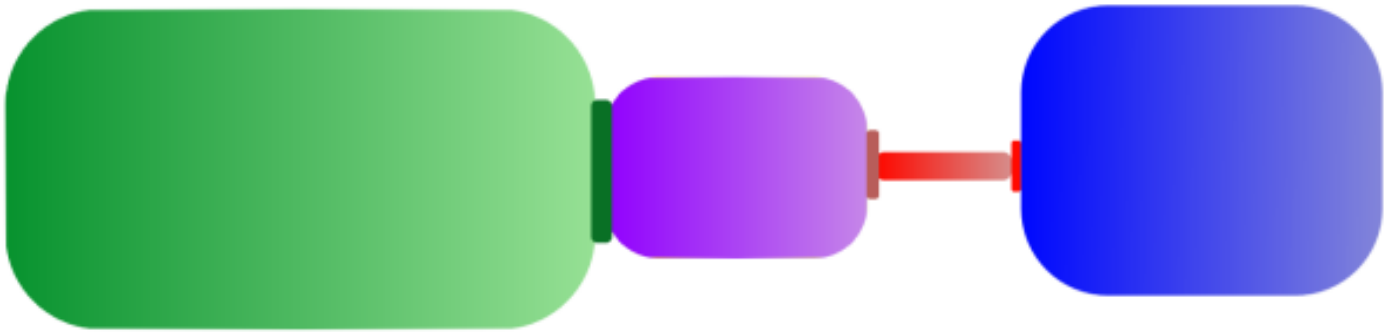
Detecting discontinuities using deep learning

Deep Ray
EPFL, Switzerland
deep.ray@epfl.ch
http://deepray.github.io

12 April, 2019

Motivation

Good numerical methods developed over the past several decades



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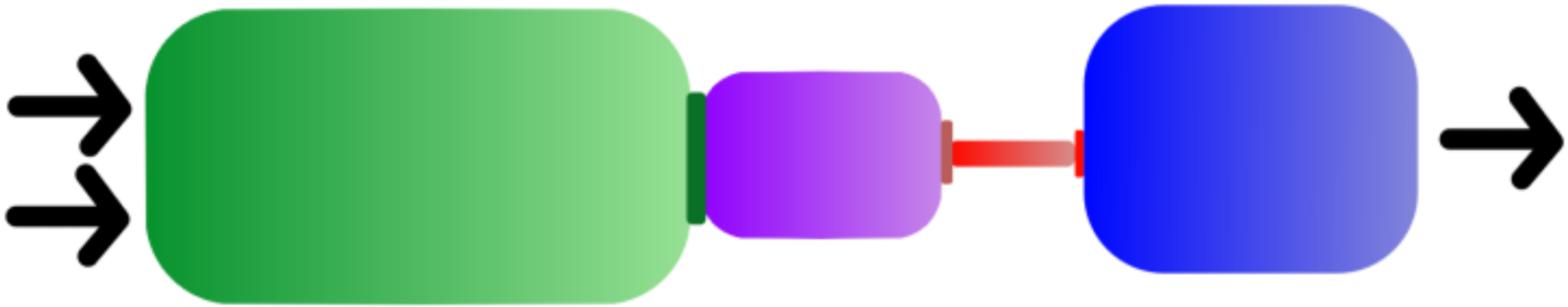

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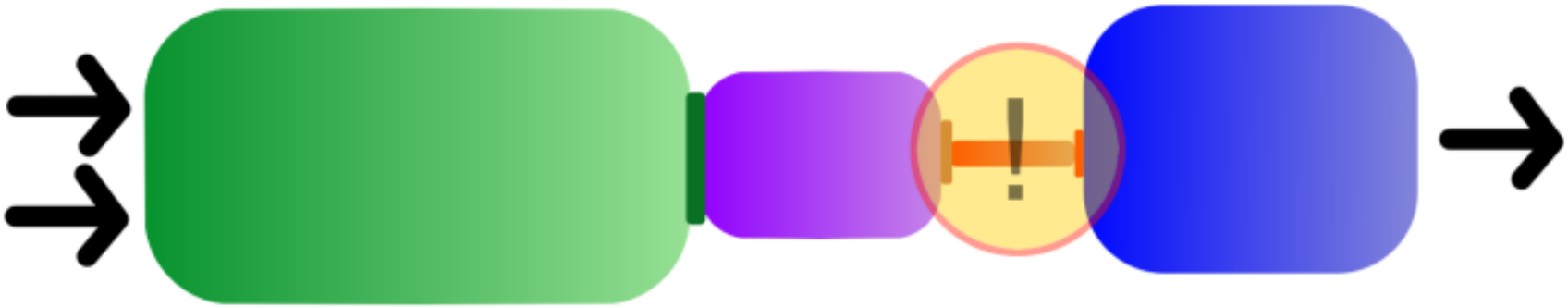

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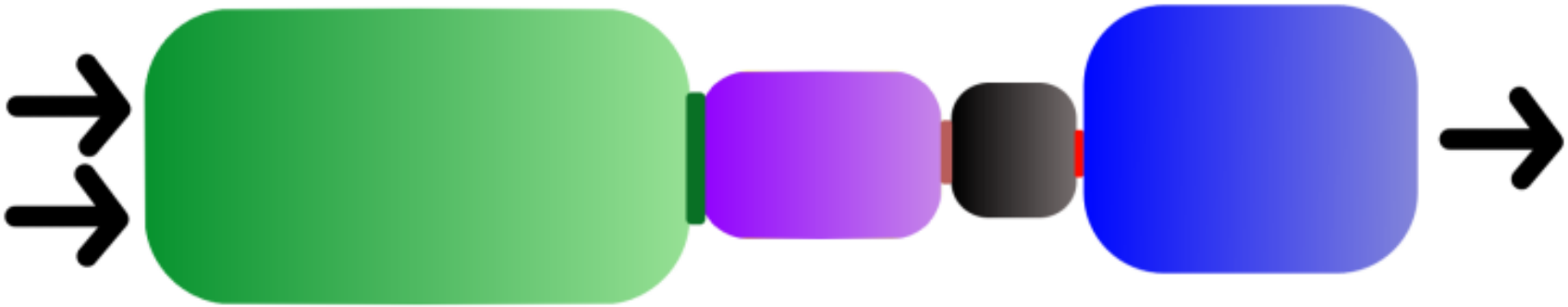
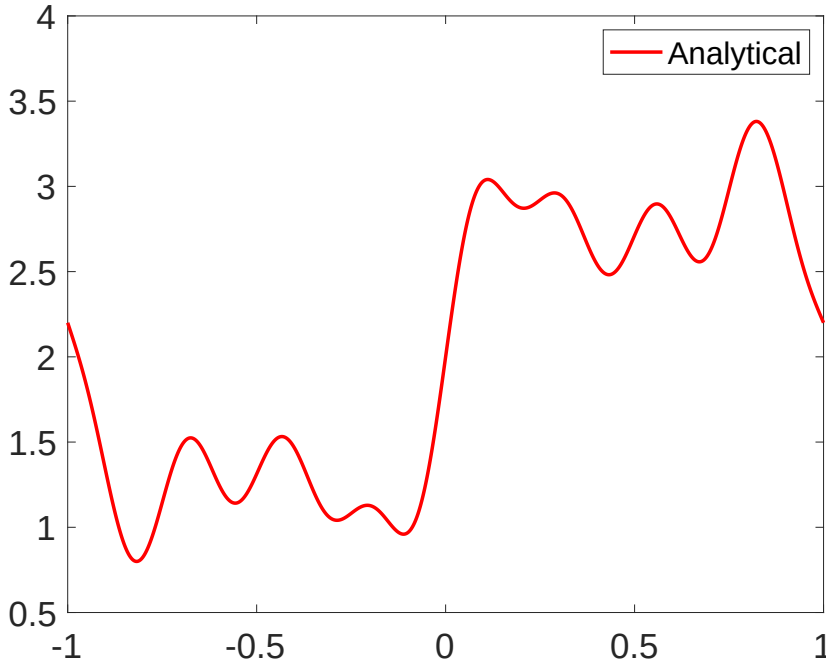
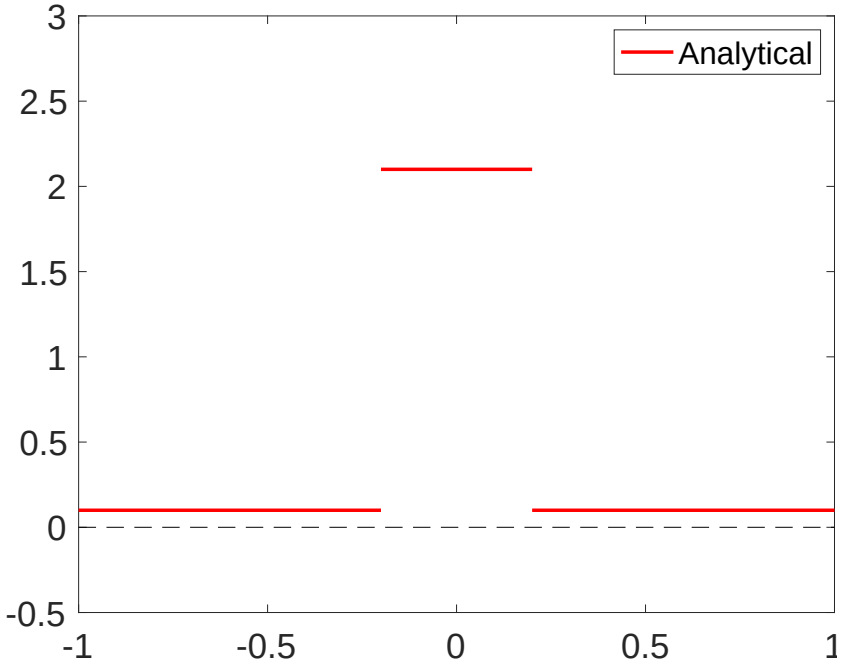


Startegy: Replace (only) the problematic part with deep learning black box

Controlling spurious oscillations

Smooth vs discontinuous





Discontinuities in real life

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(courtesy Nicole Honeywill)

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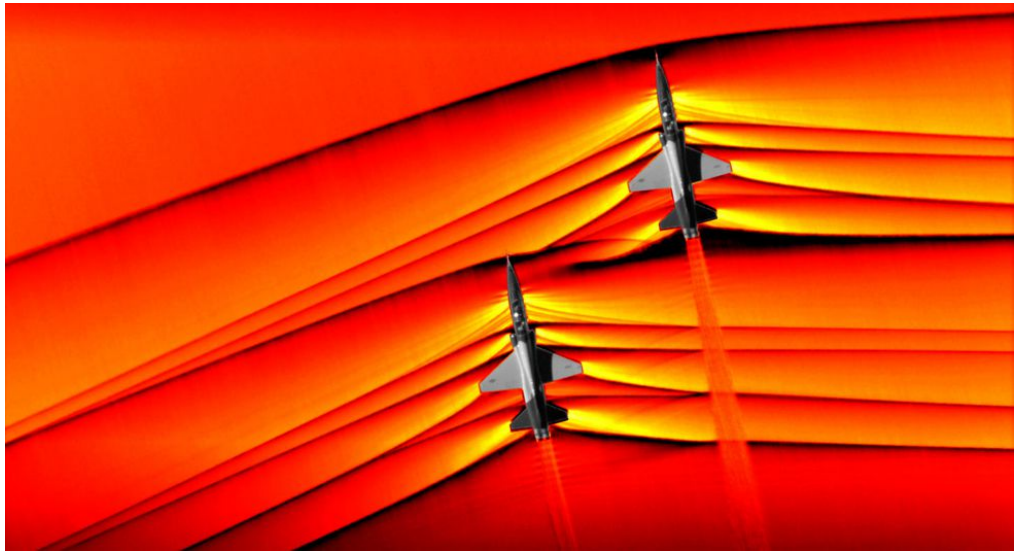

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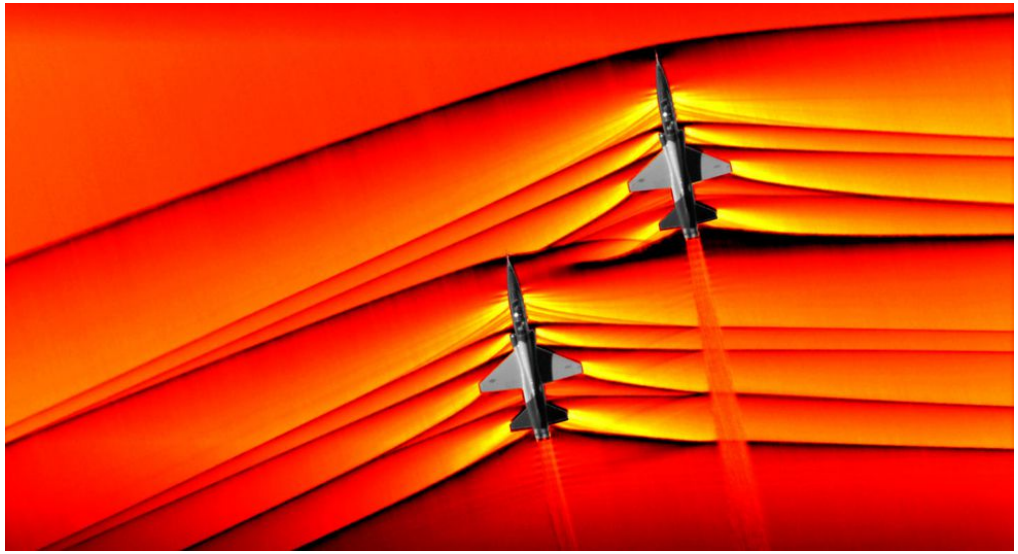

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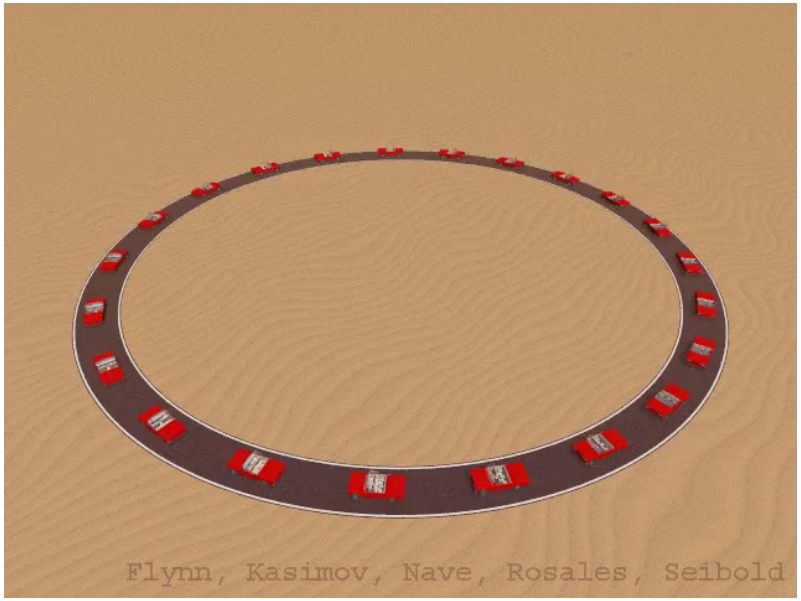
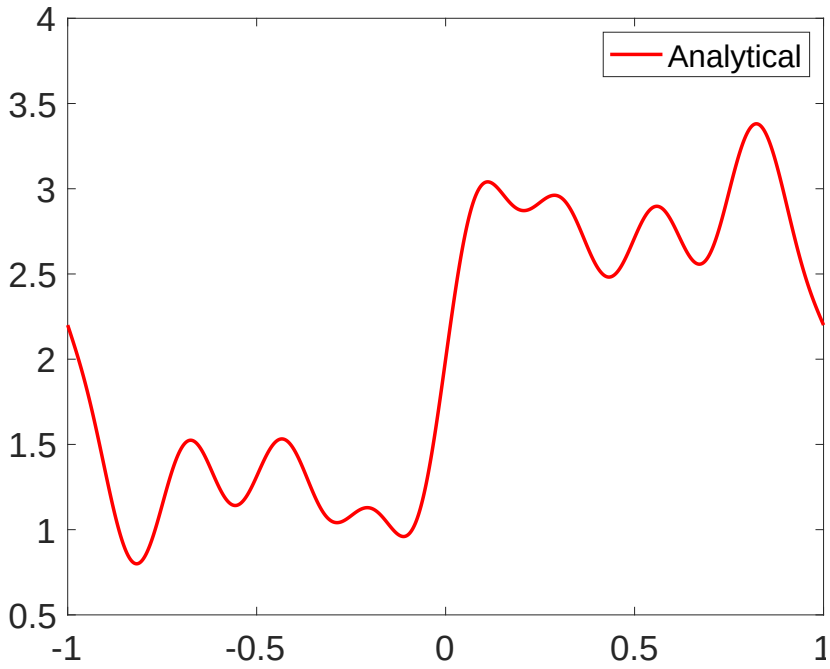
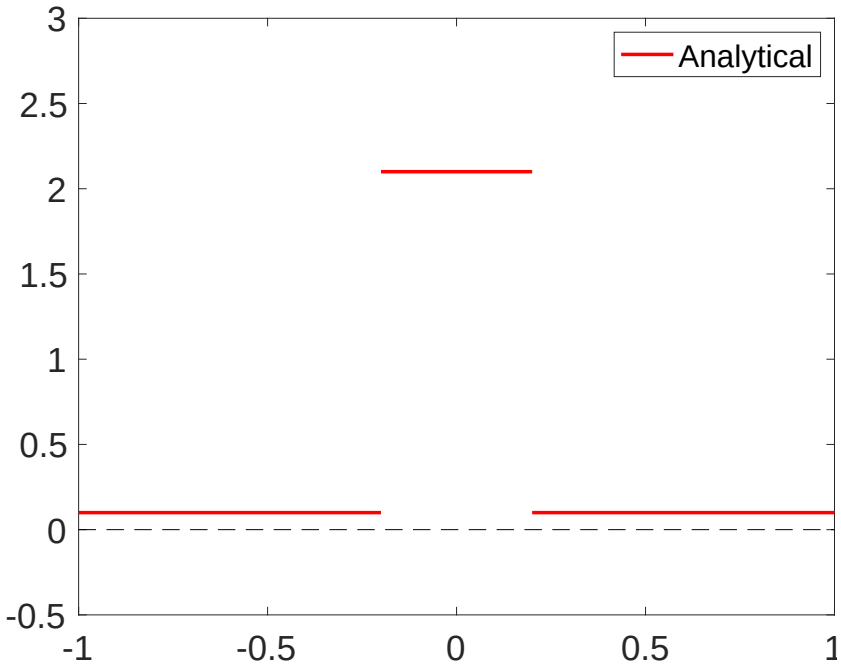


(Flynn et al.)

