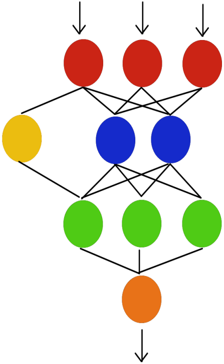
RICE ENGINEERING
Computational and Applied Mathematics



Deep learning enhancements of numerical methods

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CAAM Colloquium
9 September 2019

In collaboration with ...

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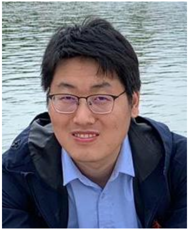
Director MCSS
EPFL



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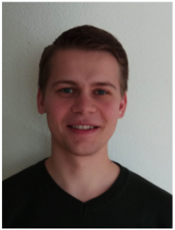
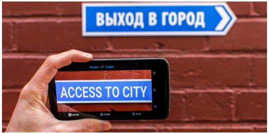
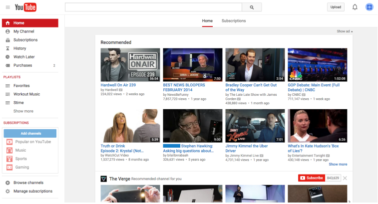
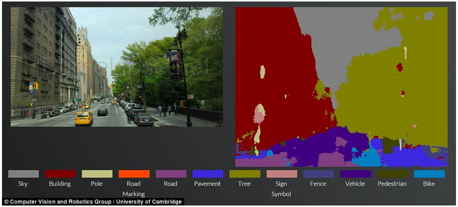


Lukas Schwander
Master student
ETH Zürich

Deep learning in action – conventional applications



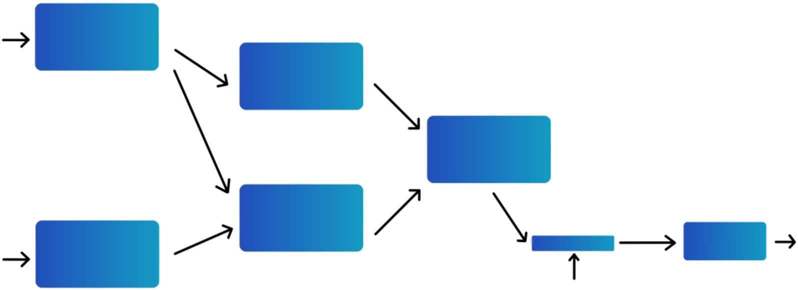




Blending deep learning and numerics

- Solving differential equations [Lagaris et al., 1998; Golak et al., 2007; Rudd et al., 2015; Tompson et al., 2017; Long et al. 2017; Raissi et al., 2018, Magiera et al., 2019]
- Subgrid scale modelling/LES/RANS [Tracey et al., 2013; Zhang et al., 2015; Ling et al., 2016; Kurian et al. 2018; Beck et al.; Duraisamy et al., 2019; Maulik et al., 2019]
- Uncertainty quantification [Tripathy et al., 2018, Kwon et al. 2018; Schwab et al, 2018; Mishra et al., 2019; Wang et al., 2019]
- Reduced order modelling [Kutz et al, 2016; Hartman et al., 2017; Carlberg et al. 2018; Willcox et al., 2019; Wang et al., 2019]
- Inverse problems [Schönlieb et al. 2017, Lunz et al., 2018; Chang et al., 2018; Raissi et al. 2019]
- Shape optimization [Timnaka et al., 2017; Baque at al., 2018; Duraisamy et al., 2019, Sasaki et al. 2019]
- ...

Motivation



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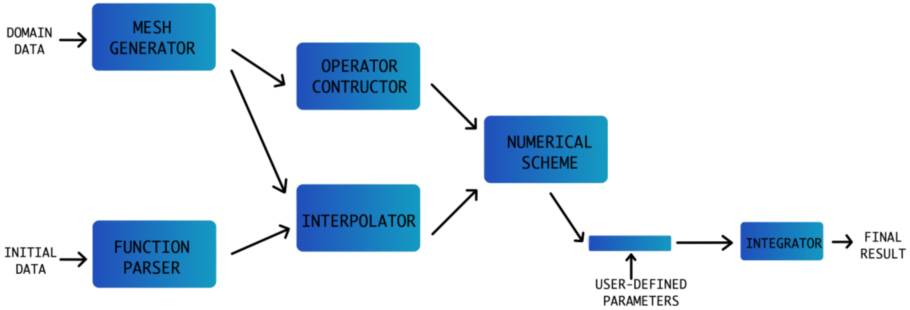
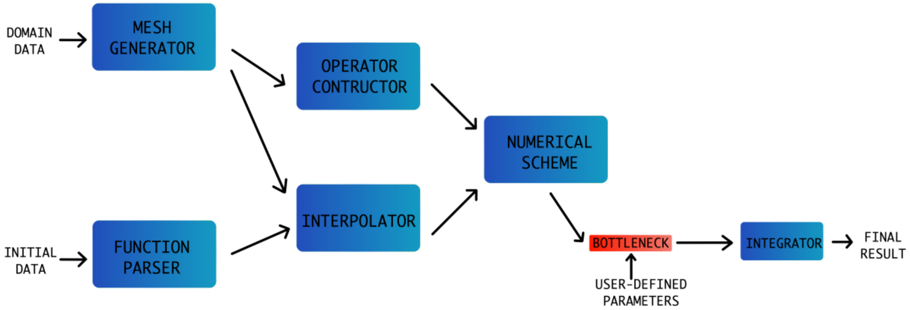

DOMAIN DATA
MESH GENERATOR
INITIAL DATA
FUNCTION PARSER
OPERATOR CONTRUCTOR
INTERPOLATOR
NUMERICAL SCHEME
USER-DEFINED PARAMETERS
INTEGRATOR
FINAL RESULT

