

# Graph Convolutional Networks and some applications

Corentin MENGEL,

under the supervision of Vincent VIGON, Emmanuel FRANCK,  
Laurent NAVORET and Laurène HUME

August 24, 2021

# Introduction

continuation of the previous project

# Introduction

continuation of the previous project

GCNs achieve good results even after modifications of the graph

# Introduction

continuation of the previous project

GCNs achieve good results even after modifications of the graph

develop a new model and use it in two problems:

# Introduction

continuation of the previous project

GCNs achieve good results even after modifications of the graph

develop a new model and use it in two problems:

- ▶ discontinuities detection and Burgers' equation

# Introduction

continuation of the previous project

GCNs achieve good results even after modifications of the graph

develop a new model and use it in two problems:

- ▶ discontinuities detection and Burgers' equation
- ▶ interpolation problem and linear transport equation

# Definitions

# Definitions: Graph Convolutional Networks

# Definitions: Graph Convolutional Networks

GCN: sequence of layers put one after the other

# Definitions: Graph Convolutional Networks

GCN: sequence of layers put one after the other

graph convolutional layer:

- ▶ takes  $d$  dimensional node features as input

# Definitions: Graph Convolutional Networks

GCN: sequence of layers put one after the other

graph convolutional layer:

- ▶ takes  $d$  dimensional node features as input
- ▶ computes  $d'$  dimensional representations of the nodes

# Definitions: Graph Convolutional Networks

GCN: sequence of layers put one after the other

graph convolutional layer:

- ▶ takes  $d$  dimensional node features as input
- ▶ computes  $d'$  dimensional representations of the nodes
- ▶ uses recursive neighborhood diffusion and message passing

# Definitions: Graph Convolutional Networks

GCN: sequence of layers put one after the other

graph convolutional layer:

- ▶ takes  $d$  dimensional node features as input
- ▶ computes  $d'$  dimensional representations of the nodes
- ▶ uses recursive neighborhood diffusion and message passing
- ▶ each graph node gathers features from its neighbors

## Definitions: pooling layers

inconvenient: convolutional layers do not change the mesh structure

## Definitions: pooling layers

inconvenient: convolutional layers do not change the mesh structure

new layers reducing the graph resolutions

## Definitions: pooling layers

inconvenient: convolutional layers do not change the mesh structure

new layers reducing the graph resolutions

enlarge receptive field for better performance and generalization

## Definitions: pooling layers

inconvenient: convolutional layers do not change the mesh structure

new layers reducing the graph resolutions

enlarge receptive field for better performance and generalization

⇒ pooling layers

## Definitions: Top-k pooling

inputs: mesh  $\Omega$ , nodes features  $X$ , integer  $k$ ,

output: new mesh with  $k$  nodes

## Definitions: Top-k pooling

inputs: mesh  $\Omega$ , nodes features  $X$ , integer  $k$ ,

output: new mesh with  $k$  nodes

selects subset of nodes to form a smaller graph

## Definitions: Top-k pooling

inputs: mesh  $\Omega$ , nodes features  $X$ , integer  $k$ ,

output: new mesh with  $k$  nodes

selects subset of nodes to form a smaller graph

a score  $y_i \in \mathbb{R}$  is associated to each node  $n_i$  of  $\Omega$

## Definitions: Top-k pooling

inputs: mesh  $\Omega$ , nodes features  $X$ , integer  $k$ ,

output: new mesh with  $k$  nodes

selects subset of nodes to form a smaller graph

a score  $y_i \in \mathbb{R}$  is associated to each node  $n_i$  of  $\Omega$

$$y_i = X_i \cdot p / \|p\|$$

$p$  trainable vector

## Definitions: Top-k pooling

inputs: mesh  $\Omega$ , nodes features  $X$ , integer  $k$ ,

output: new mesh with  $k$  nodes

selects subset of nodes to form a smaller graph

a score  $y_i \in \mathbb{R}$  is associated to each node  $n_i$  of  $\Omega$

$$y_i = X_i \cdot p / \|p\|$$

$p$  trainable vector

the new mesh has the  $k$  nodes with the highest score

# Top-k pooling example

$X_i = \text{node position}, p = (1, 1)$

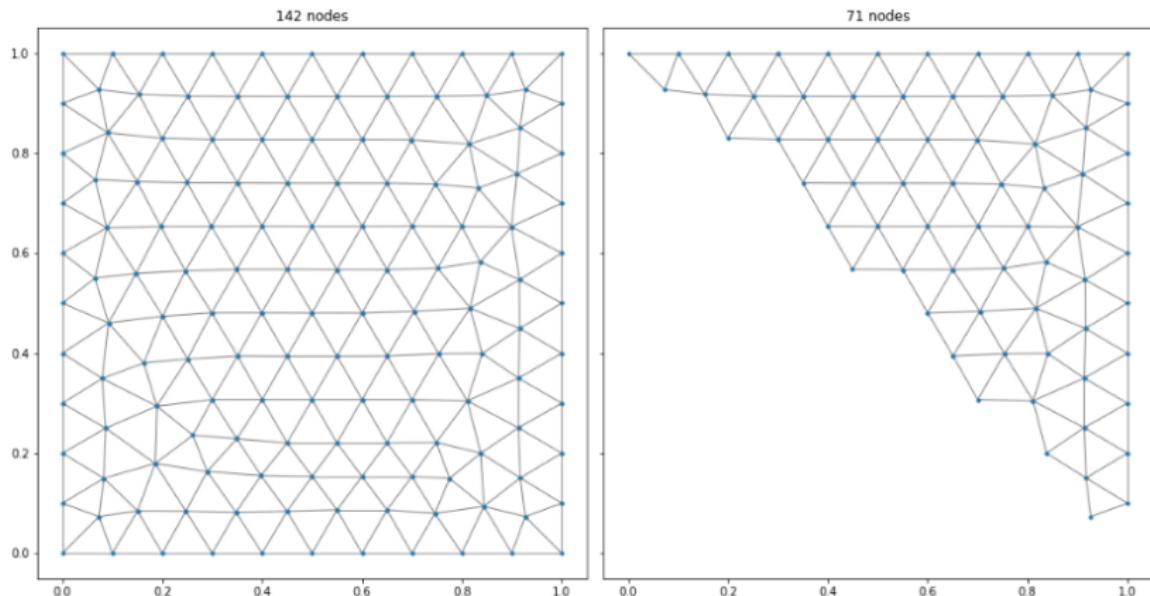


Figure: Initial mesh (left) and pooled mesh (right).