Approximating functions





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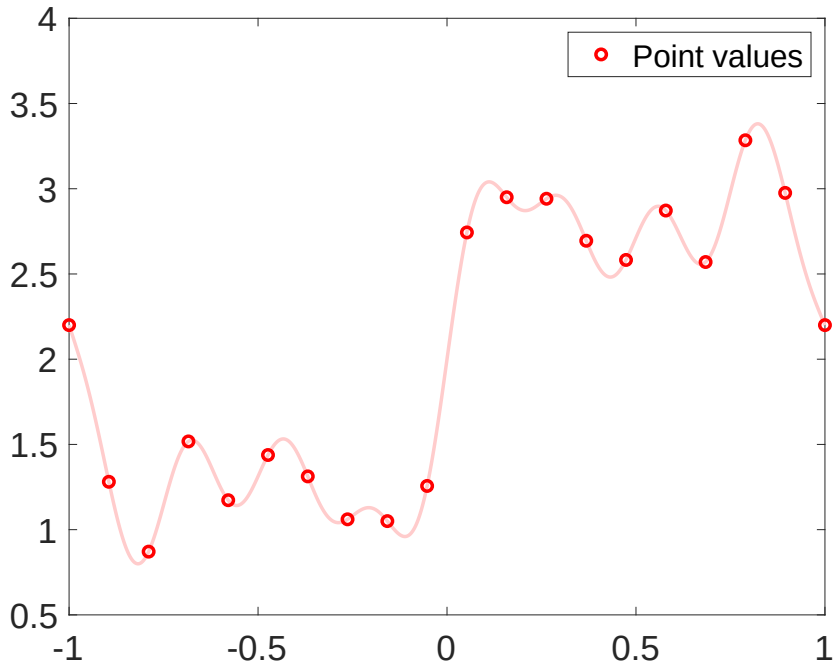

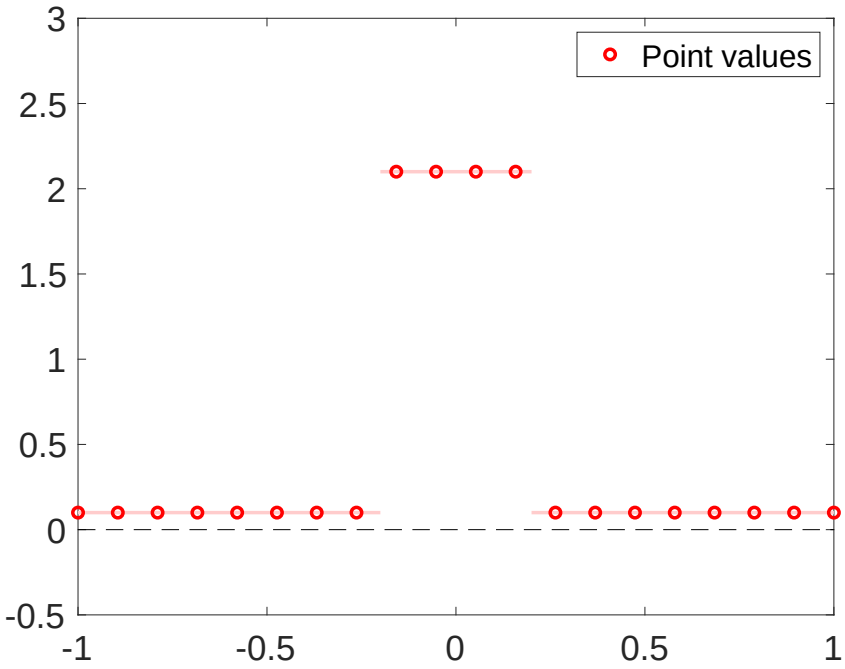

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Approximating the function using a smooth basis

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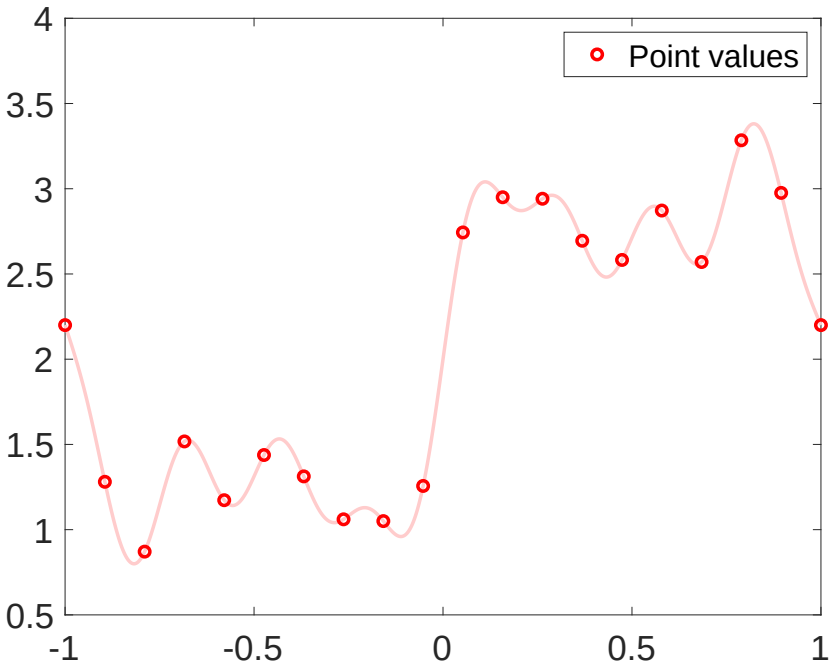

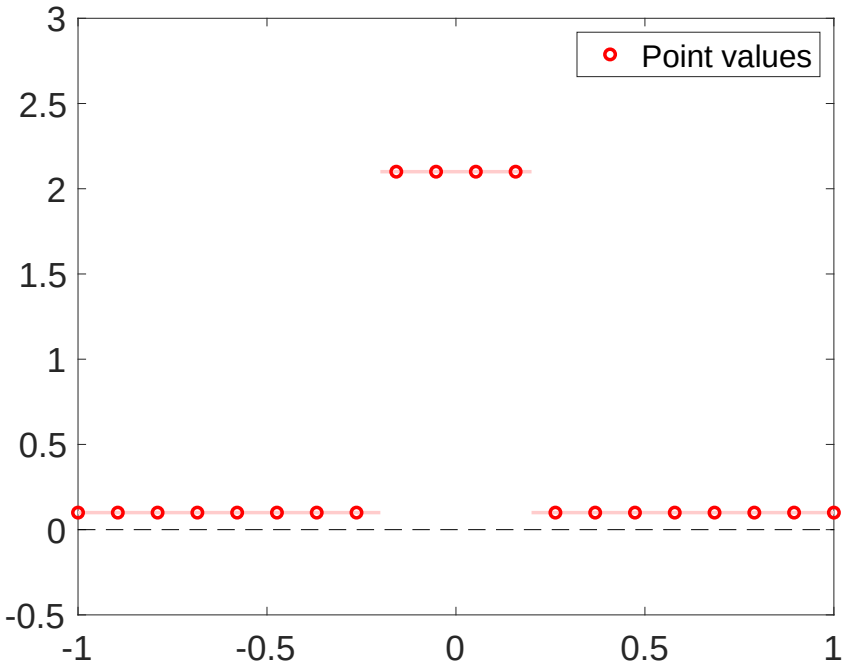

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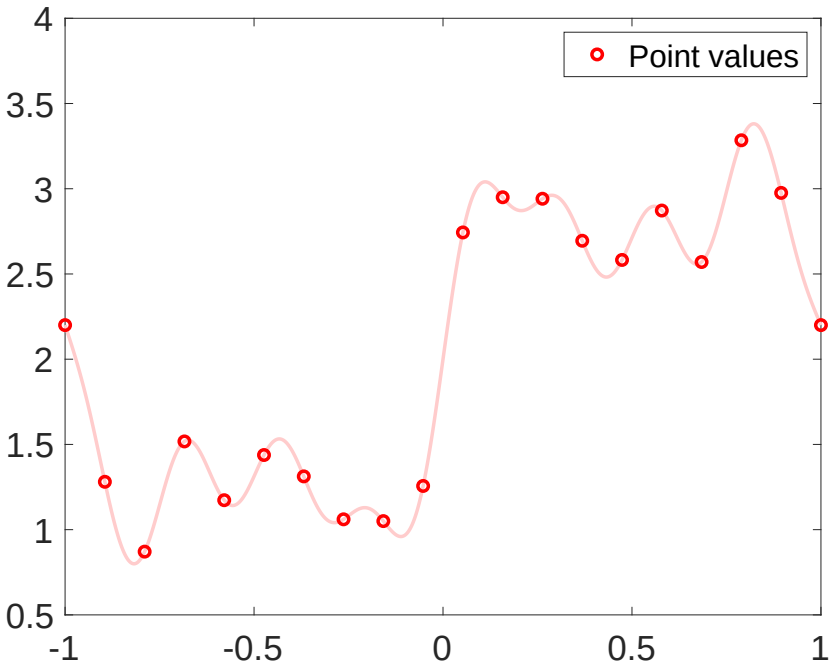

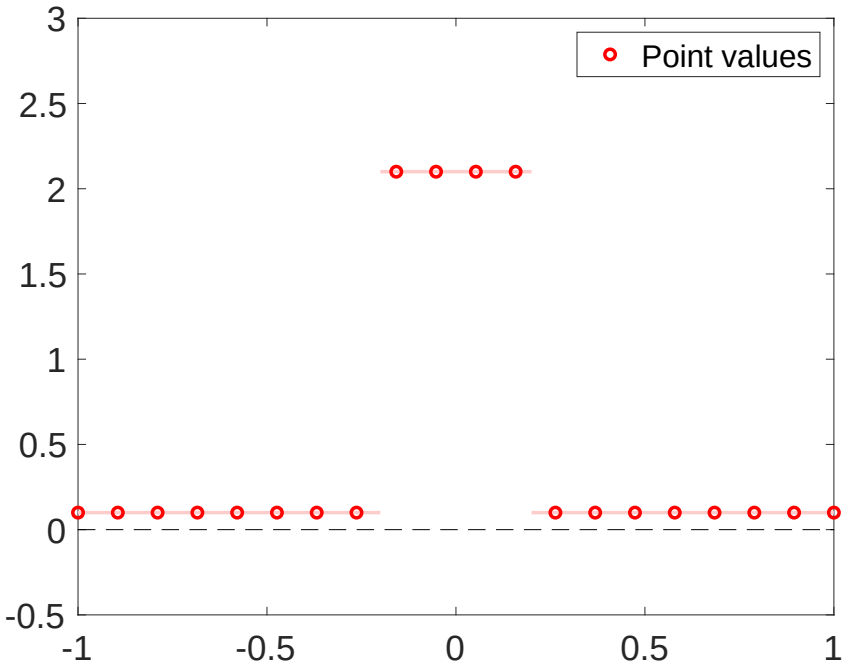

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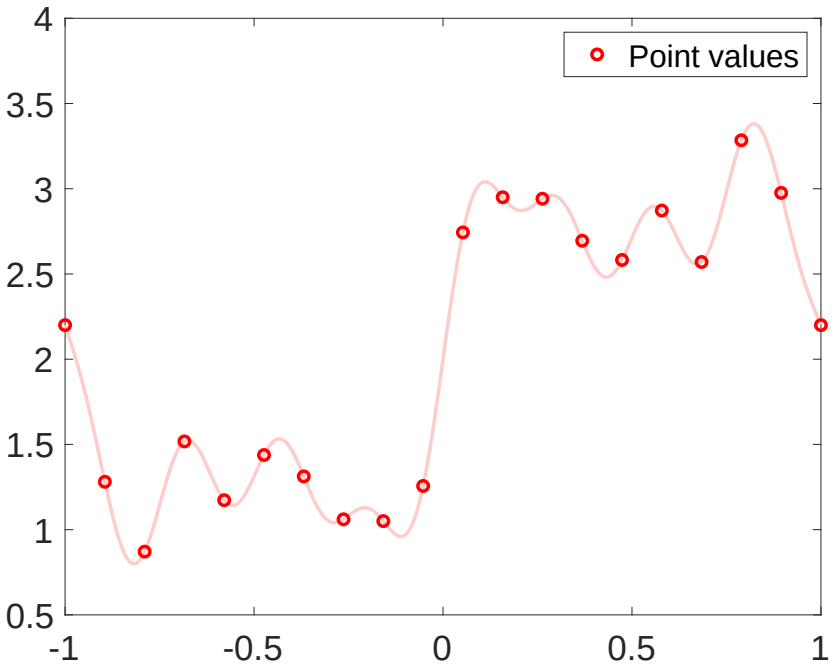

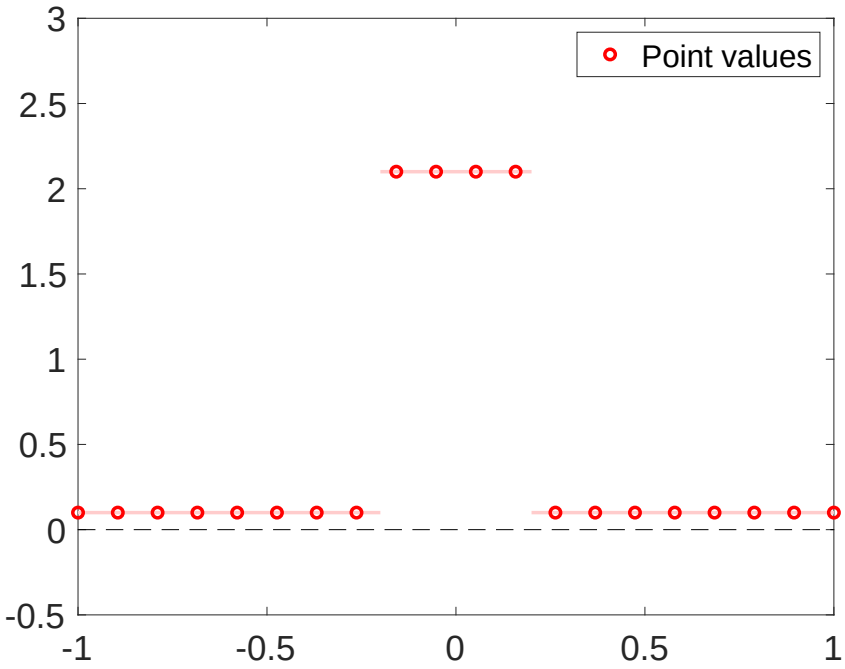

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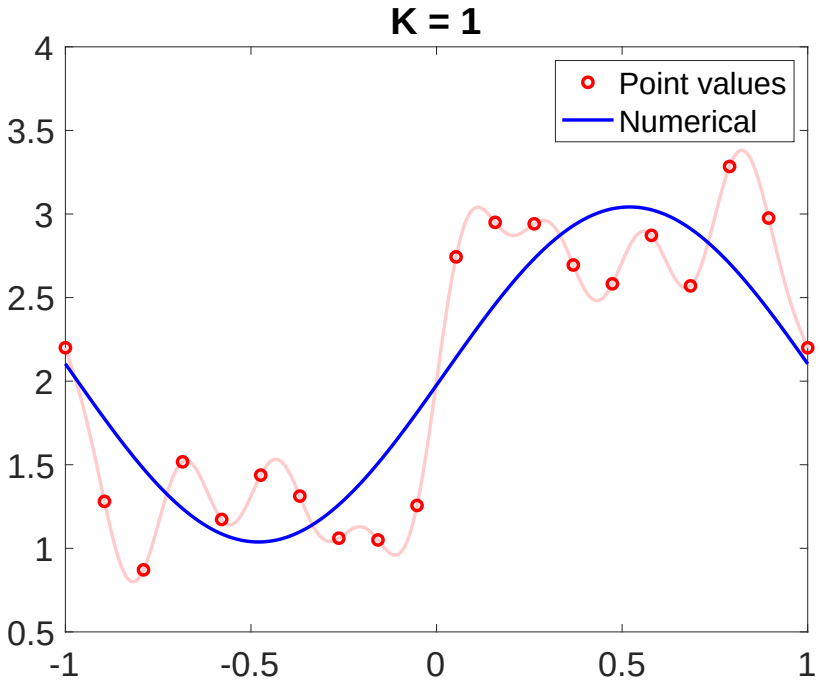

