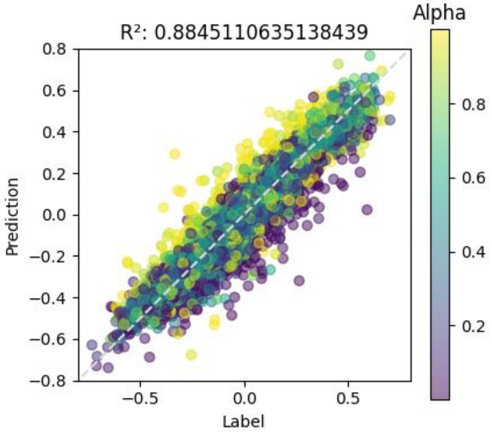



# Prediction error

- α has non-uniform distribution
- Curvature prediction, a large error at “marginal α”
  - A large α: the prediction is larger than the label
  - A small α: the prediction is smaller than the label
- This should be taken into consideration when implemented in real simulations




Histogram of α




Curvature (left) prediction vs label

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# Conclusions & Perspectives

Conclusion

1. **Graph Neural Networks** can be an alternative to the conventional surface reconstruction methods
2. GNNs could be a promising reconstruction approach to unstructured grids

Perspectives

1. Employ the model in a CFD code (i.e. OpenFOAM)
2. Assessment of time performance of the model
3. Treatment of boundary conditions

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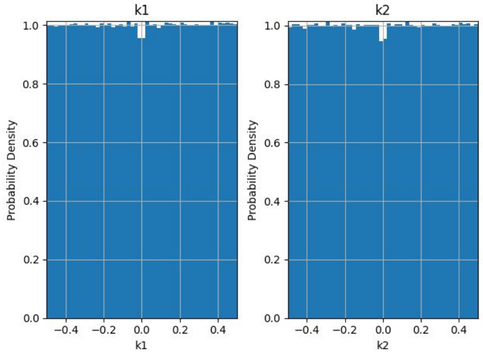
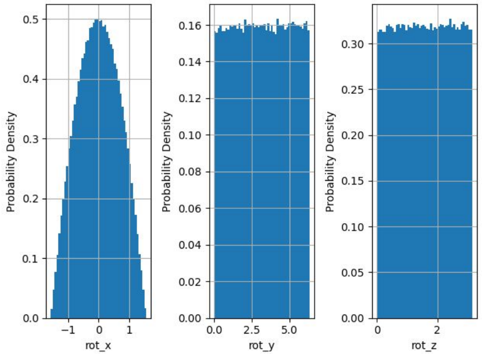
# Distribution in the dataset

PDF

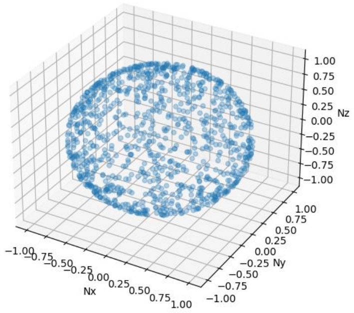



Normalized histogram of $\kappa_1, \kappa_2$

PDF

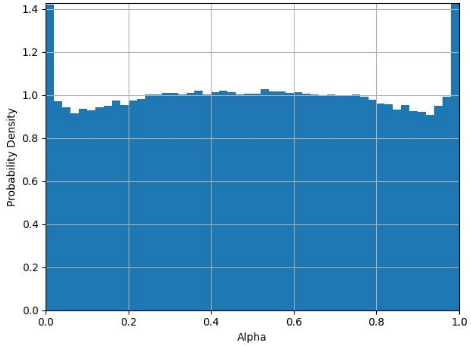



Normalized histogram of $rot_{x,y,z}$




Normal (1k graphs displayed for the simplicity)