## Definitions: k-Means pooling

pooling based on the k-Means clustering algorithm

## Definitions: k-Means pooling

pooling based on the k-Means clustering algorithm

inputs: mesh  $\Omega$ , integer  $k$ , output: new mesh with  $k$  nodes

## Definitions: k-Means pooling

pooling based on the k-Means clustering algorithm

inputs: mesh  $\Omega$ , integer  $k$ , output: new mesh with  $k$  nodes

- ▶ compute  $k$  clusters of the nodes of  $\Omega$

## Definitions: k-Means pooling

pooling based on the k-Means clustering algorithm

inputs: mesh  $\Omega$ , integer  $k$ , output: new mesh with  $k$  nodes

- ▶ compute  $k$  clusters of the nodes of  $\Omega$
- ▶ center of the  $k$  clusters → nodes of the new mesh

## Definitions: k-Means pooling

pooling based on the k-Means clustering algorithm

inputs: mesh  $\Omega$ , integer  $k$ , output: new mesh with  $k$  nodes

- ▶ compute  $k$  clusters of the nodes of  $\Omega$
- ▶ center of the  $k$  clusters  $\rightarrow$  nodes of the new mesh
- ▶ new node features = average of the node features in the clusters

# k-Means example

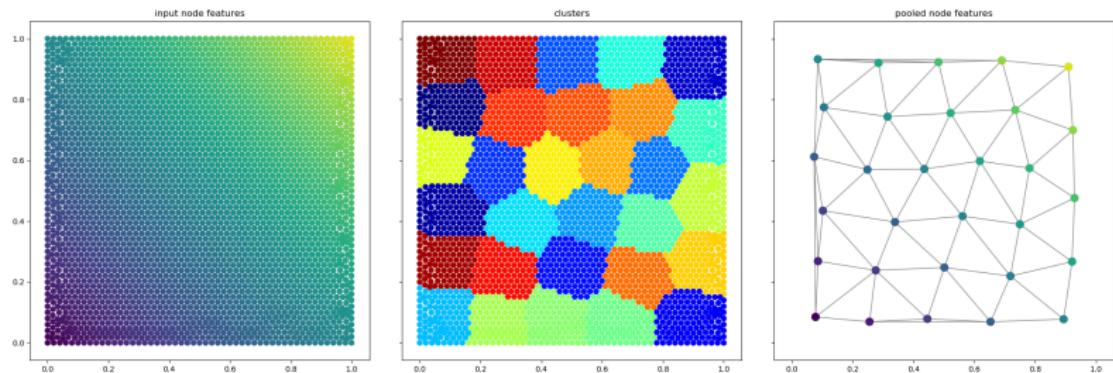


Figure: Initial mesh (left), clusters (center), and pooled mesh (right).

## Frontier detection problem

## Frontier detection: dataset

problem: detect the frontier between two areas on a mesh

# Frontier detection: dataset

problem: detect the frontier between two areas on a mesh

3 types of areas:

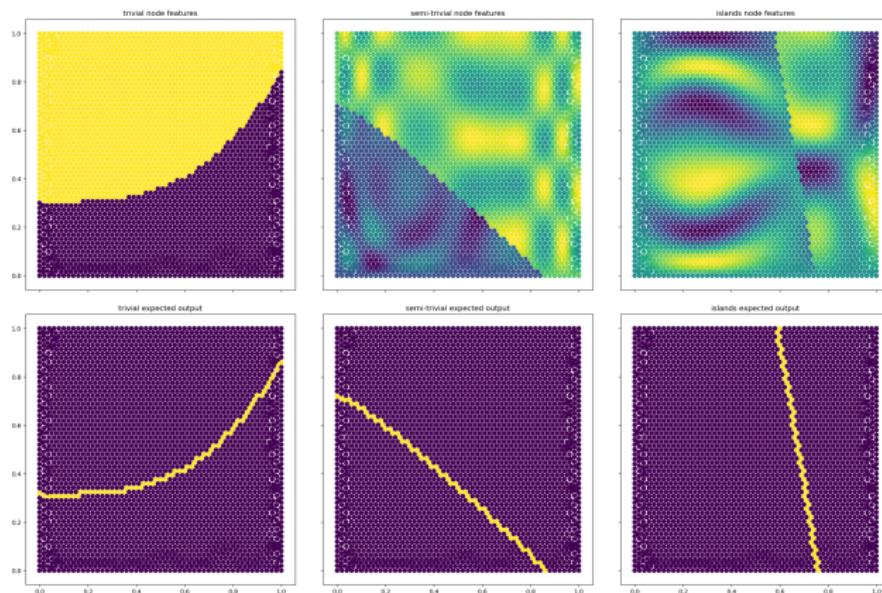


Figure: Trivial dataset (left), semi-trivial dataset (center) and islands dataset (right).

## Frontier detection: previous results

simple sequential model: GCN layers put one after the other

## Frontier detection: previous results

simple sequential model: GCN layers put one after the other

worked only on the trivial dataset

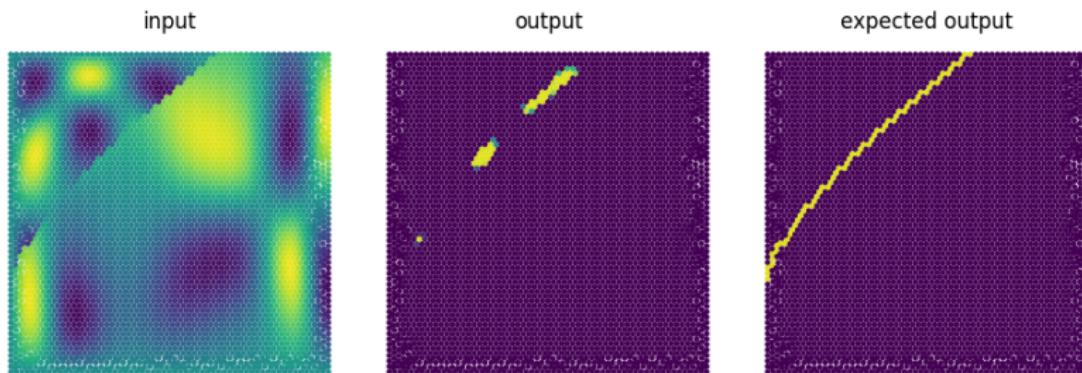


Figure: Old model results on the islands dataset.