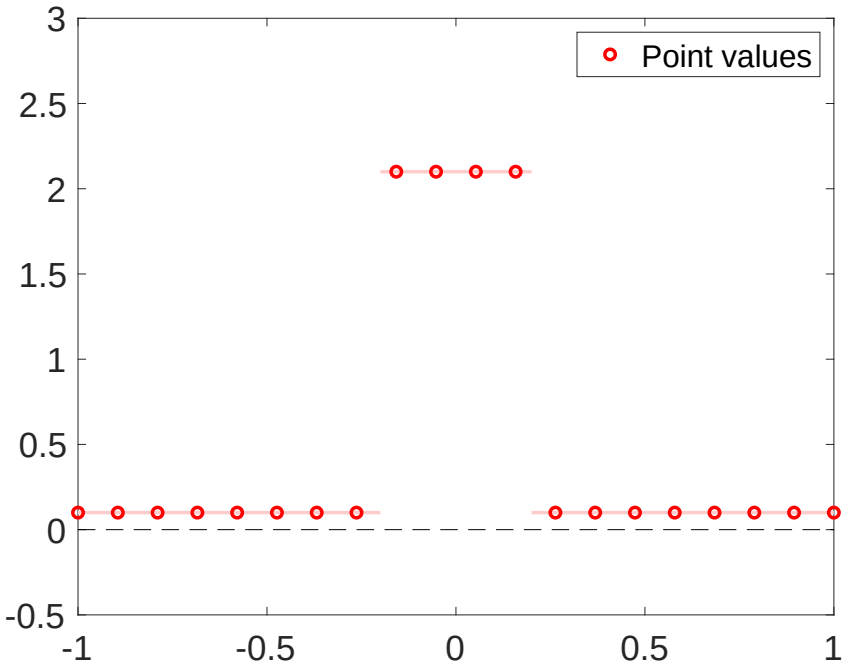

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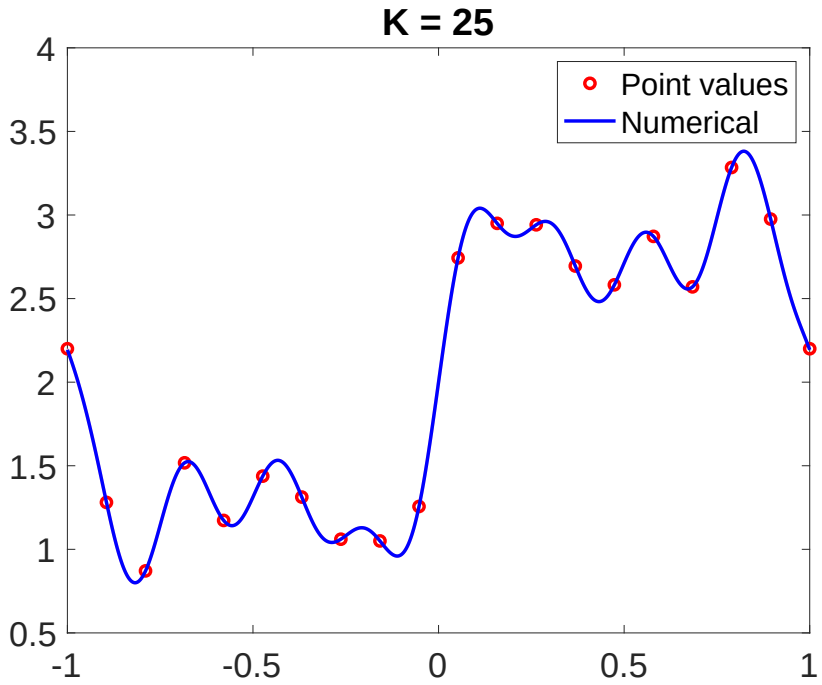

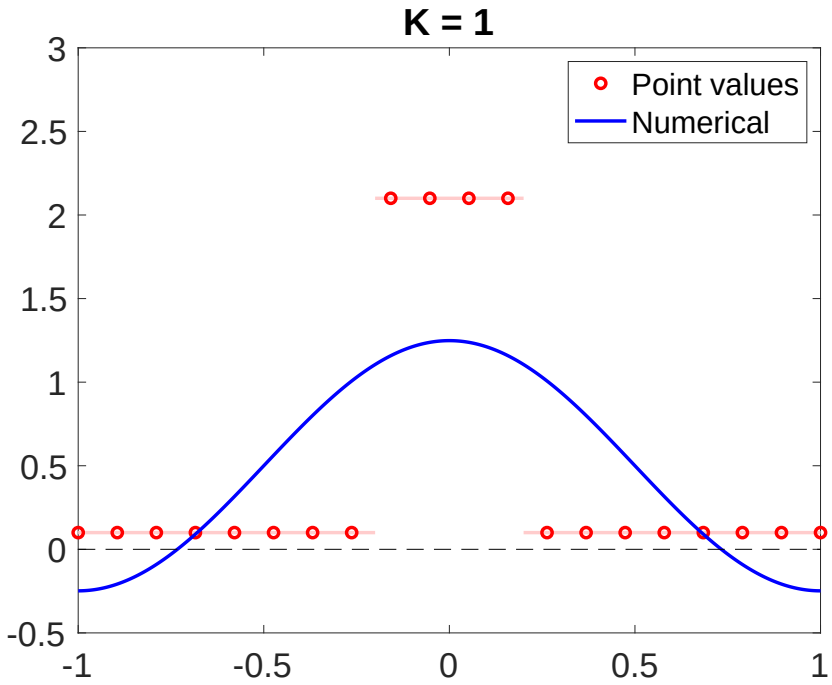

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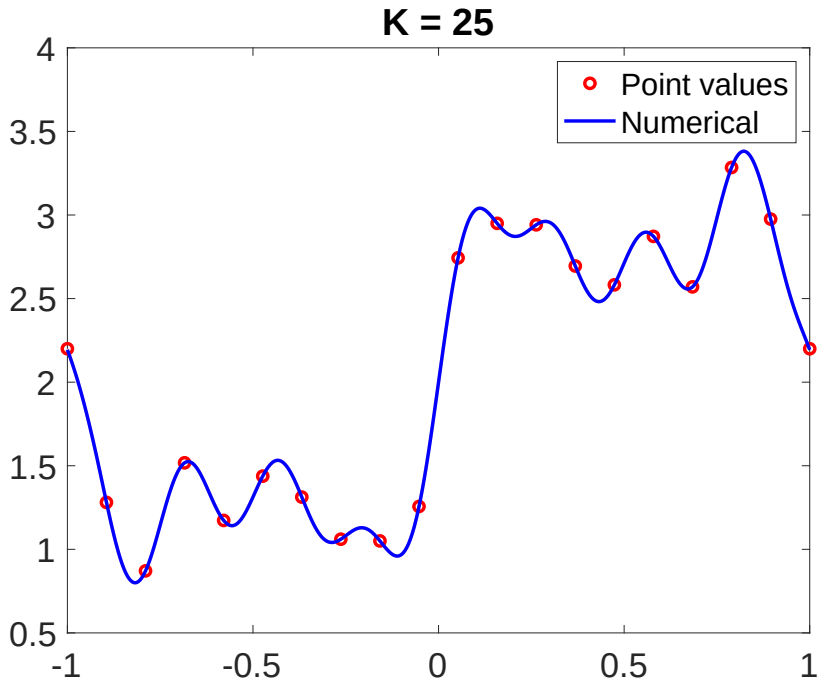
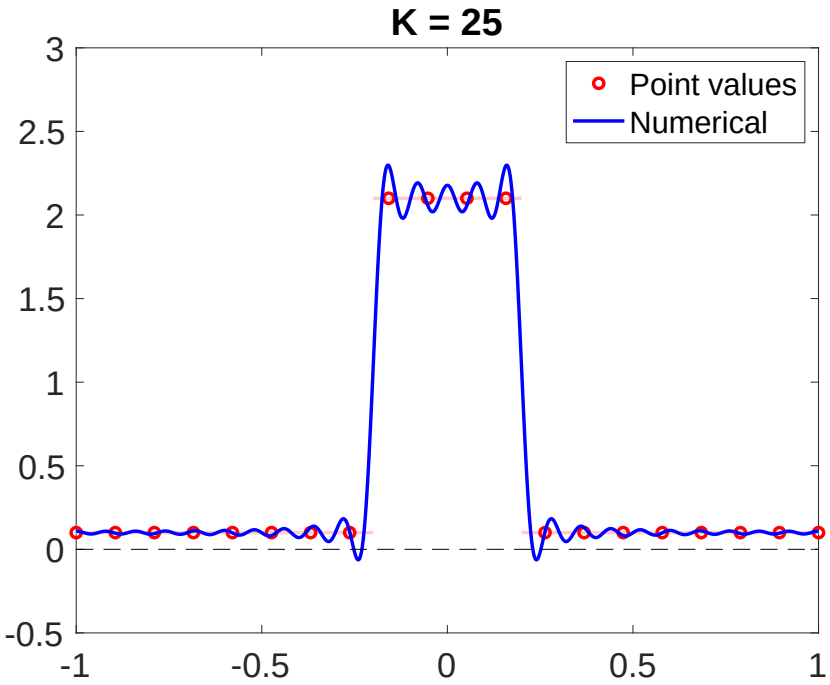
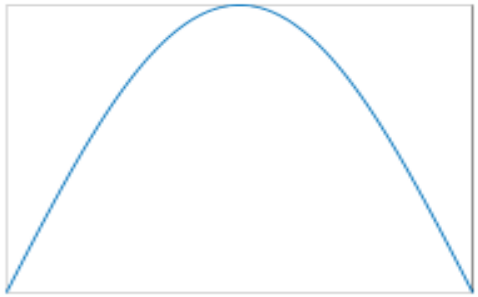
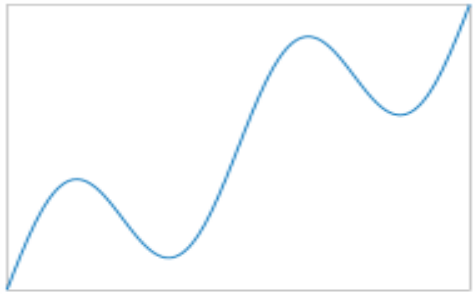


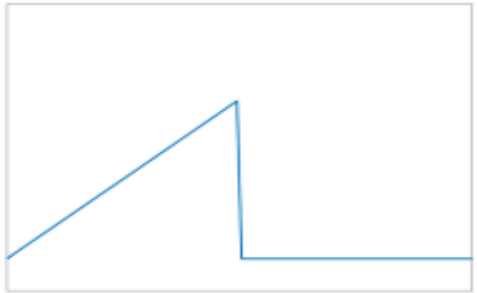


Unphysical/spurious oscillations $\Longrightarrow$ loss of positivity!

Approximating functions







Conservation laws

Consider the partial differential equation

$$\frac{\partial \mathbf{u}}{\partial t} + \frac{\partial \mathbf{f}(\mathbf{u})}{\partial x} = 0$$
$$\mathbf{u}(x, 0) = \mathbf{u}_0(x)$$

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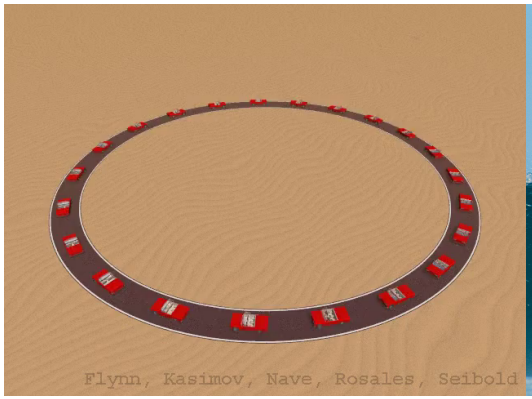


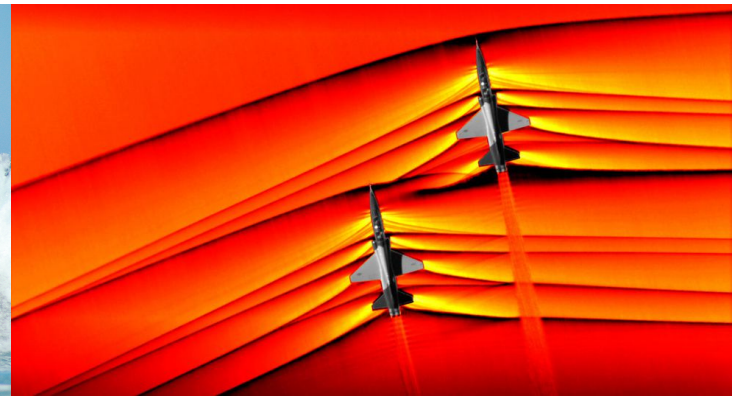

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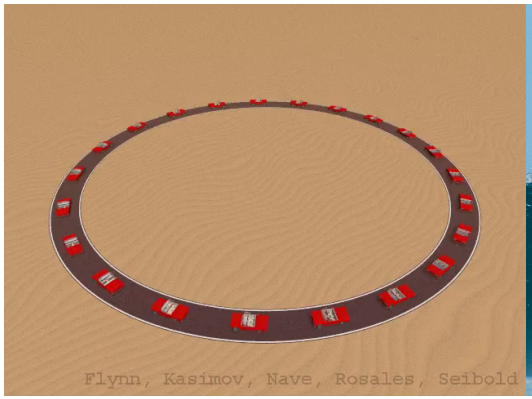

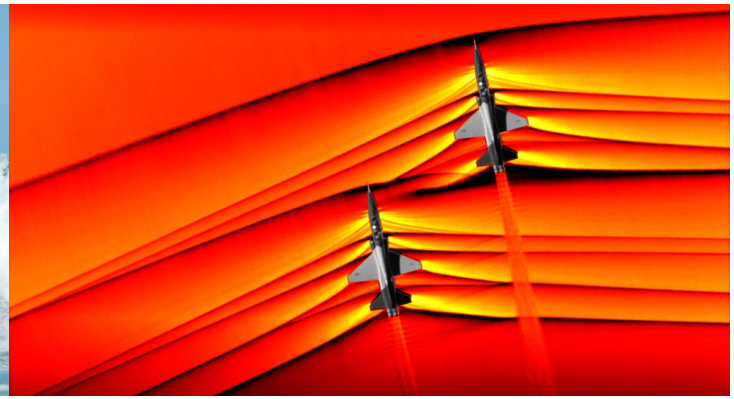

Lighthill-Whitham-Richards model

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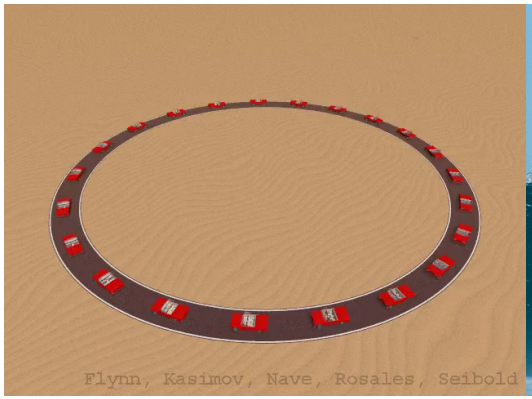
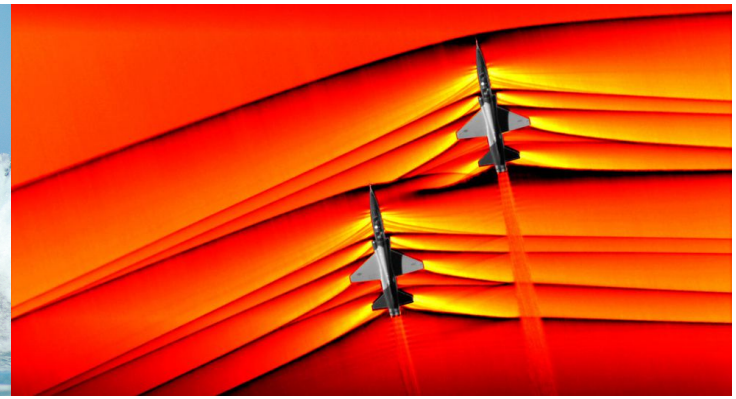