PDF



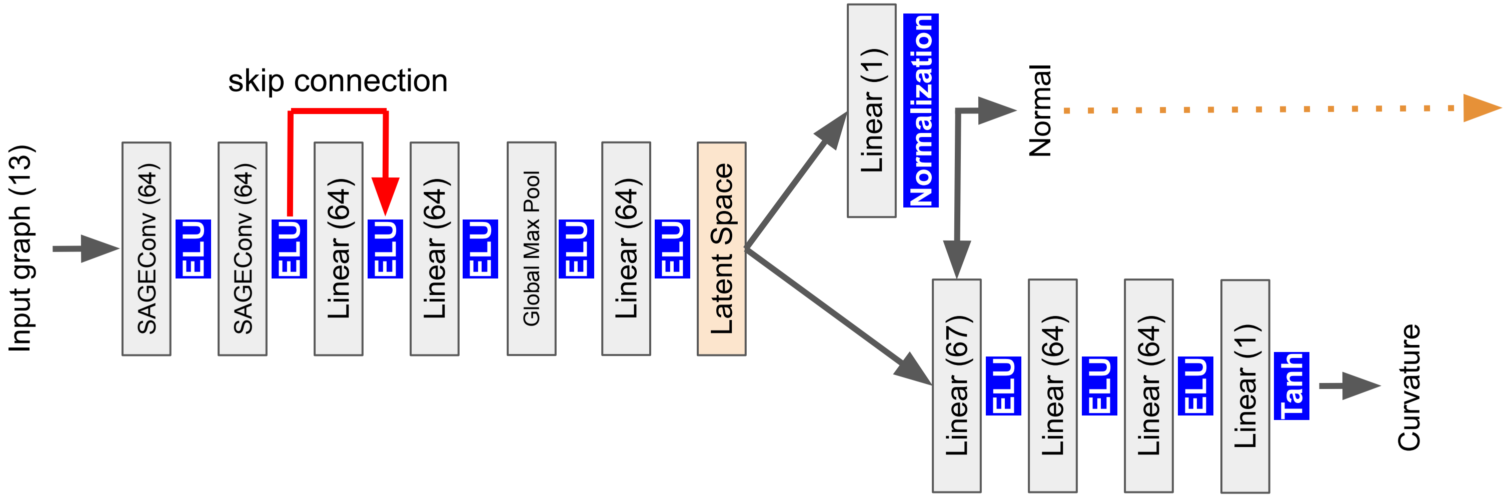

Alpha

- $\kappa_1, \kappa_2 \sim \pm[0.001, 0.5]$ (uniforme distribution)
- $(rot_x, rot_y, rot_z) = \cos^{-1}(2u_2 - 1), \pi u_2, 2\pi u_2$ (uniform rotation in 3D)
- Alpha distribution is uncontrollable in advance => quasi-uniform is generated
- Center of graph randomized

=> **A non-biased dataset has been then generated**

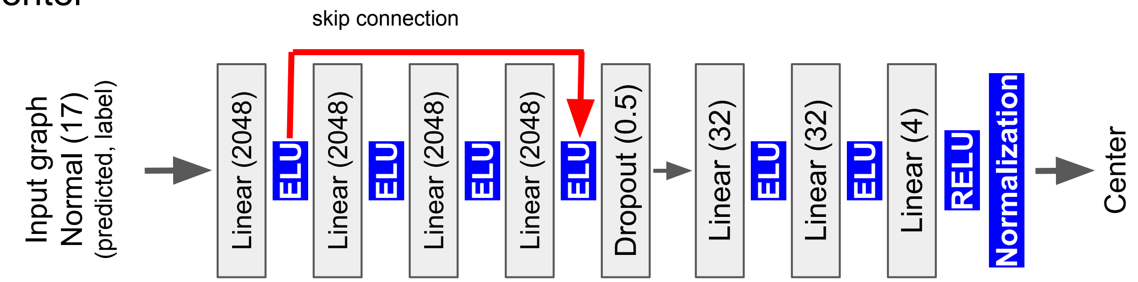
# Architecture

Normal, Curvature

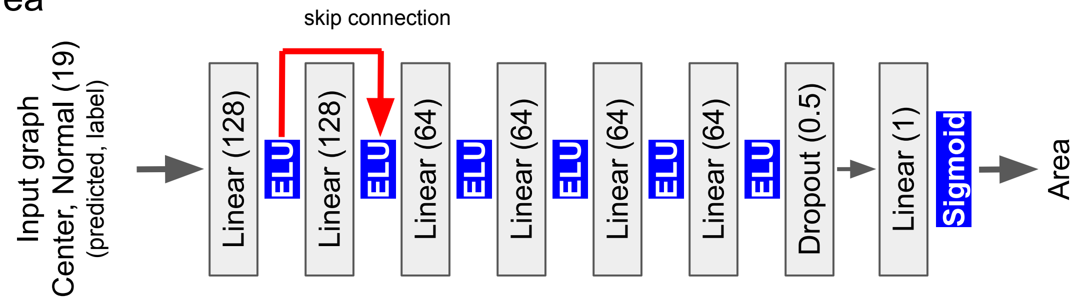


# Architecture

## Center




## Area



## Loss function

$$\text{Loss}_{\text{total}} = \text{Loss}_{\text{normal}} + \text{Loss}_{\text{curv}} + \text{Loss}_{\text{c:wl}} + \text{Loss}_{\text{a:wl}} + \text{Loss}_{\text{c:wol}} + \text{Loss}_{\text{a:wol}}$$