# Frontier detection: U-Net architecture

more complex architecture

# Frontier detection: U-Net architecture

more complex architecture

model: contractive + expansive path

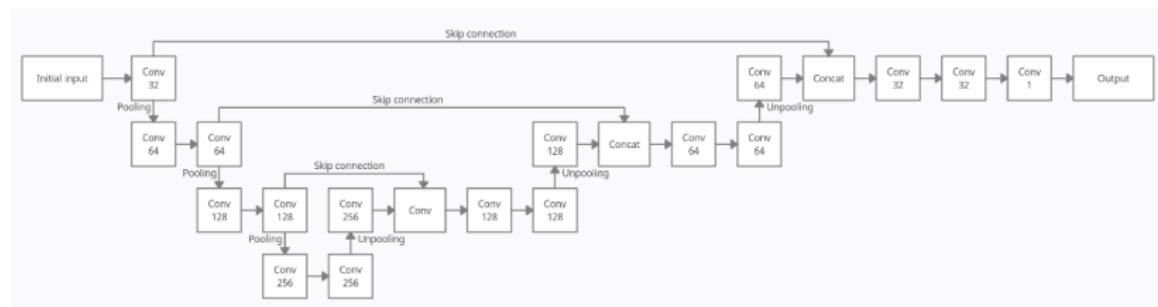


Figure: Architecture of the model used.

# Frontier detection: U-Net architecture

more complex architecture

model: contractive + expansive path

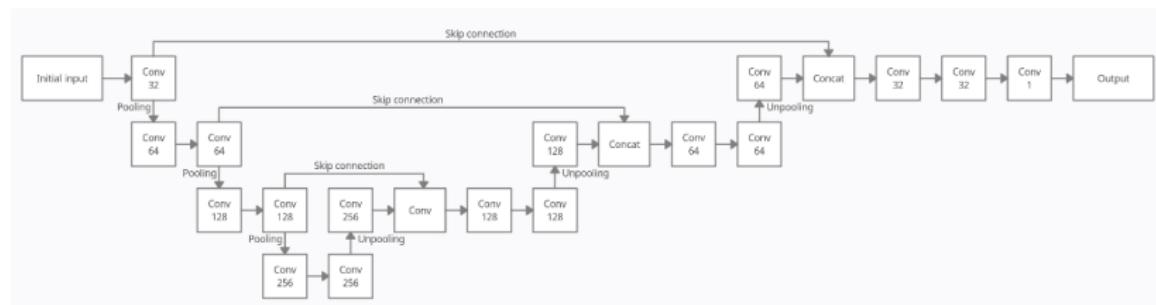


Figure: Architecture of the model used.

3 pooling layers and 3 unpooling layers

## Frontier detection: results

first model: U-Net with Vanilla GCN layers and Top-k pooling layers

## Frontier detection: results

first model: U-Net with Vanilla GCN layers and Top-k pooling layers

⇒ bad results: Top-k pooling discard big portions of the graph

## Frontier detection: results

first model: U-Net with Vanilla GCN layers and Top-k pooling layers

⇒ bad results: Top-k pooling discard big portions of the graph

second model: replace Top-k pooling by k-Means pooling

## Frontier detection: results

first model: U-Net with Vanilla GCN layers and Top-k pooling layers

⇒ bad results: Top-k pooling discard big portions of the graph

second model: replace Top-k pooling by k-Means pooling

⇒ good results on trivial/semi-trivial dataset

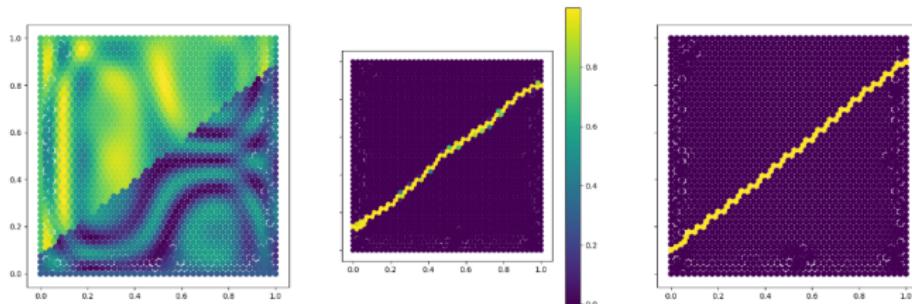


Figure: Input (left), model prediction (middle), expected output (right).

## Frontier detection: results

second model still unable to detect the border on the islands dataset

## Frontier detection: results

second model still unable to detect the border on the islands dataset

third model: replace VanillaGCN with ChebConv layers

## Frontier detection: results

second model still unable to detect the border on the islands dataset

third model: replace VanillaGCN with ChebConv layers  
⇒ model more complex/more trainable weights

## Frontier detection: results

second model still unable to detect the border on the islands dataset

third model: replace VanillaGCN with ChebConv layers  
⇒ model more complex/more trainable weights

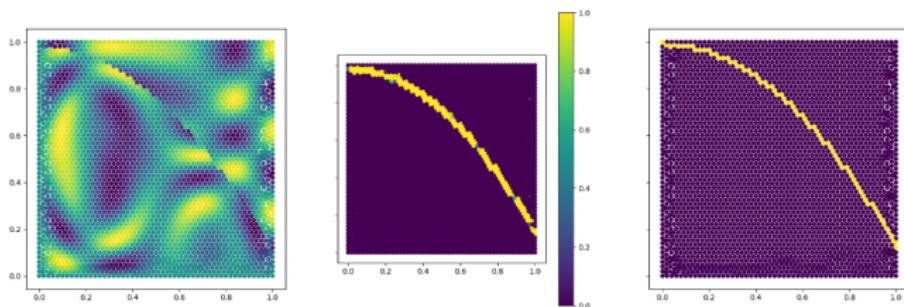


Figure: Input (left), model prediction (middle), expected output (right).