Lighthill-Whitham-Richards model

Shallow water equations



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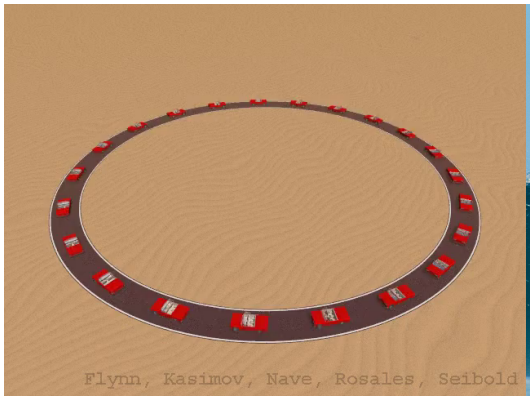

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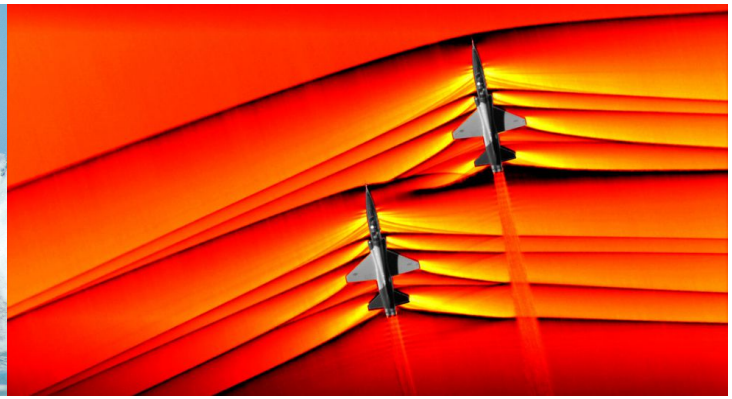

Euler equations

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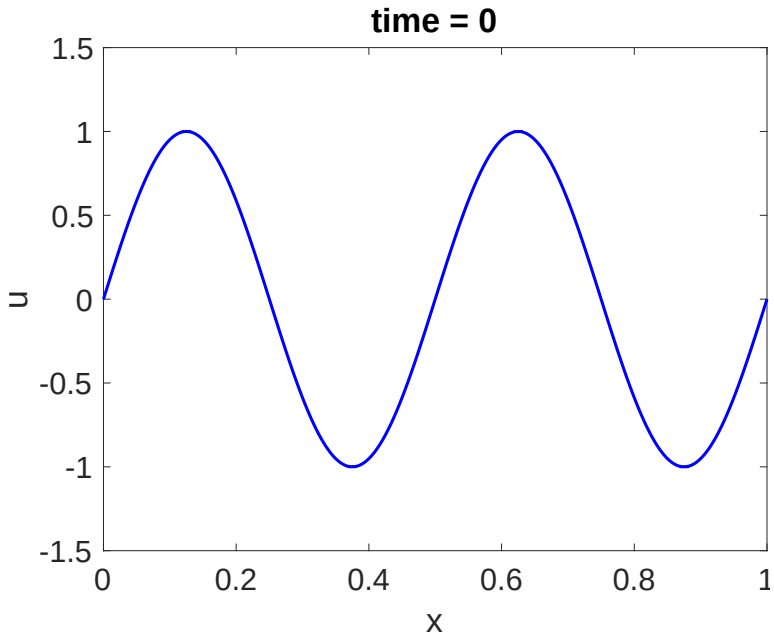
Non-linearity

$\Longrightarrow$

Discontinuities in finite time



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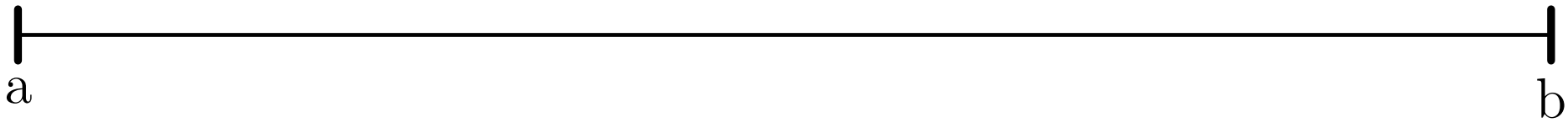
$$0 \leq t \leq T_f \qquad\qquad a \leq x \leq b$$



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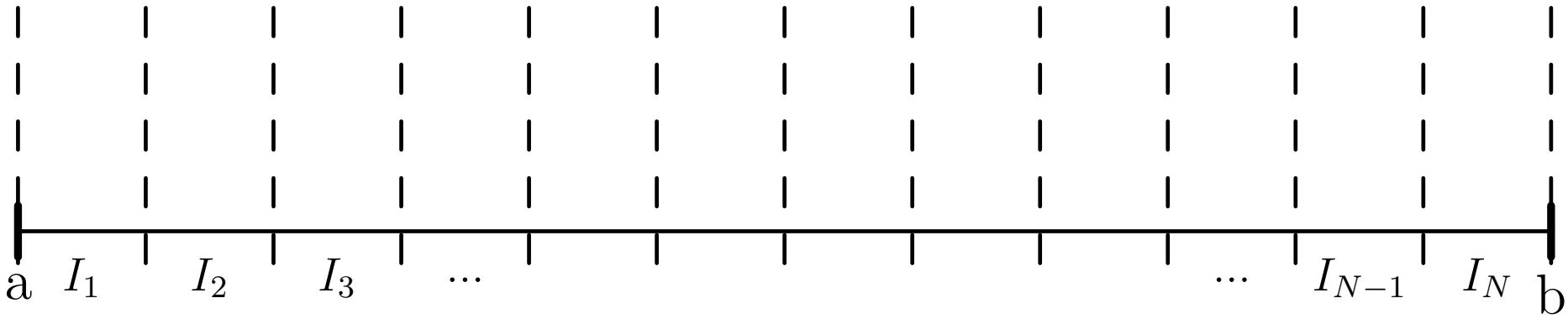

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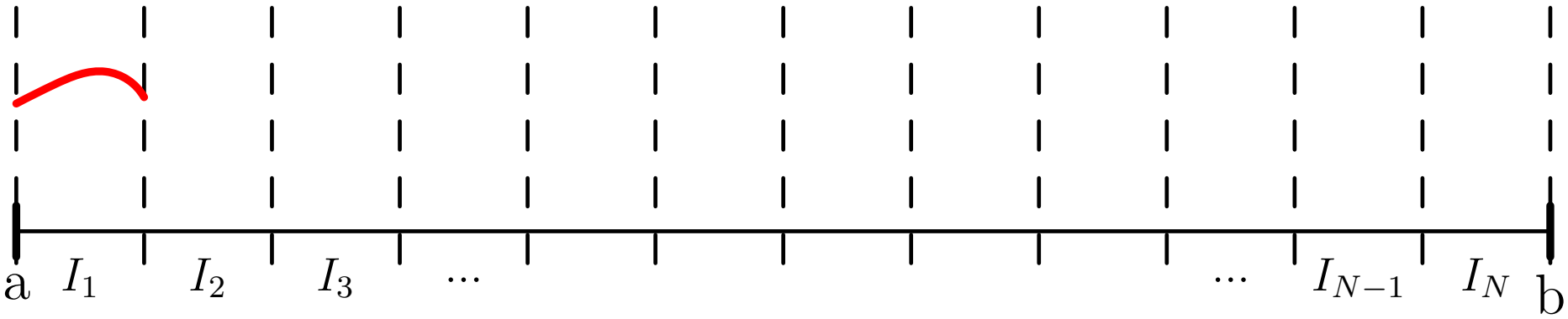

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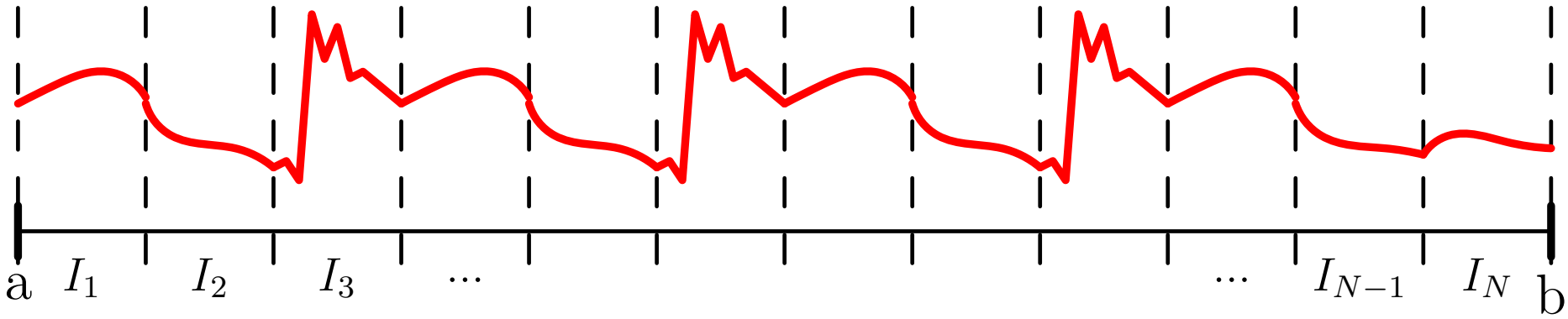

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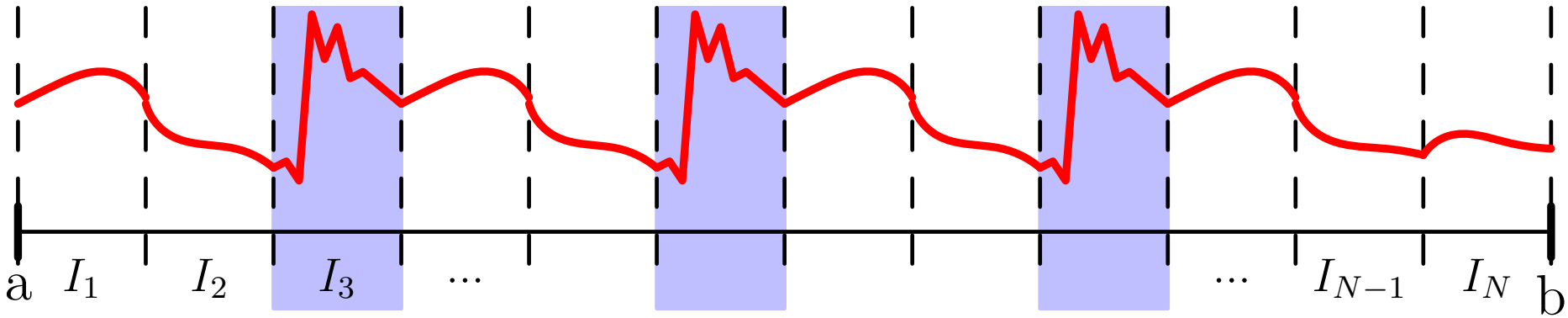
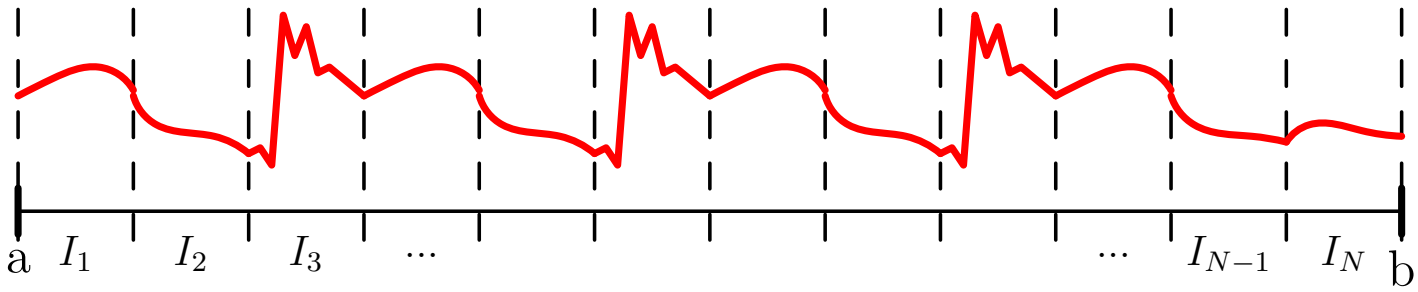


Detecting and limiting

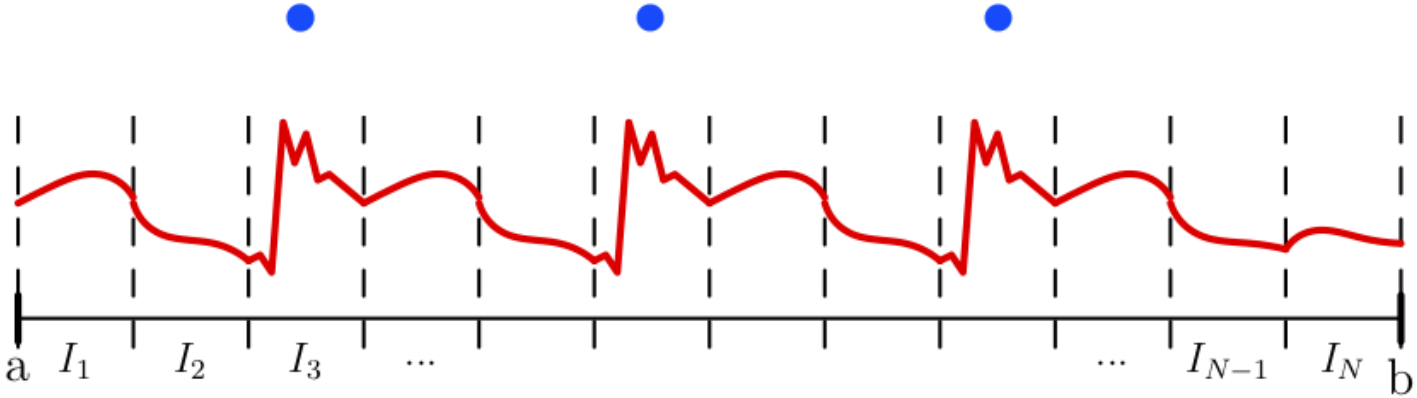
Strategy:



Detecting and limiting

Strategy:

1. Find troubled-cells



Detecting and limiting

Strategy:

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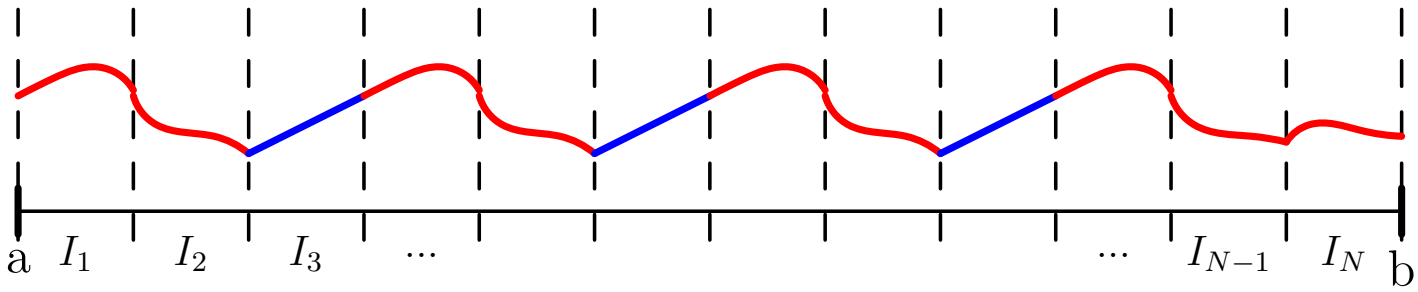
2. Limit solution in flagged cells



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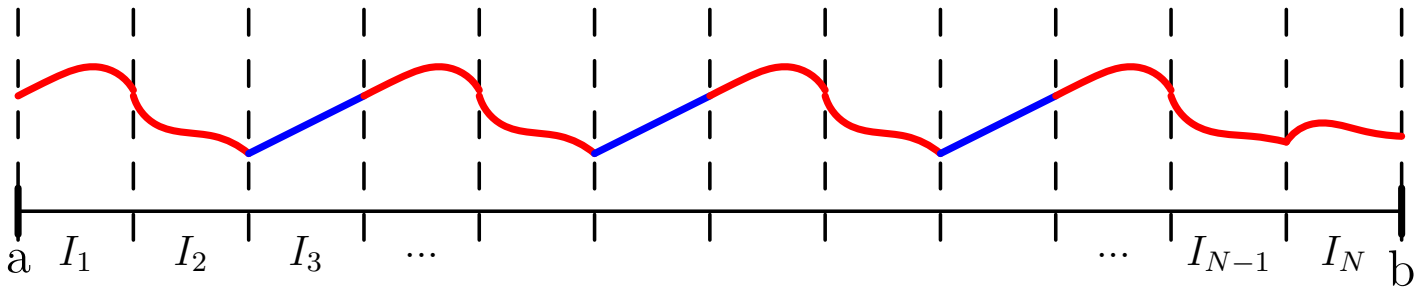