$$\text{Loss}_{\text{normal}} = \frac{1}{N_b}\sum_{b=1}^{N_b}\sum_{i=1}^{3}\frac{(N_{b,i,label} - N_{b,i,pred})^2}{3}$$

$$\text{Loss}_{\text{c:wl,wol}} = \frac{1}{N_b}\sum_{b=1}^{N_b}\sum_{i=1}^{4}\frac{(p_{b,i,label} - p_{b,i,pred})^2}{4}$$

$$\text{Loss}_{\text{curv,a:wl,wol}} = \frac{1}{N_b}\sum_{b=1}^{N_b}(y_{b,label} - y_{b,pred})^2$$

## Model performance

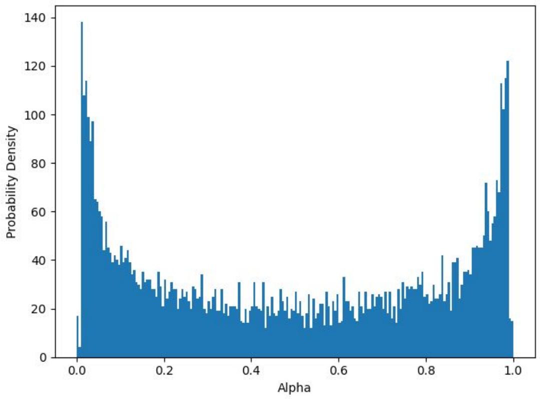
Table 1: Model performance at the 508[th] epoch

| Type of loss | Training | Validation | MSE |
|---|---|---|---|
| $\text{Loss}_{\text{total}}$ | 7.50e-3 | 9.07e-3 | 9.30e-3 |
| $\text{Loss}_{\text{normal}}$ | 2.30e-3 | 2.39e-3 | 2.41e-3 |
| $\text{Loss}_{\text{curv}}$ | 4.13e-3 | 5.26e-3 | 5.40e-3 |
| $\text{Loss}_{\text{c:wl}}$ | 1.10e-4 | 2.01e-4 | 1.84e-4 |
| $\text{Loss}_{\text{c:wol}}$ | 6.66e-4 | 9.76e-4 | 1.05e-3 |
| $\text{Loss}_{\text{a:wl}}$ | 1.03e-4 | 5.53e-5 | 5.51e-5 |
| $\text{Loss}_{\text{a:wol}}$ | 1.99e-4 | 1.95e-4 | 2.03e-4 |

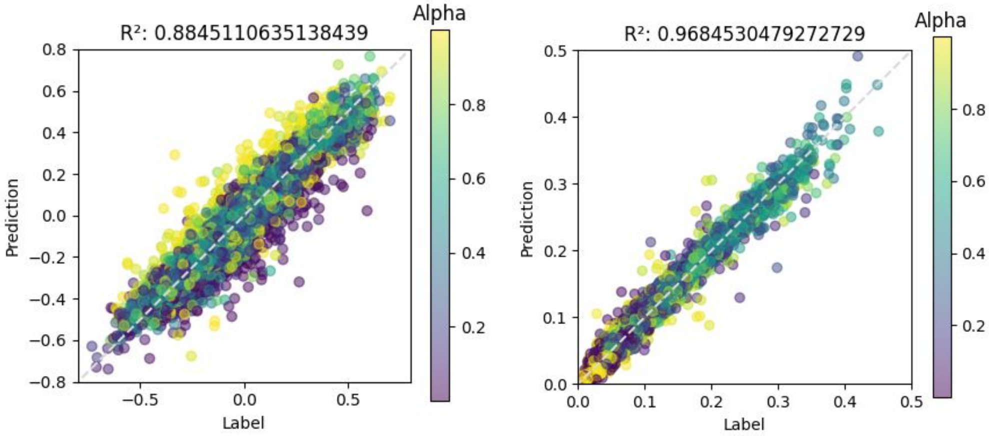
Table 2: The model performance the test-No.1

| Predicted variable | Median |
|---|---|
| $N_{error} = \Vert\mathbf{N}_{label} - \mathbf{N}_{pred}\Vert$ | 5.61e-2 |
| $H_{error} = \vert H_{label} - H_{pred}\vert$ | 4.16e-2 |
| $M_{error} = \Vert\mathbf{M}_{label} - \mathbf{M}_{pred}\Vert$ | 1.98e-2 |
| $A_{error} = \vert A_{label} - A_{pred}\vert$ | 7.57e-3 |

# Prediction error




Histogram of α




Curvature (left), Area (right) prediction vs label