## Burgers' equation and dynamic refining

# Burgers' equation and dynamic refining

PDE used for example in fluid mechanics or traffic flow

# Burgers' equation and dynamic refining

PDE used for example in fluid mechanics or traffic flow

$$\partial_t \rho(t, x) + \nabla \cdot \left( a \frac{\rho(t, x)^2}{2} \right) = 0 \quad (1)$$

with  $\rho : \mathbb{R}_+ \times \mathbb{R}^2 \rightarrow \mathbb{R}$ ,  $a \in \mathbb{R}^2$  and  $t \in [0, T]$ .

## Burgers' equation and dynamic refining

PDE used for example in fluid mechanics or traffic flow

$$\partial_t \rho(t, x) + \nabla \cdot \left( a \frac{\rho(t, x)^2}{2} \right) = 0 \quad (1)$$

with  $\rho : \mathbb{R}_+ \times \mathbb{R}^2 \rightarrow \mathbb{R}$ ,  $a \in \mathbb{R}^2$  and  $t \in [0, T]$ .

multiple methods: kinetic relaxation or finite volume method

# Burgers' equation and dynamic refining

PDE used for example in fluid mechanics or traffic flow

$$\partial_t \rho(t, x) + \nabla \cdot \left( a \frac{\rho(t, x)^2}{2} \right) = 0 \quad (1)$$

with  $\rho : \mathbb{R}_+ \times \mathbb{R}^2 \rightarrow \mathbb{R}$ ,  $a \in \mathbb{R}^2$  and  $t \in [0, T]$ .

multiple methods: kinetic relaxation or finite volume method

transforms PDE into algebraic equations

# Finite Volume Method

mesh  $\Omega$ , triangles  $\Omega_j$ ,  $t_n$  discretization of  $[0, T]$

# Finite Volume Method

mesh  $\Omega$ , triangles  $\Omega_j$ ,  $t_n$  discretization of  $[0, T]$

final scheme:

$$\rho_j^{n+1} = \rho_j^n - \frac{\Delta t}{|\Omega_j|} \sum_{k \in E_j} d_{jk} F(\rho_j^n, \rho_k^n).$$

where:

$$F(\rho_j^n, \rho_k^n) = \frac{1}{2} \left[ a \cdot n_{jk} \left( \rho_j^{n2} + \rho_j^{n2} \right) + \max(|a \cdot n_{jk} \rho_j^n|, |a \cdot n_{jk} \rho_k^n|) (\rho_j^n - \rho_k^n) \right]$$

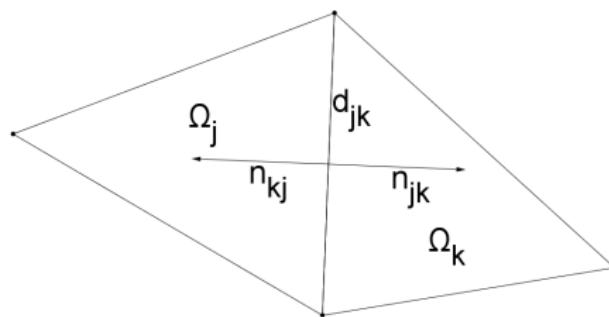


Figure: Notations.

## Example of solutions

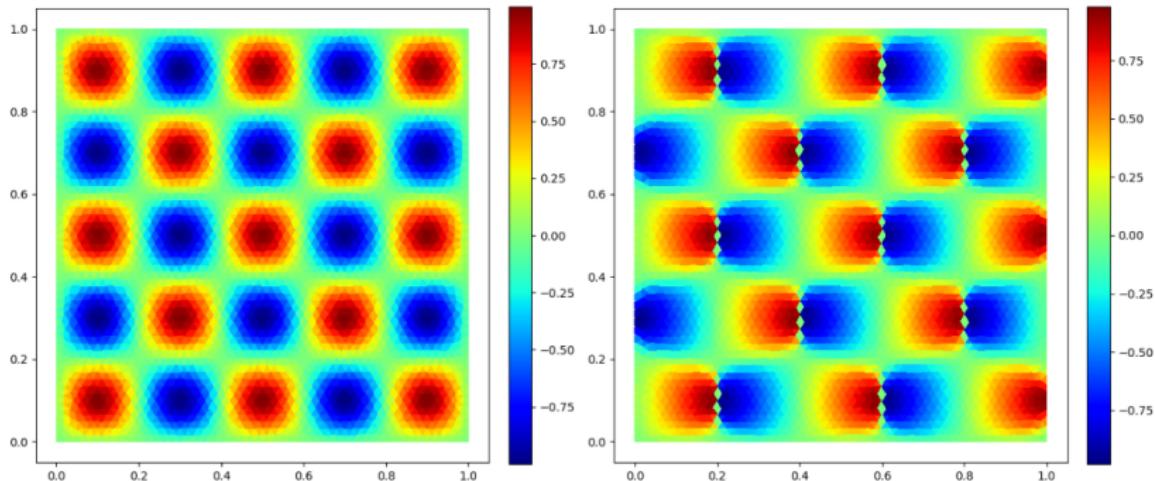


Figure: Initial solution (left) and final solution (right) at  $t = 0.05s$ ,  
 $a = (1, 0)$ .