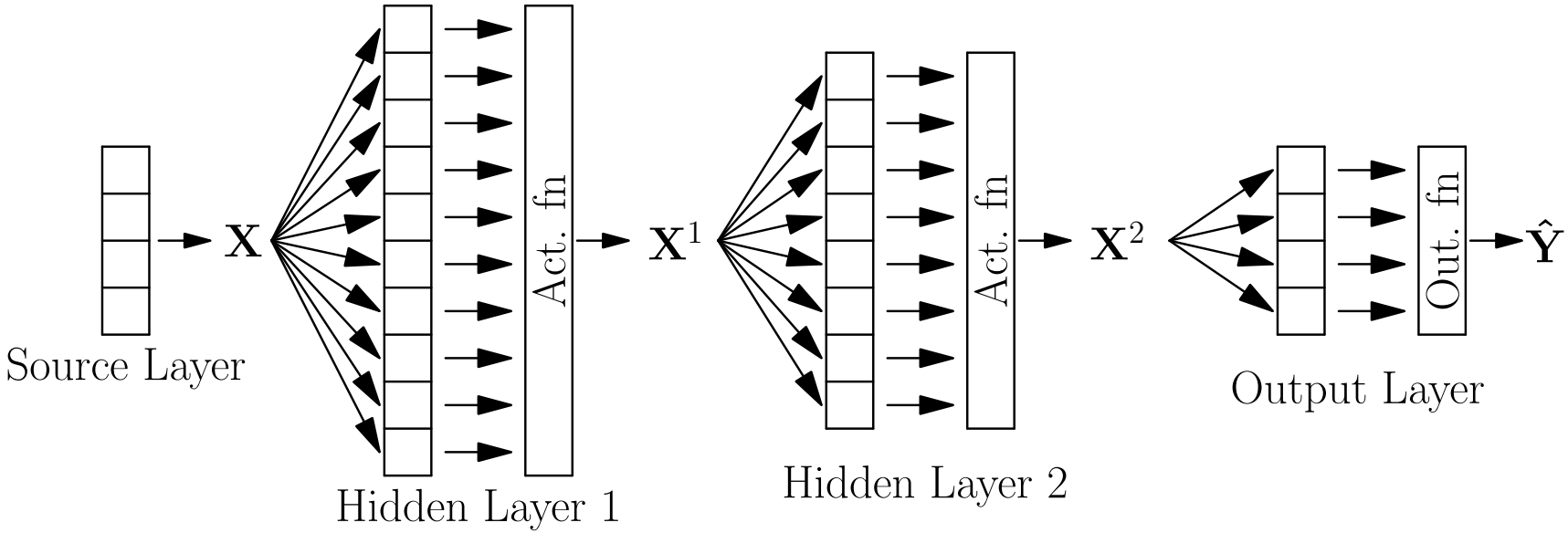
Some issues with existing detectors:

- Problem-dependent parameters
- If insufficient cells marked $\longrightarrow$ re-appearance of oscillations
- If excessive cells marked
  - Unnecessary computational cost
  - Loss of accuracy for strong limiters

AIM: Train a neural network to detect discontinuities

- Free from problem-dependent parameters
- Does not flag smooth regions

An MLP-based detector



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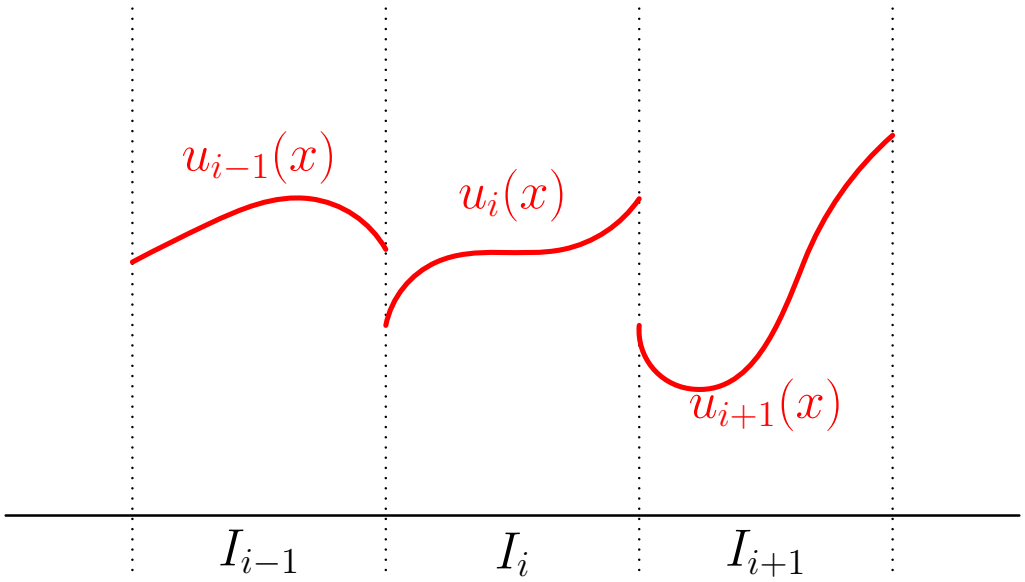
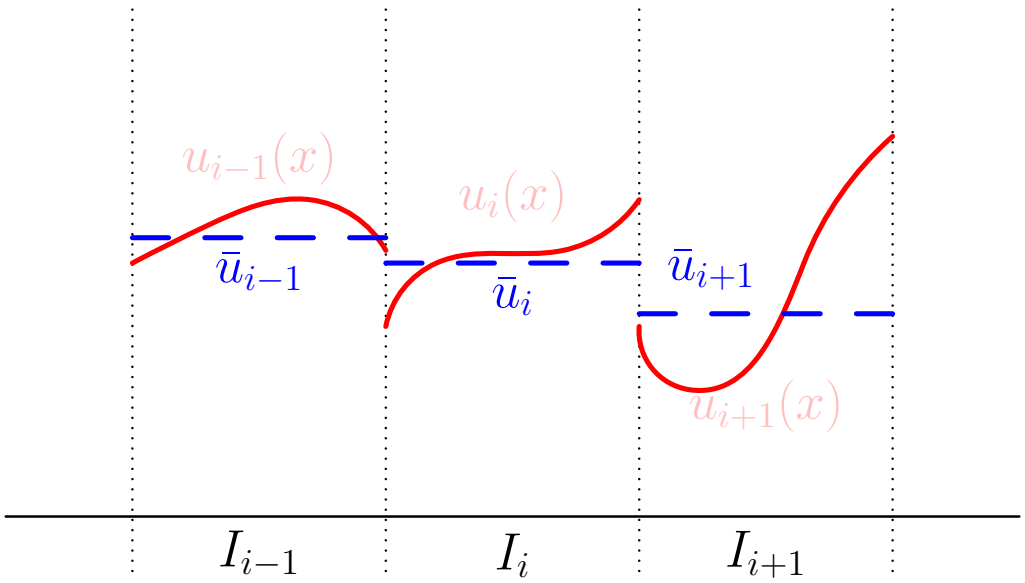


An MLP-based detector

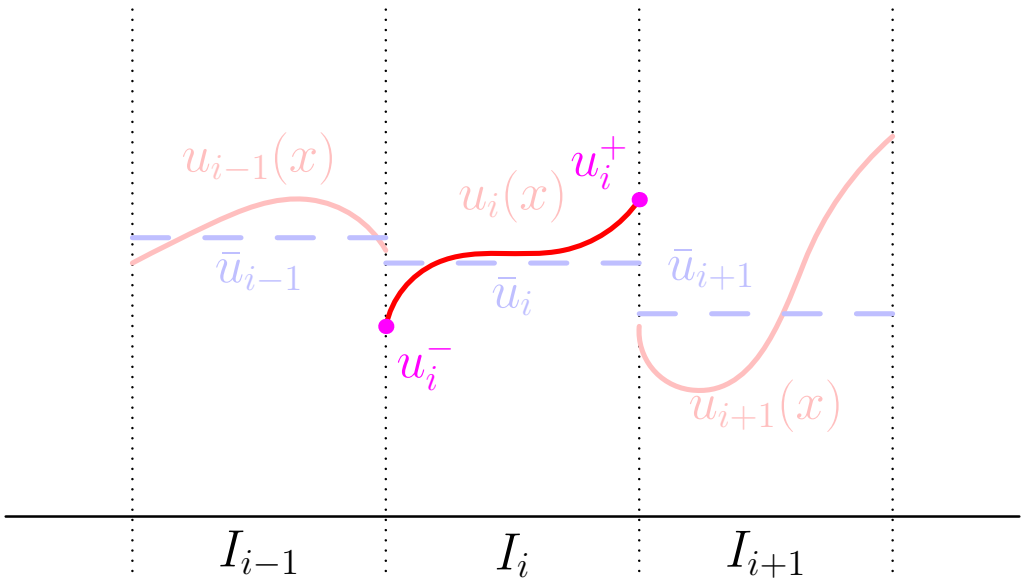
- Input $\mathbf{X} = [\overline{u}_{i-1}, \overline{u}_i, \overline{u}_{i+1} \quad]$



$$\overline{u}_j = \frac{1}{|I_j|} \int_{I_j} u_j(x) \mathrm{d}x$$

An MLP-based detector

- Input $\mathbf{X} = [\overline{u}_{i-1}, \overline{u}_i, \overline{u}_{i+1}, u_i^-, u_i^+] \in \mathbb{R}^5$



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- Input $\mathbf{X} = [\overline{u}_{i-1}, \overline{u}_i, \overline{u}_{i+1}, u_i^-, u_i^+] \in \mathbb{R}^5$
- 5 Hidden Layers with width 256, 128, 64, 32, 16

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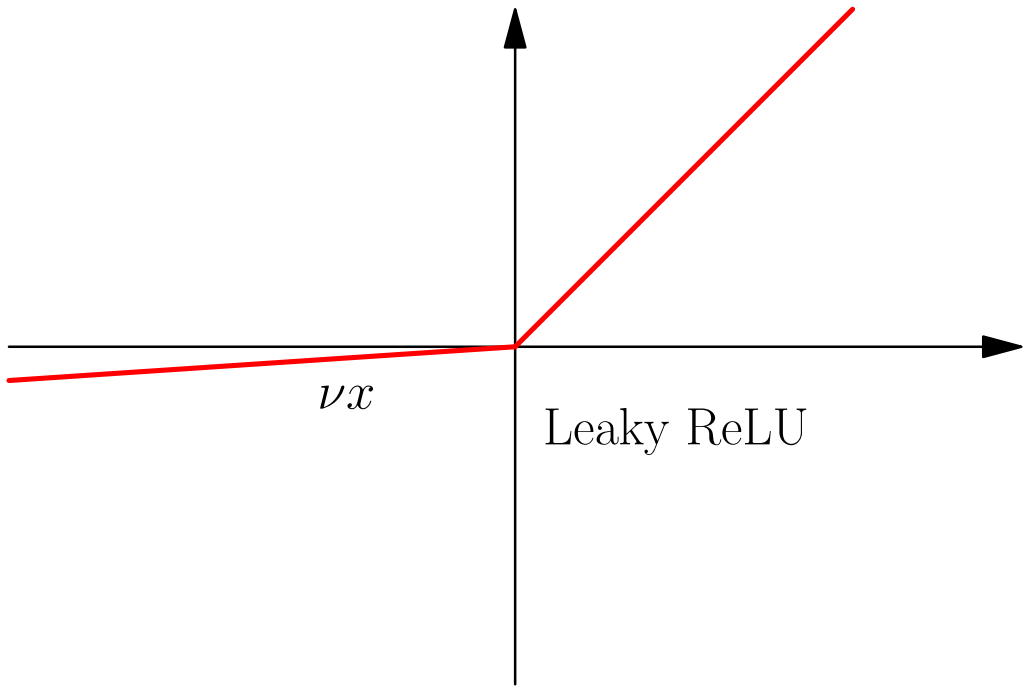

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$$\hat{Y}^{(k)} \leftarrow \frac{e^{\hat{Y}^{(k)}}}{\sum_j e^{\hat{Y}^{(j)}}} \quad \in \quad [0,1] \quad \longrightarrow \quad \text{probabilities/classification}$$

Output $\hat{Y} = [\hat{Y}^{(0)}, \hat{Y}^{(1)}] \in [0,1]^2$

Troubled-cell if $\hat{Y}^{(0)} > 0.5$

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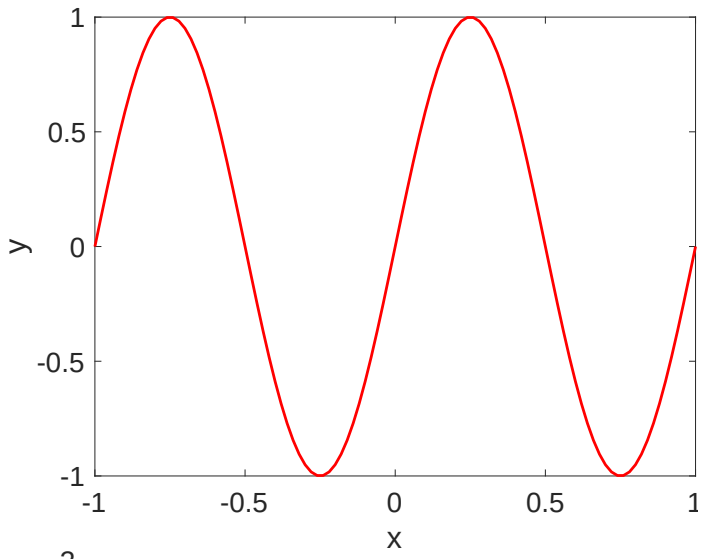
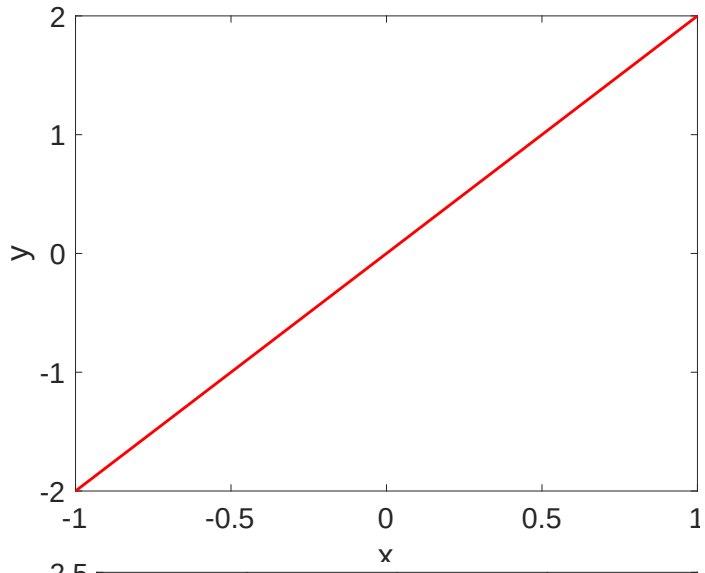
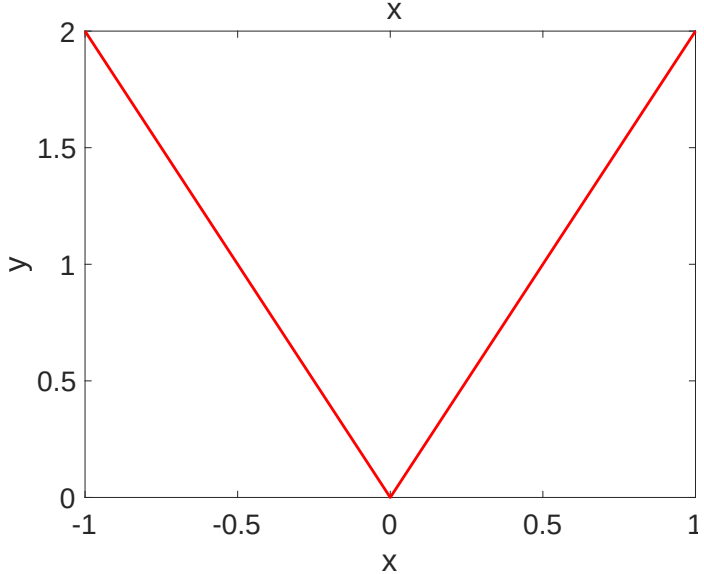
- Cost functional: L2 regularized cross-entropy

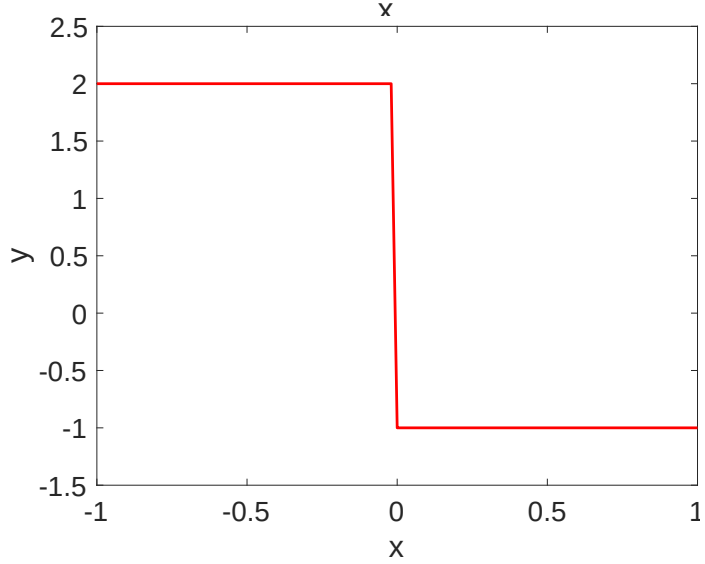
Generating the training data for indicator