## Example of solutions

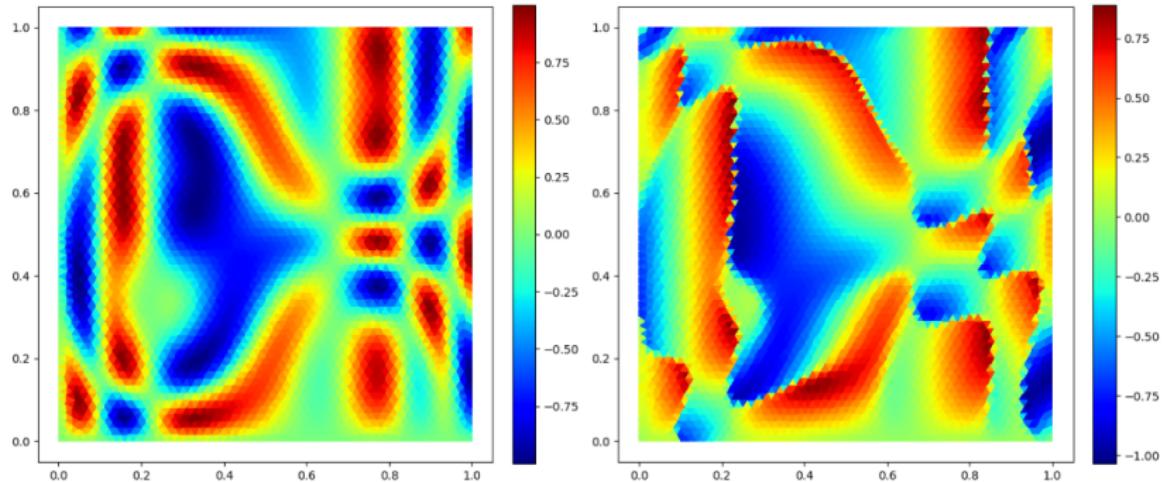


Figure: Initial solution (left) and final solution (right) at  $t = 0.05s$ ,  
 $a = (1, 1)$ .

## Dynamic refining

refine the mesh while we are computing the final solution

## Dynamic refining

refine the mesh while we are computing the final solution

use the border detection model to detect discontinuities

# Dynamic refining

refine the mesh while we are computing the final solution

use the border detection model to detect discontinuities

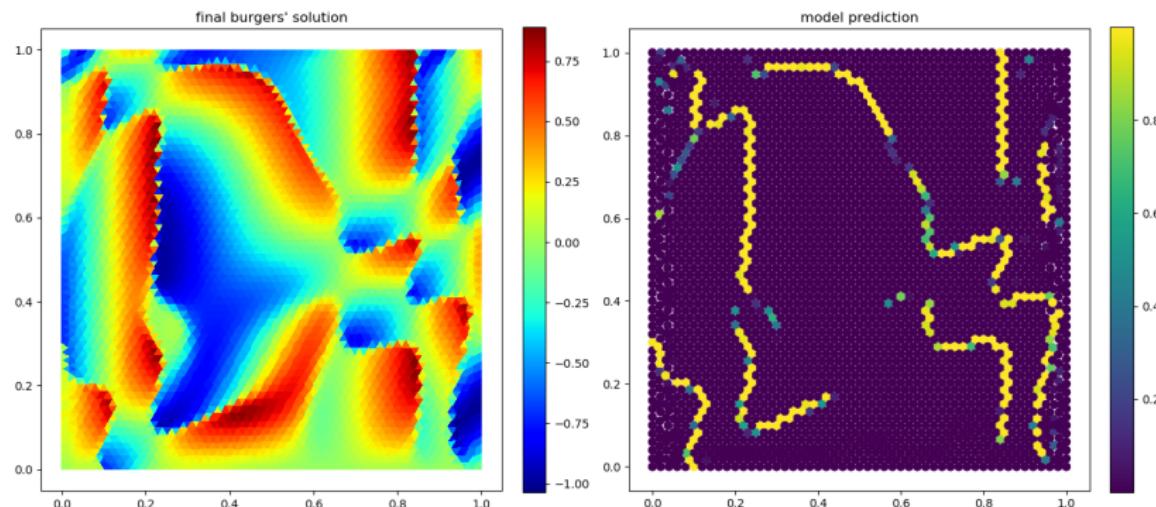


Figure: Final Burgers' solutions (left), and model predictions (right).

# Dynamic refining

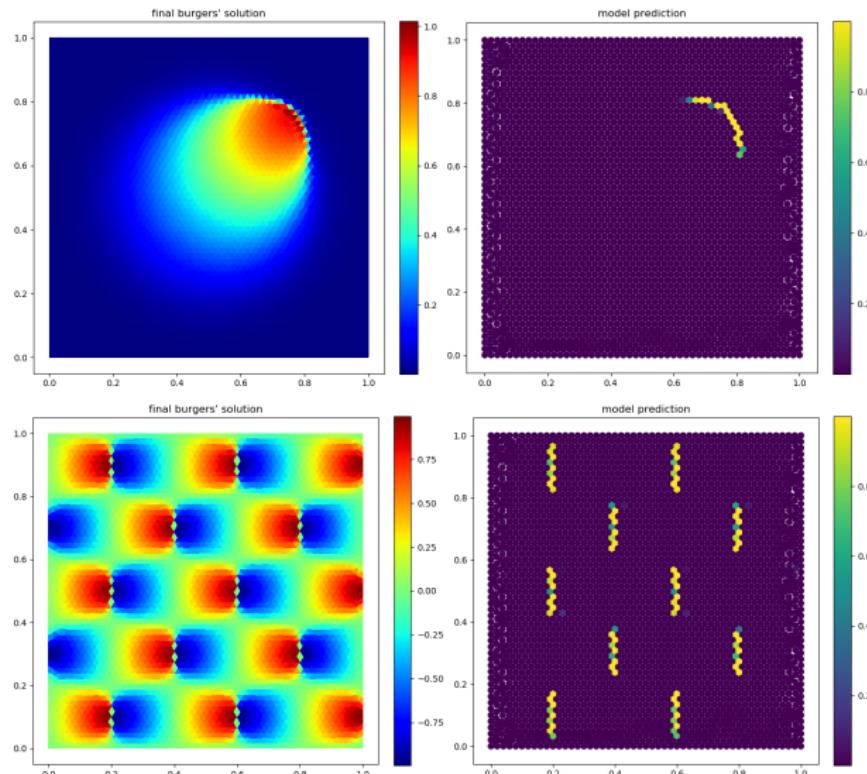


Figure: Final Burgers' solutions (left), and model predictions (right).

# Results

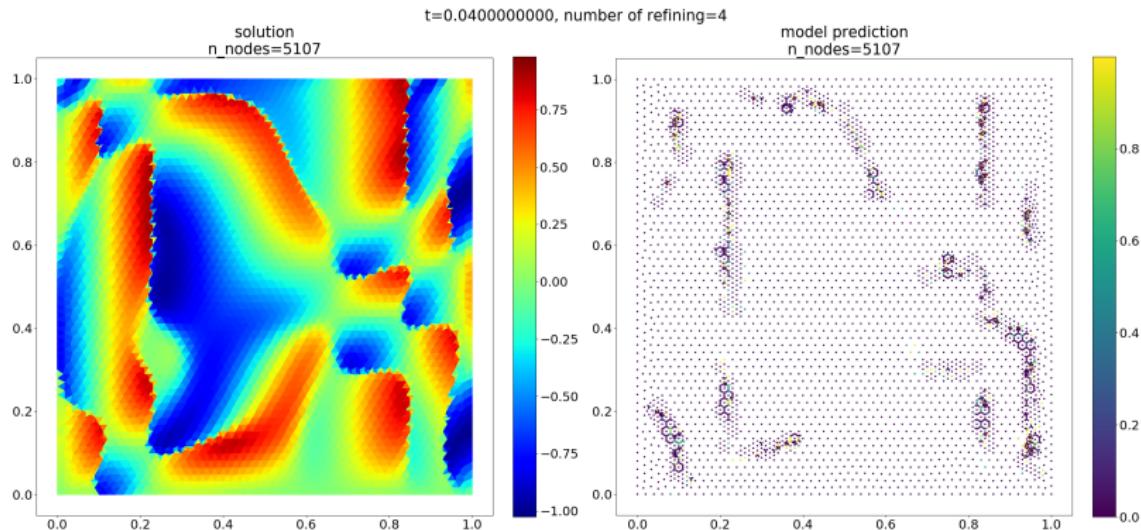


Figure: Solution with refinements (left), and model prediction (right).

# Results

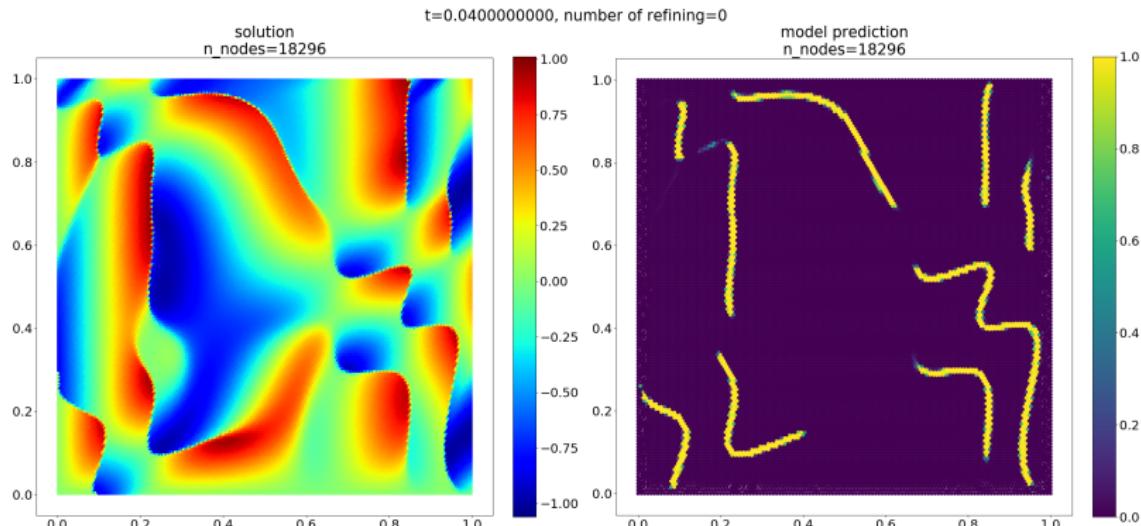


Figure: Finer solution (left), and model prediction (right).

# Results

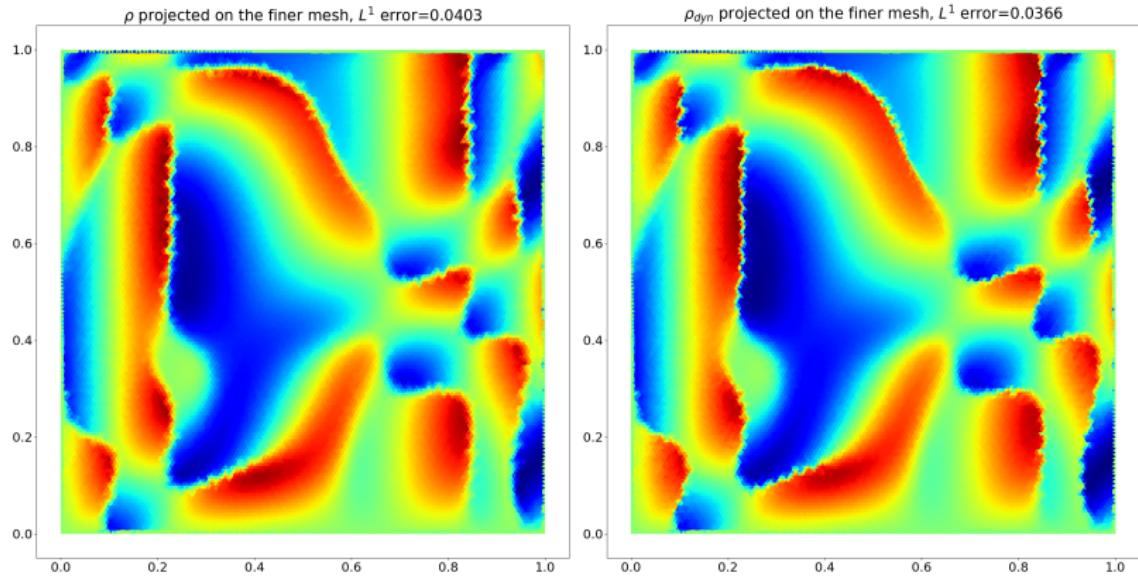


Figure: Projections and errors on the finer mesh.