Types of functions used:









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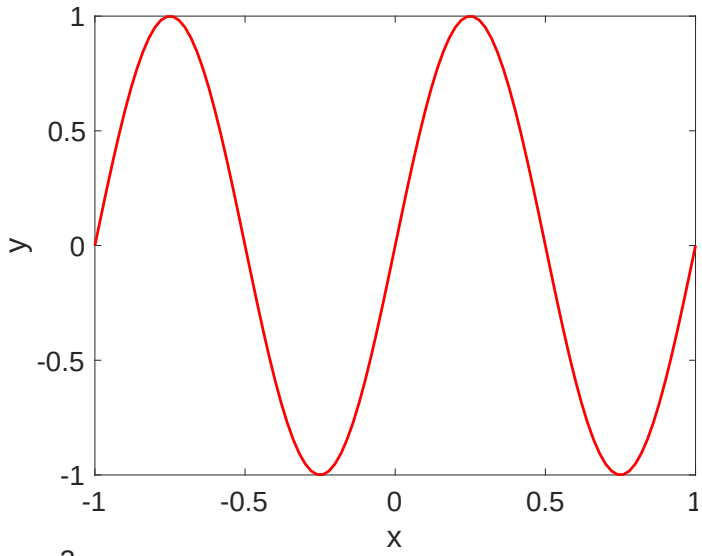
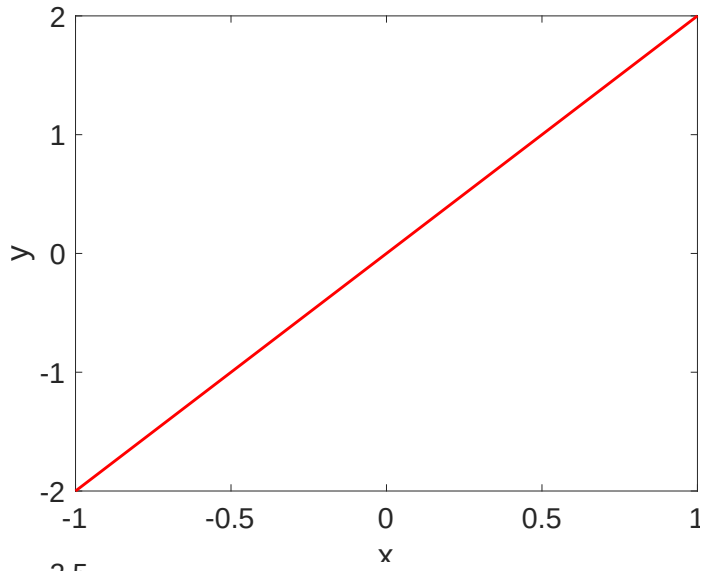
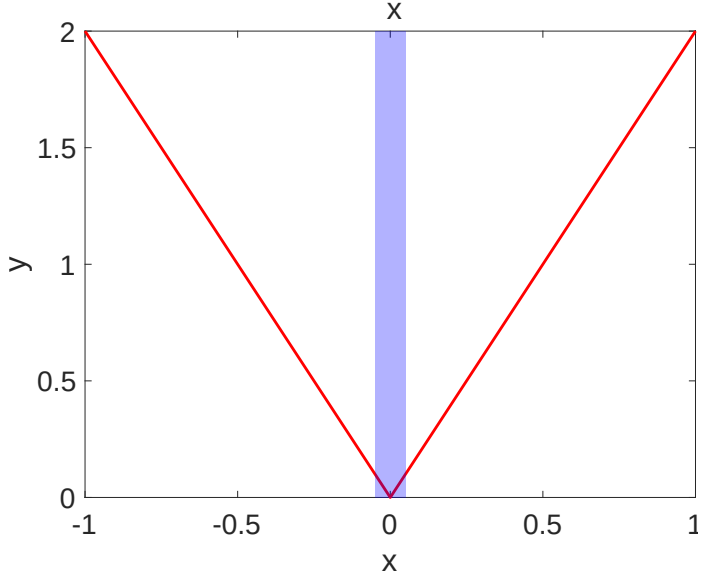
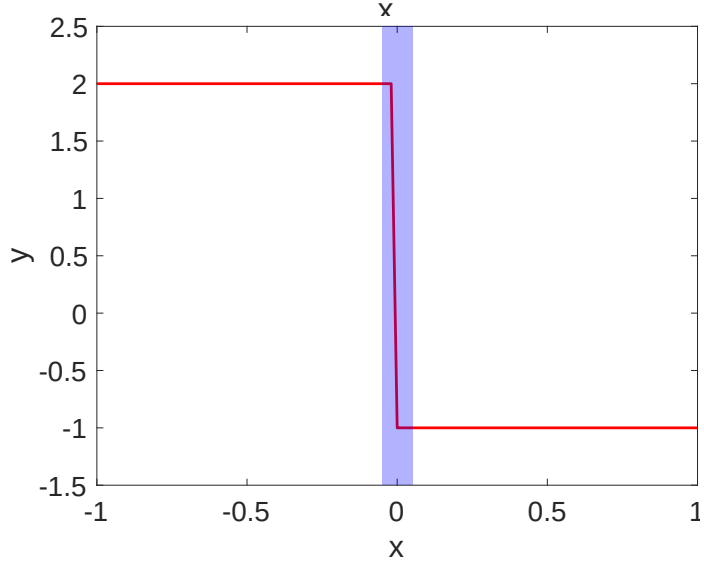


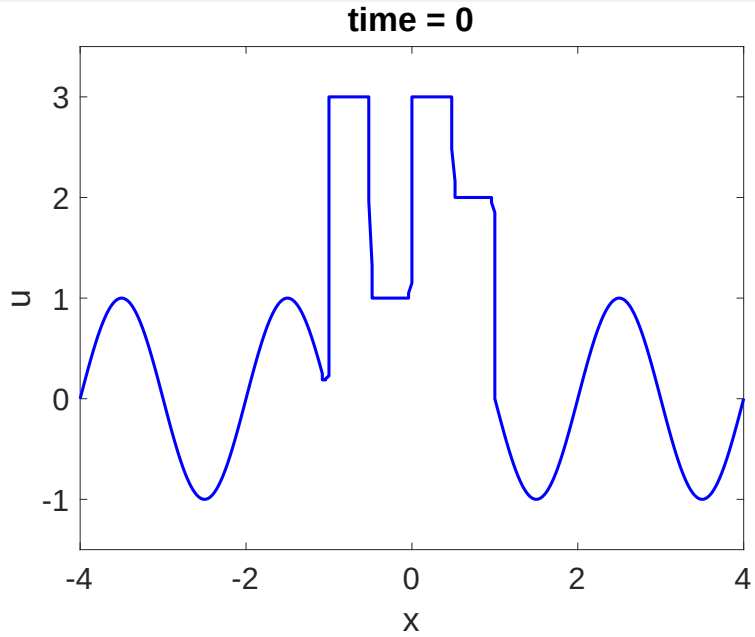


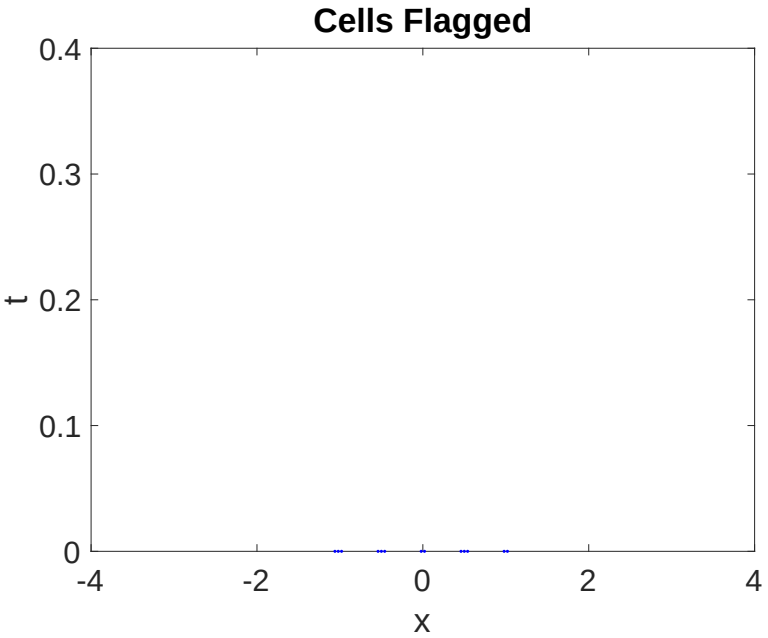




Burgers' equation

$$\partial_t u + \partial_x \left(\frac{u^2}{2} \right) = 0$$





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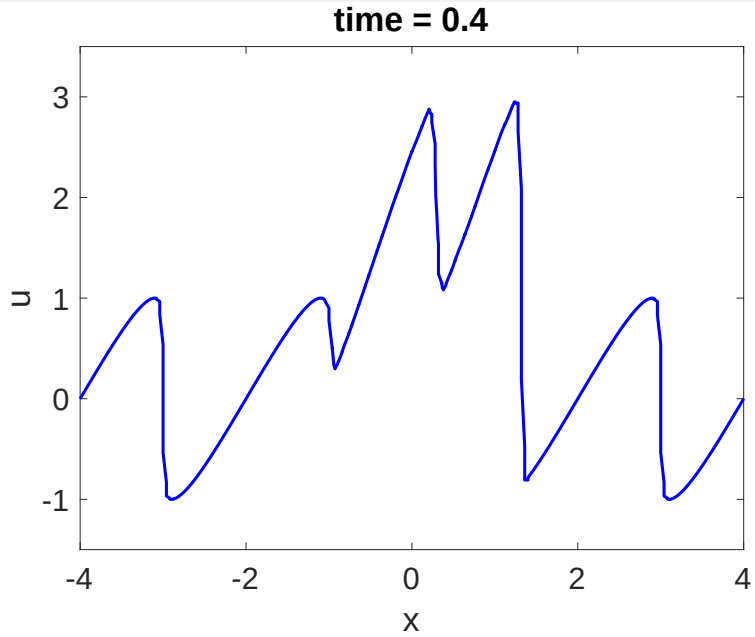

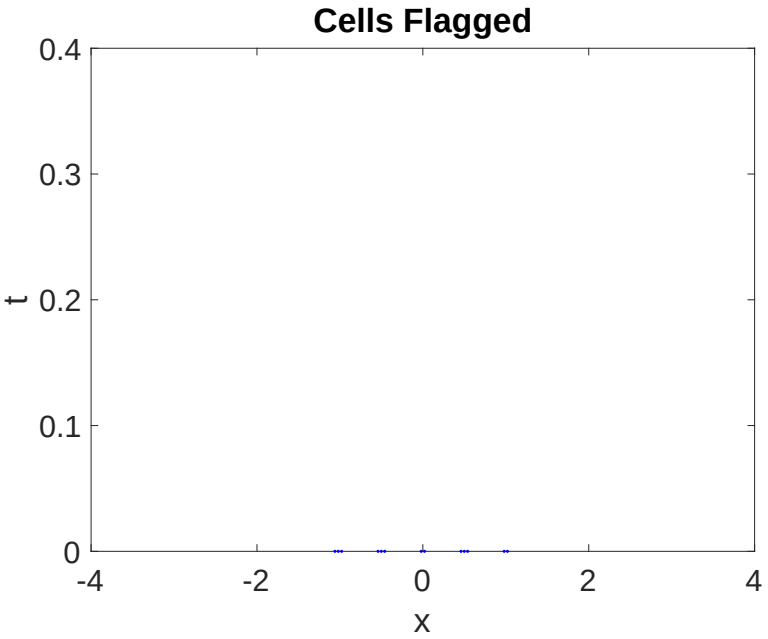

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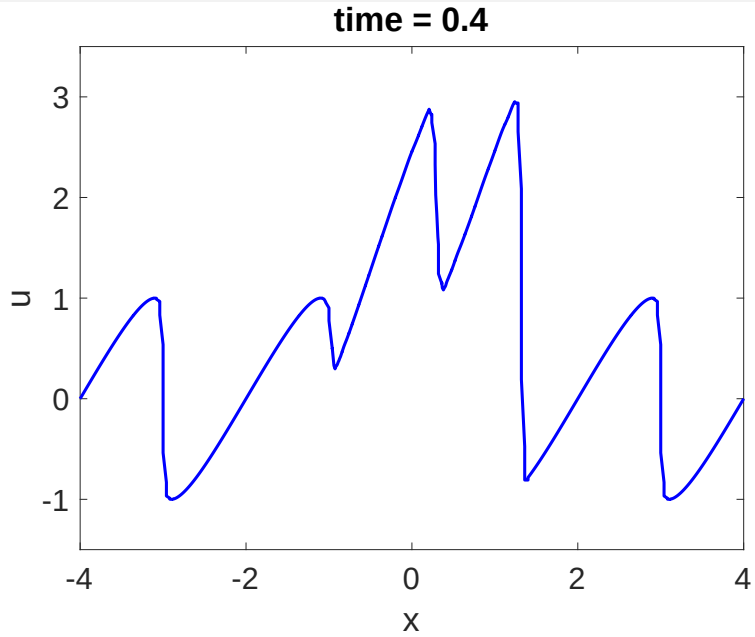
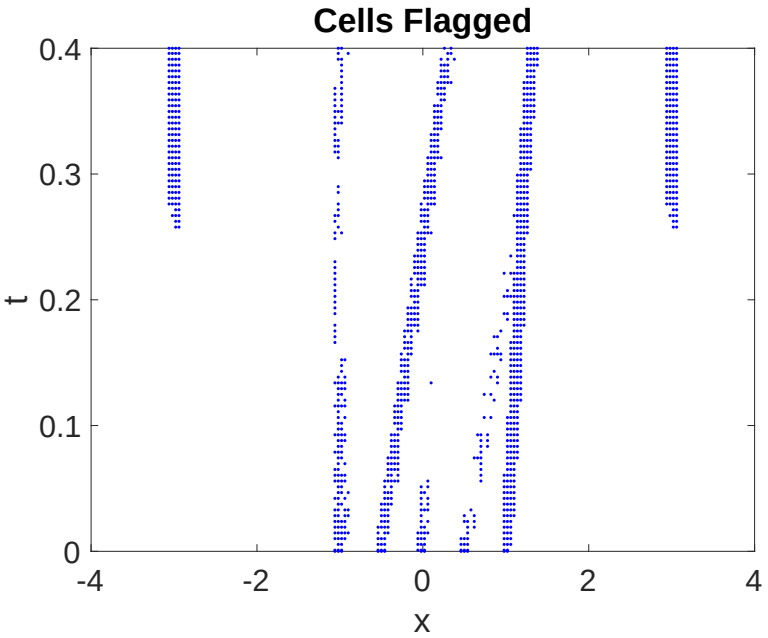




Euler equations

$$\frac{\partial}{\partial t}\begin{pmatrix}\rho\\ \rho u\\ E\end{pmatrix}+\frac{\partial}{\partial x}\begin{pmatrix}\rho u\\ p+\rho u^2\\ (E+p)u\end{pmatrix}=0$$

$$E=\rho\left(\frac{u^2}{2}+e\right),\qquad e=\frac{p}{(\gamma-1)\rho},\qquad \gamma=1.4$$