## Transport equation and interpolation problem

# Transport equation and interpolation problem

equation describing the displacement of some quantity

## Transport equation and interpolation problem

equation describing the displacement of some quantity

$$\partial_t u + a(x) \cdot \nabla_x u = 0 \quad (2)$$

with  $u : \mathbb{R}_+ \times \mathbb{R}^2 \rightarrow \mathbb{R}$ ,  $a : \mathbb{R}_+ \times \mathbb{R}^2 \rightarrow \mathbb{R}^2$  the direction.

## Transport equation and interpolation problem

equation describing the displacement of some quantity

$$\partial_t u + a(x) \cdot \nabla_x u = 0 \quad (2)$$

with  $u : \mathbb{R}_+ \times \mathbb{R}^2 \rightarrow \mathbb{R}$ ,  $a : \mathbb{R}_+ \times \mathbb{R}^2 \rightarrow \mathbb{R}^2$  the direction.

semi-Lagrangian method

# Semi-Lagrangian method

characteristic curve  $X_{s,y} : \mathbb{R}_+ \rightarrow \mathbb{R}^2$

## Semi-Lagrangian method

characteristic curve  $X_{s,y} : \mathbb{R}_+ \rightarrow \mathbb{R}^2$

$$\begin{cases} X'(t) &= a(t, X(t)), \\ X(s) &= y. \end{cases}$$

## Semi-Lagrangian method

characteristic curve  $X_{s,y} : \mathbb{R}_+ \rightarrow \mathbb{R}^2$

$$\begin{cases} X'(t) &= a(t, X(t)), \\ X(s) &= y. \end{cases}$$

the solution  $u$  can be computed as

$$u_j^{n+1} = u(t_{n+1}, x_j) = u(t_n, X_{t_{n+1}, x_j}(t_n)).$$

## Semi-Lagrangian method

characteristic curve  $X_{s,y} : \mathbb{R}_+ \rightarrow \mathbb{R}^2$

$$\begin{cases} X'(t) &= a(t, X(t)), \\ X(s) &= y. \end{cases}$$

the solution  $u$  can be computed as

$$u_j^{n+1} = u(t_{n+1}, x_j) = u(t_n, X_{t_{n+1}, x_j}(t_n)).$$

$X_{t_{n+1}, x_j}(t_n) \in \mathbb{R}^2$  is not necessarily a node of the mesh

## Semi-Lagrangian method

characteristic curve  $X_{s,y} : \mathbb{R}_+ \rightarrow \mathbb{R}^2$

$$\begin{cases} X'(t) &= a(t, X(t)), \\ X(s) &= y. \end{cases}$$

the solution  $u$  can be computed as

$$u_j^{n+1} = u(t_{n+1}, x_j) = u(t_n, X_{t_{n+1}, x_j}(t_n)).$$

$X_{t_{n+1}, x_j}(t_n) \in \mathbb{R}^2$  is not necessarily a node of the mesh

$$u(t^n, X_{t_{n+1}, x_j}(t_n)) \simeq (\Pi u^n)(X_{t_{n+1}, x_j}(t_n)),$$

$\Pi$  an interpolation operator

## Semi-Lagrangian method

characteristic curve  $X_{s,y} : \mathbb{R}_+ \rightarrow \mathbb{R}^2$

$$\begin{cases} X'(t) &= a(t, X(t)), \\ X(s) &= y. \end{cases}$$

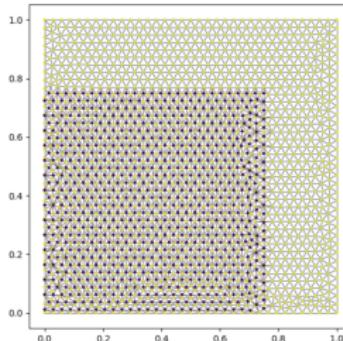
the solution  $u$  can be computed as

$$u_j^{n+1} = u(t_{n+1}, x_j) = u(t_n, X_{t_{n+1}, x_j}(t_n)).$$

$X_{t_{n+1}, x_j}(t_n) \in \mathbb{R}^2$  is not necessarily a node of the mesh

$$u(t^n, X_{t_{n+1}, x_j}(t_n)) \simeq (\Pi u^n)(X_{t_{n+1}, x_j}(t_n)),$$

$\Pi$  an interpolation operator



## Interpolation problem

constant direction  $a \Rightarrow X_{s,y}(t) = y + (t - s)a$ , and:

$$u_j^{n+1} = (\Pi u^n)(x_j - a\Delta t).$$

## Interpolation problem

constant direction  $a \Rightarrow X_{s,y}(t) = y + (t - s)a$ , and:

$$u_j^{n+1} = (\Pi u^n)(x_j - a\Delta t).$$

operator  $\Pi$ : same model than for border detection

# Interpolation problem

constant direction  $a \Rightarrow X_{s,y}(t) = y + (t - s)a$ , and:

$$u_j^{n+1} = (\Pi u^n)(x_j - a\Delta t).$$

operator  $\Pi$ : same model than for border detection

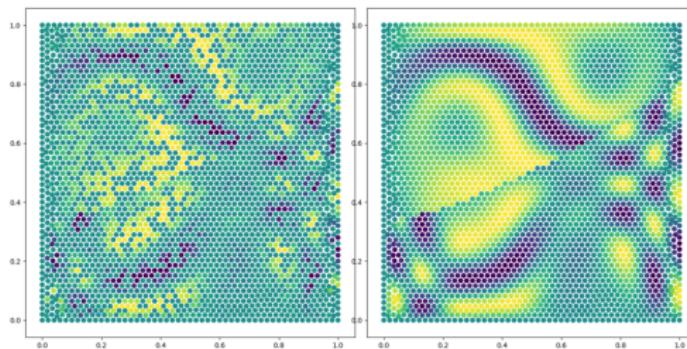


Figure: Input (left) and expected output (right).