ρ : density

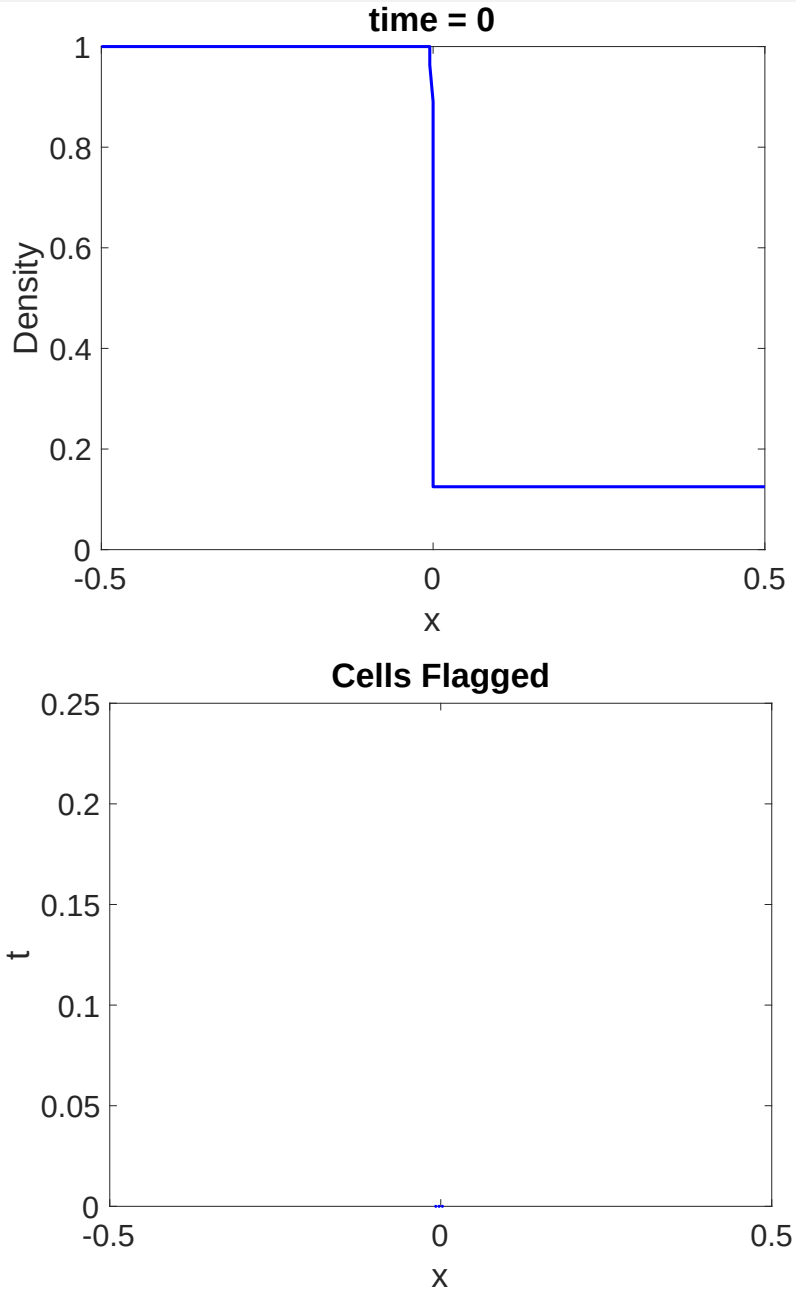
u : velocity

p : pressure

E : total energy

e : internal energy

Euler equations: Shock-tube problem



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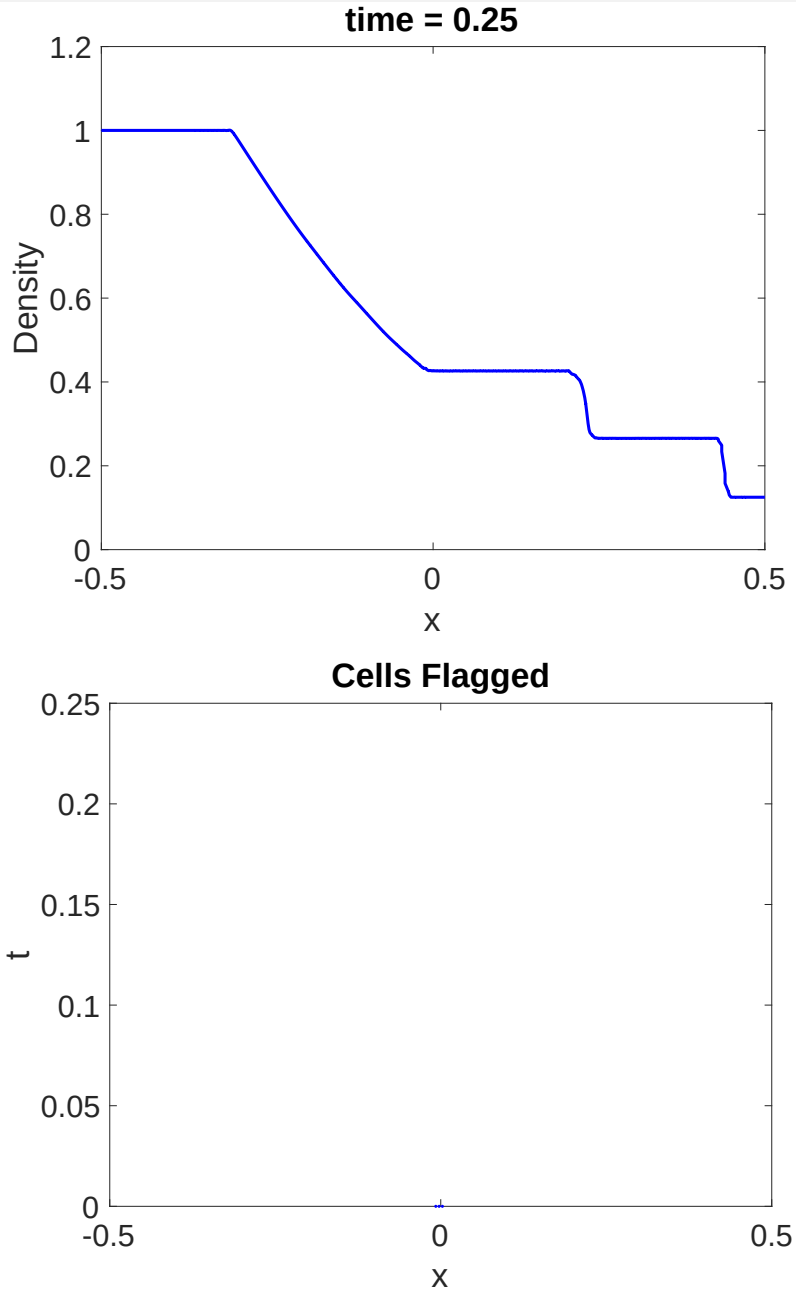

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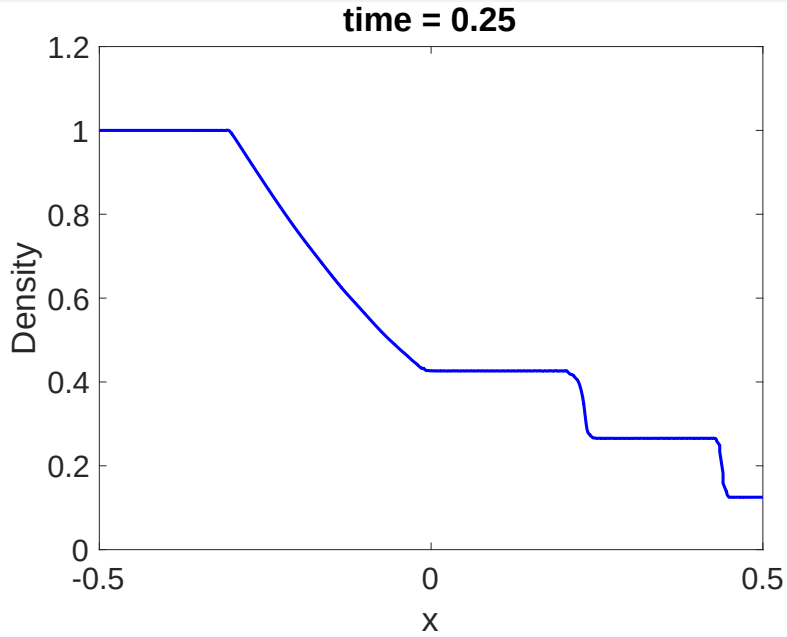
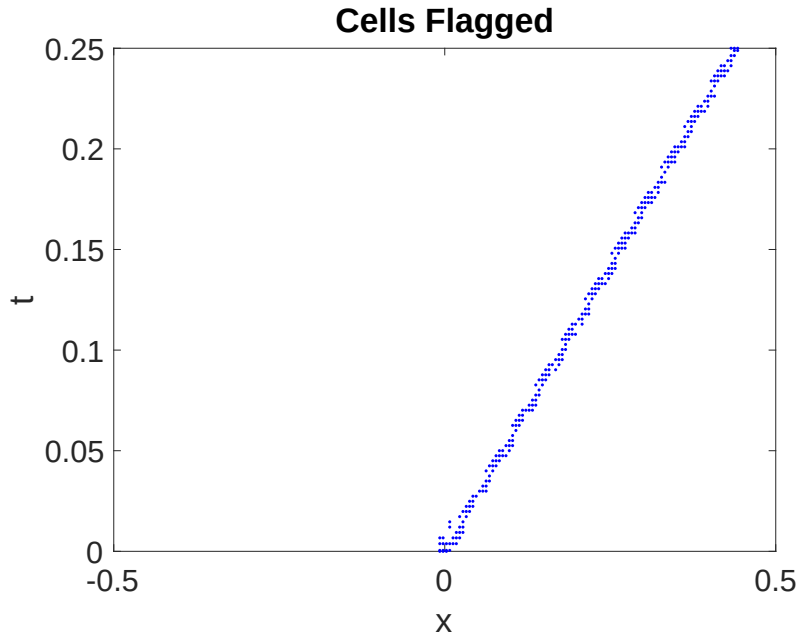
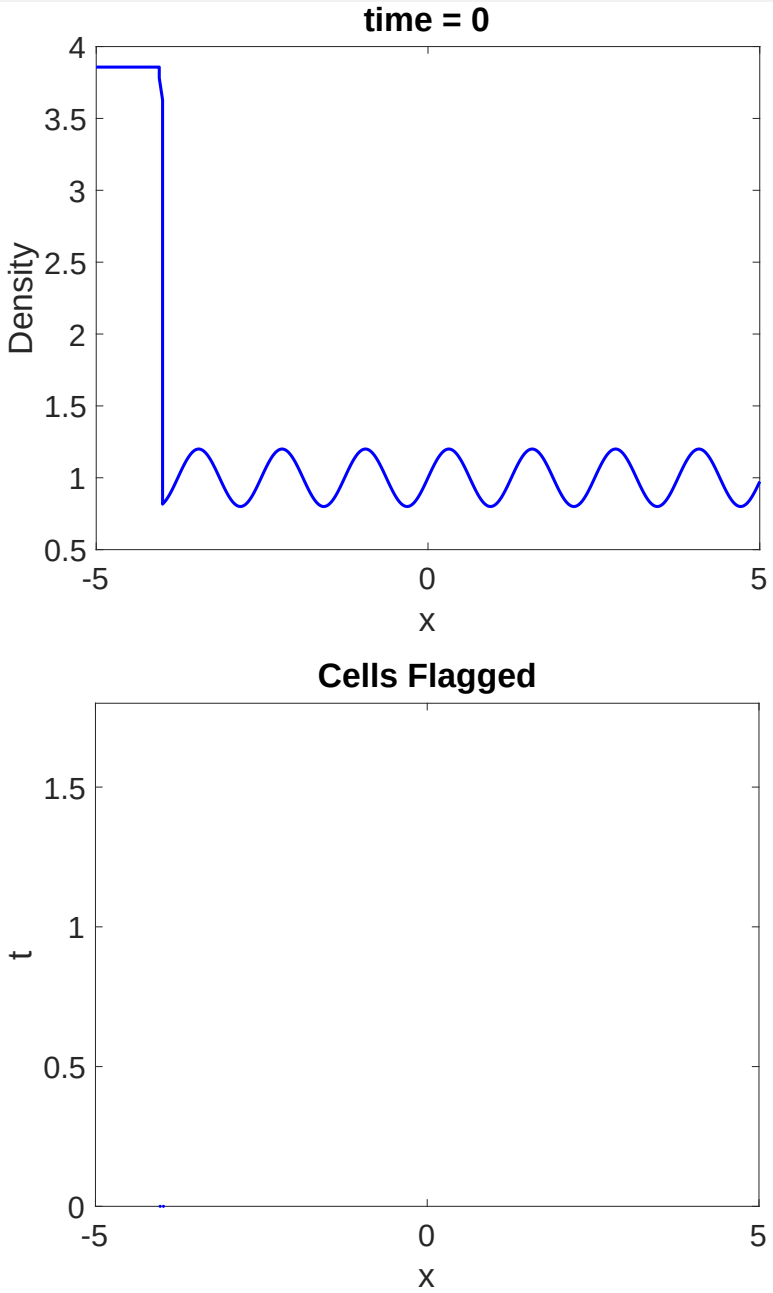
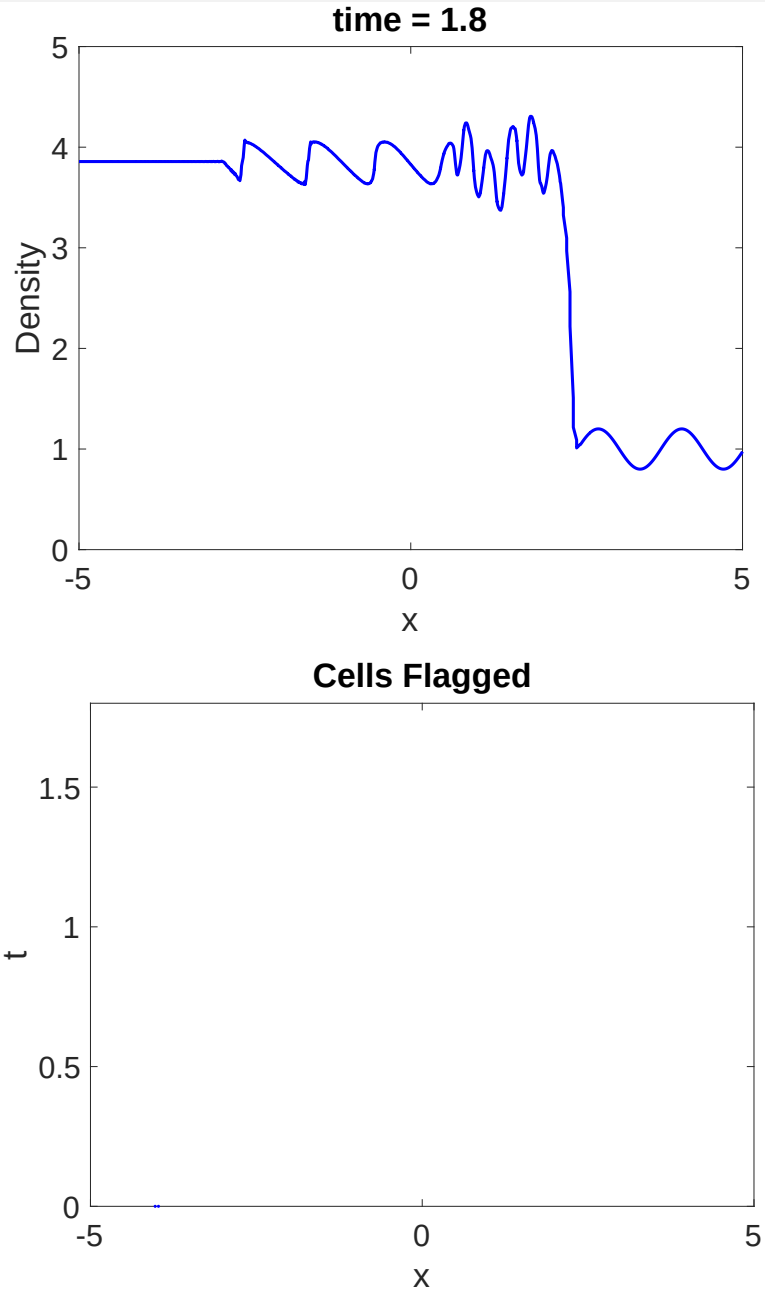




Euler equations: Shock-entropy problem



Euler equations: Shock-entropy problem



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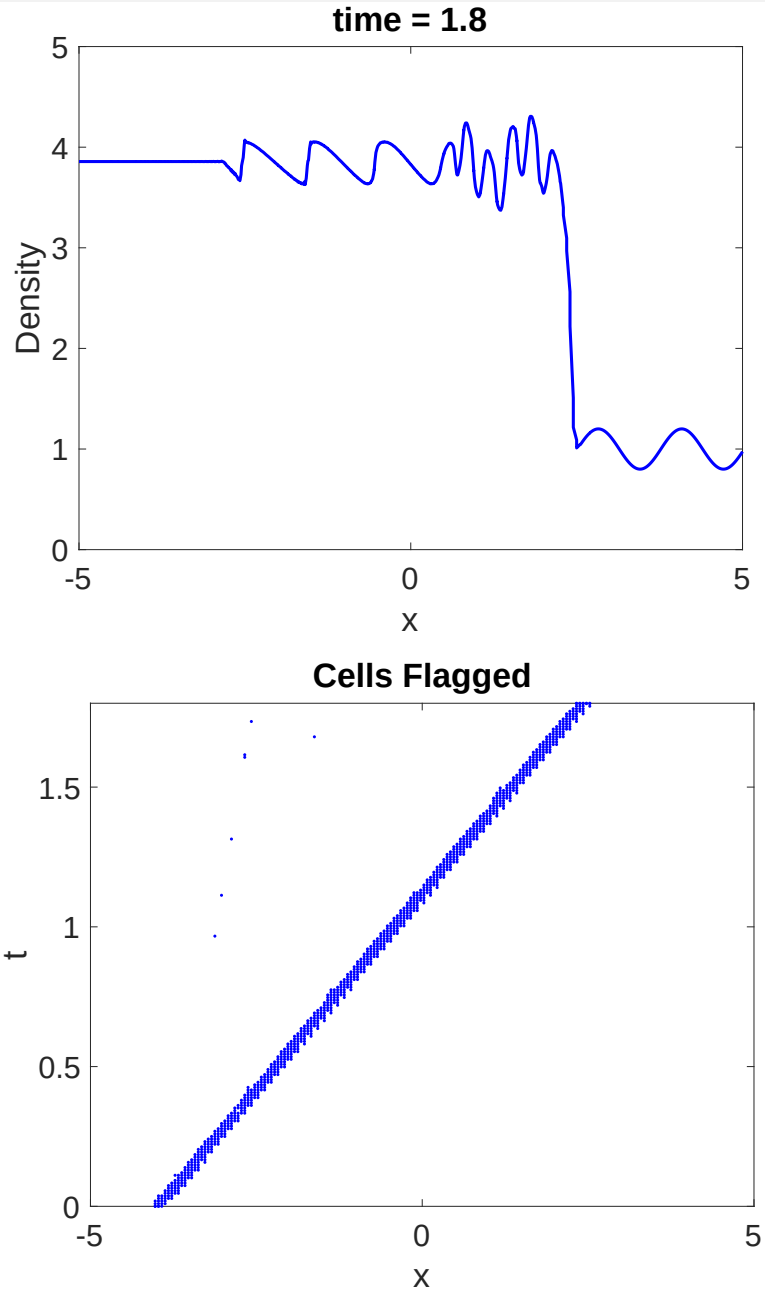
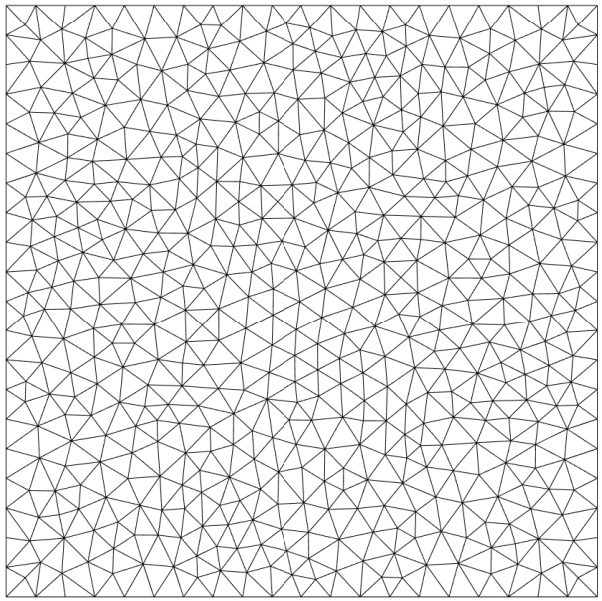
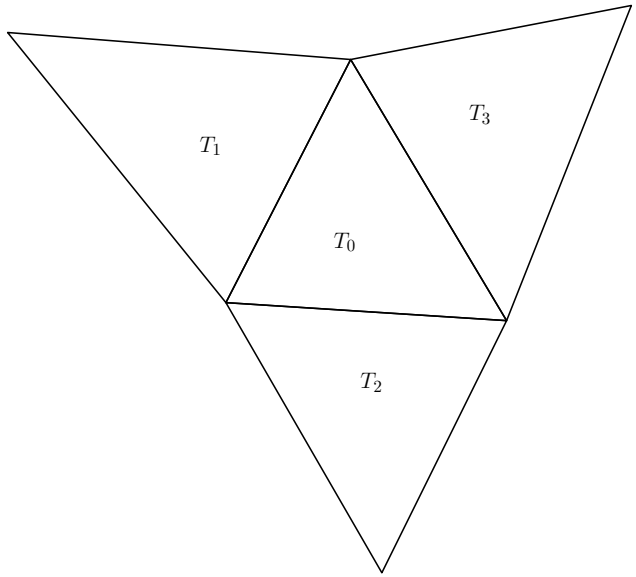


What else?

What else?

- We can also do this in 2D





What else?

- We can also do this in 2D
- Add artificial viscosity instead of limiting

$$\frac{\partial \mathbf{u}}{\partial t} + \frac{\partial \mathbf{f}(\mathbf{u})}{\partial x} = \mu \frac{\partial^2 \mathbf{u}}{\partial x^2}$$

μ based on local smoothness $\longrightarrow$ predicted by a network

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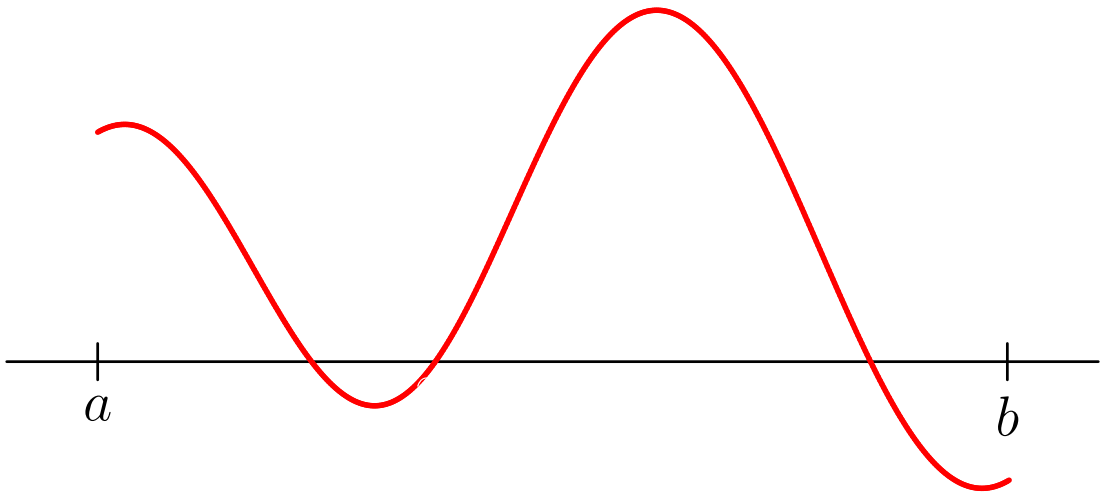
- Similar applications (see deepray.github.io/publications)

Don't replace but enhance existing numerical frameworks with deep networks

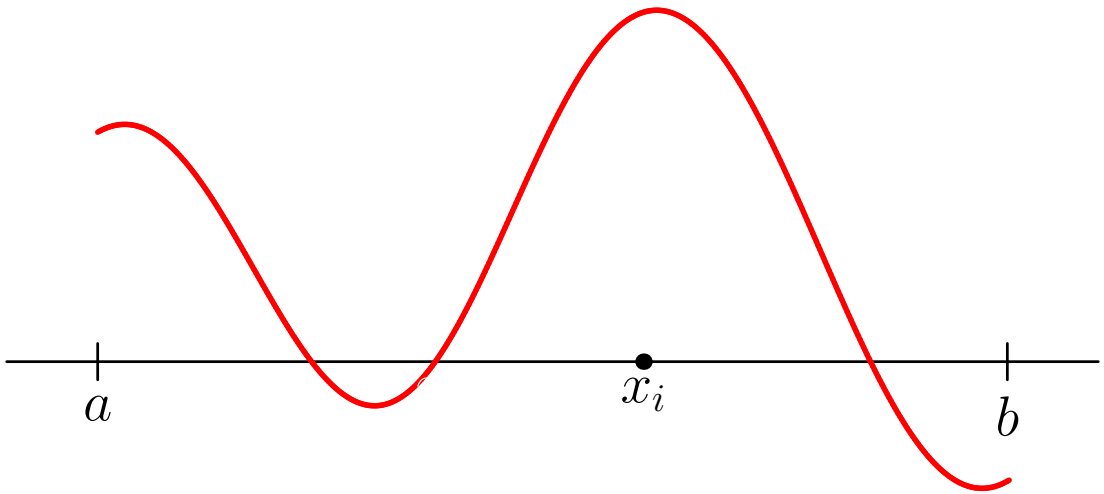
Generating the training data for indicator



Data sampling is achieved by

- Choose a known function $u(x)$ – for eg $\sin(x)$, x^p, etc

Generating the training data for indicator



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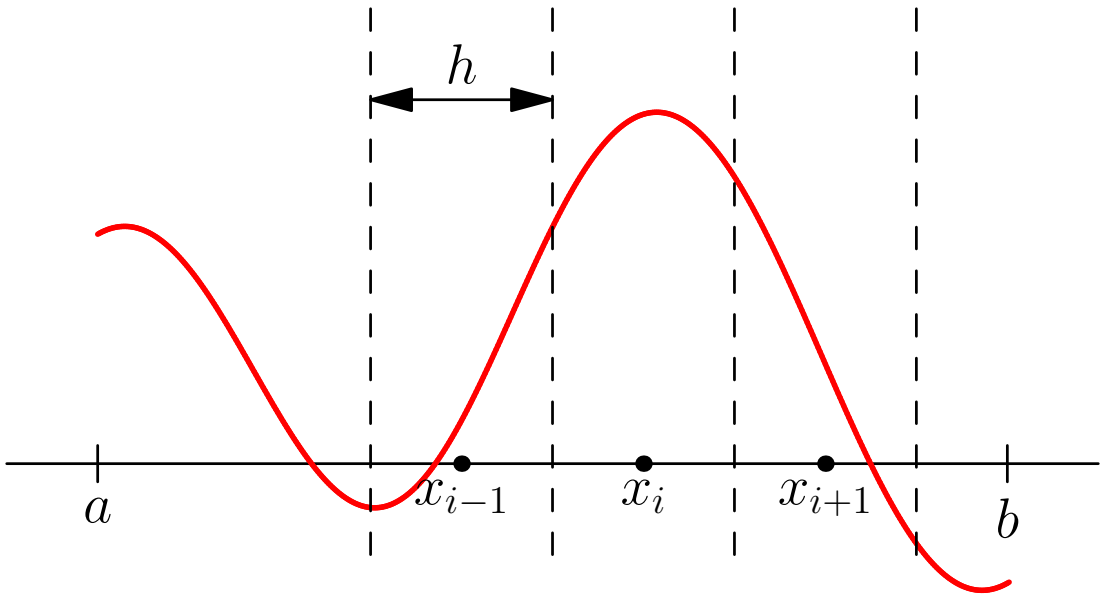

Data sampling is achieved by

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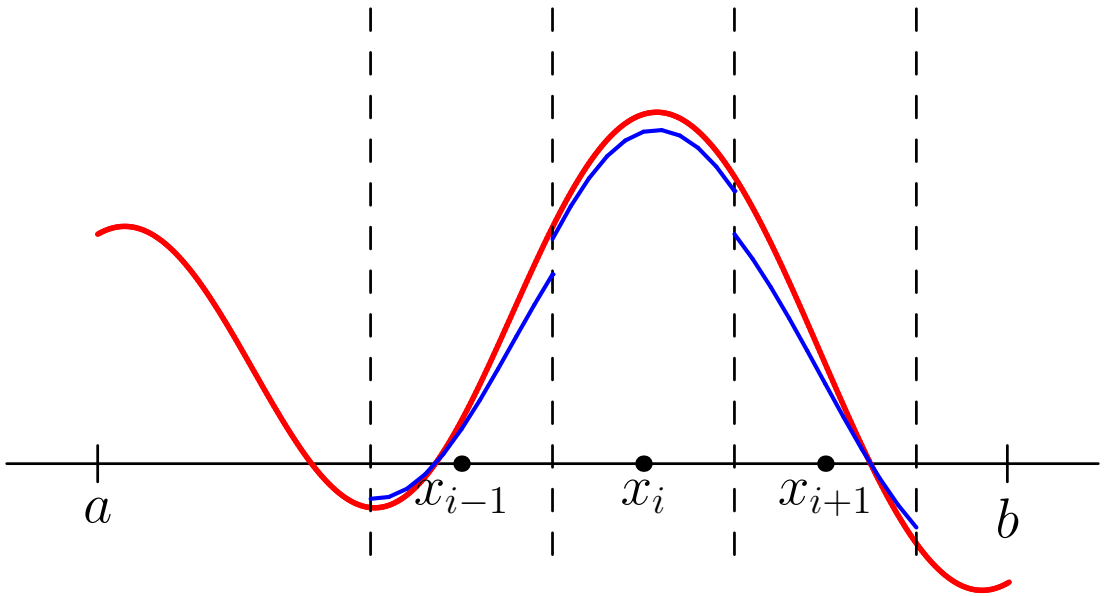
- Pick a cell size h and make stencil

Generating the training data for indicator



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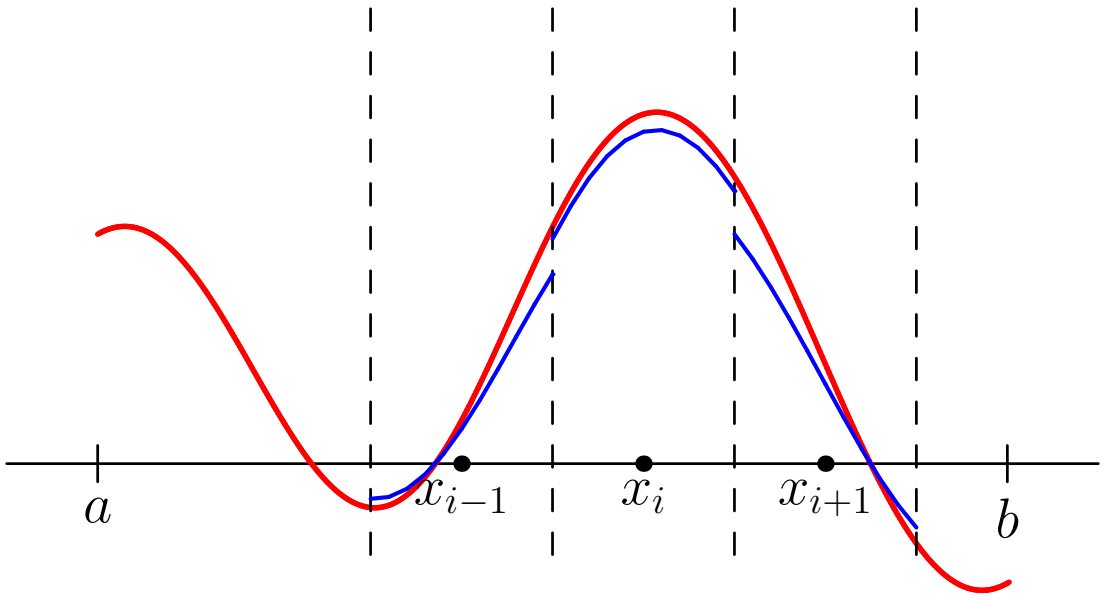
Generating the training data for indicator



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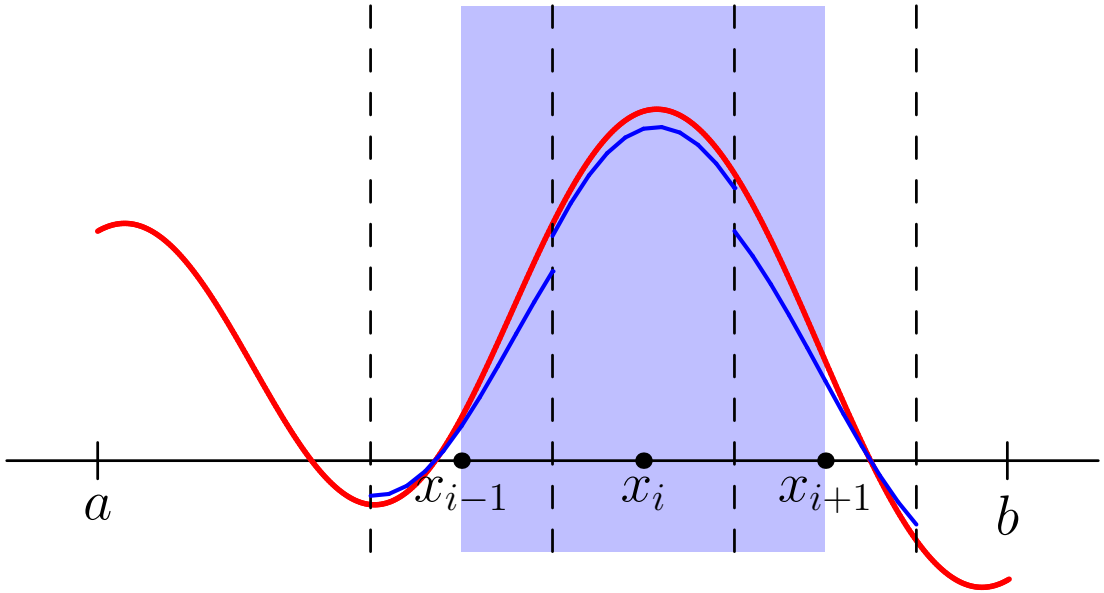

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- Flag cell if discontinuity in $[x_{i-\frac{1}{2}} - h/2, x_{i+\frac{1}{2}} + h/2]$