# Results

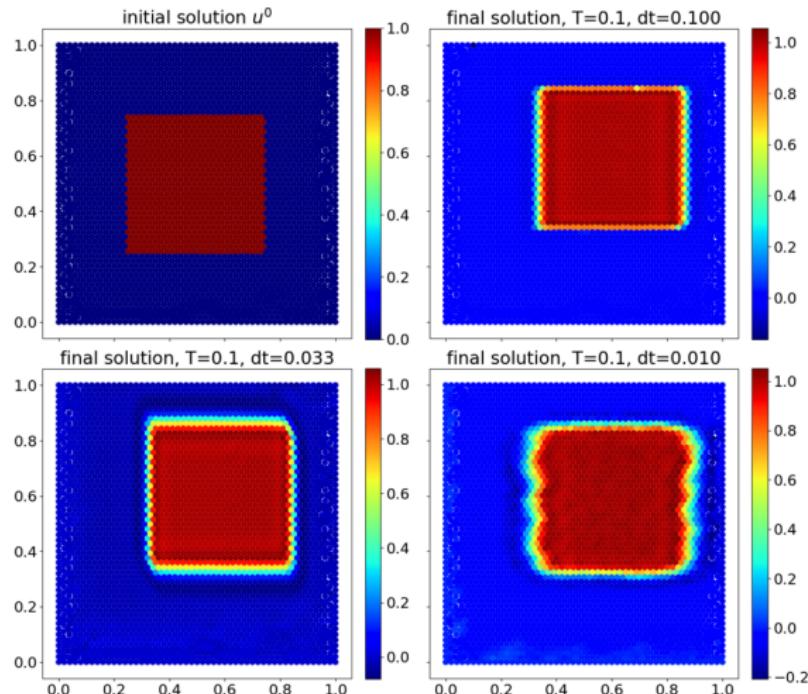


Figure: Solutions computed using the U-Net interpolation model.

# Results

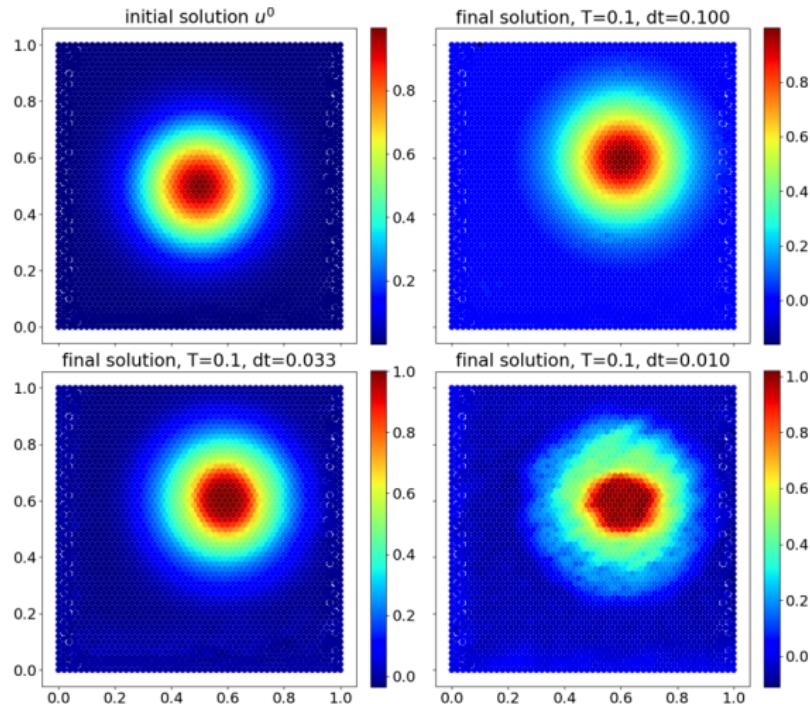


Figure: Solutions computed using the U-Net interpolation model.

# Conclusion

U-Net architecture is efficient

# Conclusion

U-Net architecture is efficient  
⇒ allowed us to solve the frontier problem

# Conclusion

U-Net architecture is efficient  
⇒ allowed us to solve the frontier problem

good results on Burgers' equation but:

# Conclusion

U-Net architecture is efficient  
⇒ allowed us to solve the frontier problem

good results on Burgers' equation but:

- ▶ limitation on number of refinements

# Conclusion

U-Net architecture is efficient  
⇒ allowed us to solve the frontier problem

good results on Burgers' equation but:

- ▶ limitation on number of refinements
- ▶ use a solving method without time constraints

# Conclusion

U-Net architecture is efficient  
⇒ allowed us to solve the frontier problem

good results on Burgers' equation but:

- ▶ limitation on number of refinements
- ▶ use a solving method without time constraints

we made an interpolation operator, but instable

# Conclusion

U-Net architecture is efficient  
⇒ allowed us to solve the frontier problem

good results on Burgers' equation but:

- ▶ limitation on number of refinements
- ▶ use a solving method without time constraints

we made an interpolation operator, but instable

possible corrections:

# Conclusion

U-Net architecture is efficient  
⇒ allowed us to solve the frontier problem

good results on Burgers' equation but:

- ▶ limitation on number of refinements
- ▶ use a solving method without time constraints

we made an interpolation operator, but instable

possible corrections:

- ▶ modify the training dataset

# Conclusion

U-Net architecture is efficient  
⇒ allowed us to solve the frontier problem

good results on Burgers' equation but:

- ▶ limitation on number of refinements
- ▶ use a solving method without time constraints

we made an interpolation operator, but instable

possible corrections:

- ▶ modify the training dataset
- ▶ modify the training process

## Tools used

totality of this project is coded in Python

# Tools used

totality of this project is coded in Python

- ▶ Tensorflow/Keras (model training)
- ▶ Spektral (convolutional layers)
- ▶ Github
- ▶ PyGMSH (generate meshes)

## Tools used

totality of this project is coded in Python

- ▶ Tensorflow/Keras (model training)
- ▶ Spektral (convolutional layers)
- ▶ Github
- ▶ PyGMSH (generate meshes)

v100 GPU for training sessions