Motivation



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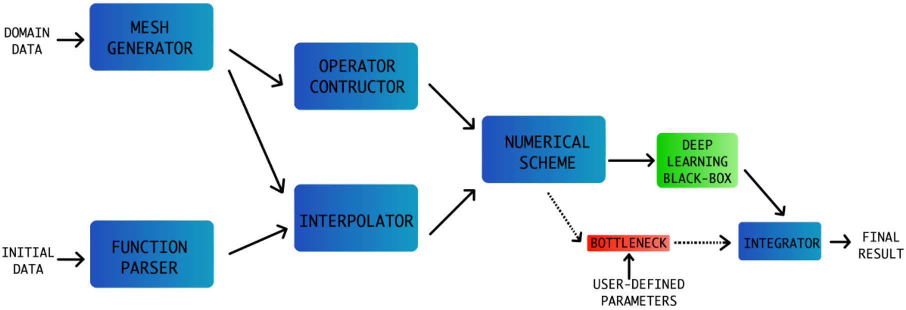
DOMAIN
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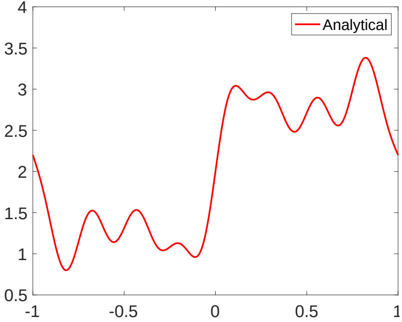
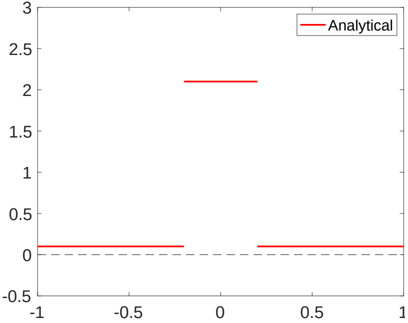
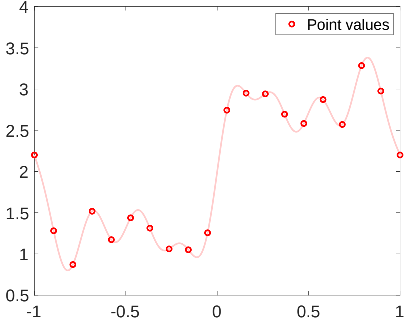
Today's bottleneck – controlling spurious oscillations

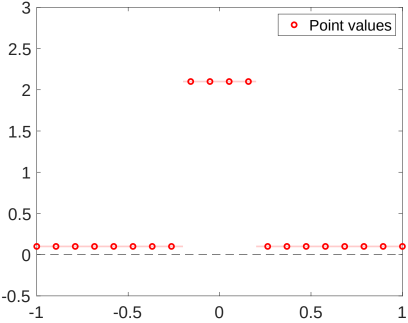




Today’s bottleneck – controlling spurious oscillations

Approximate the function using discrete data e.g. point values





Today's bottleneck – controlling spurious oscillations

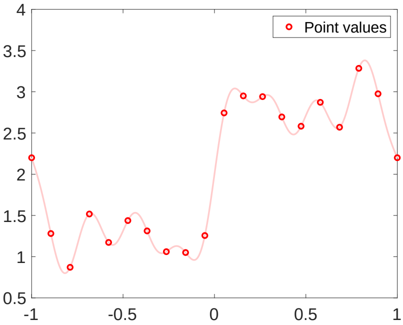
Approximate the function using discrete data e.g. point values

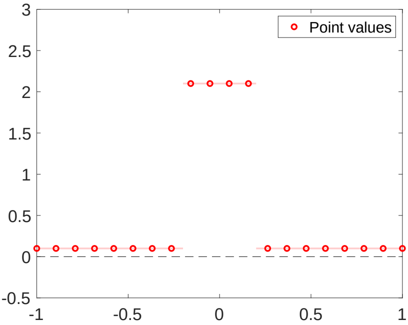
Use a smooth basis

$$u(x) \approx \sum_{p=1}^{K} u_p \phi_p(x)$$

$1, x, x^2, x^3, ...$

$\sin\left(\frac{\pi p}{K}\right), \cos\left(\frac{\pi p}{K}\right)$





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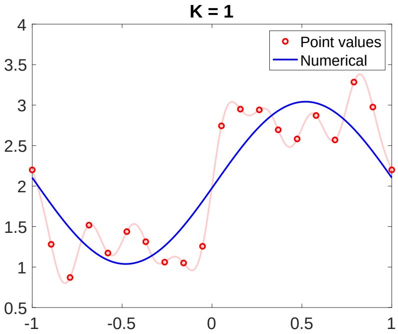

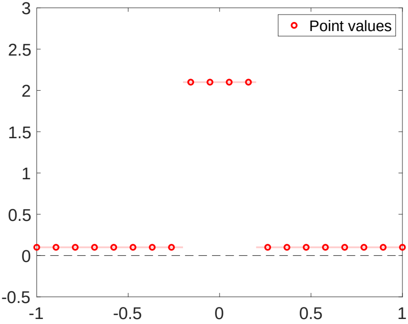

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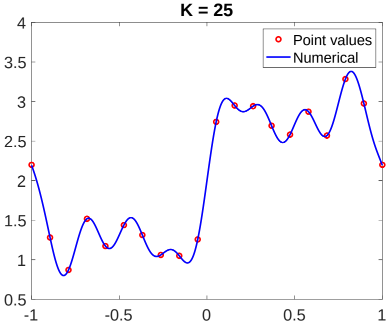
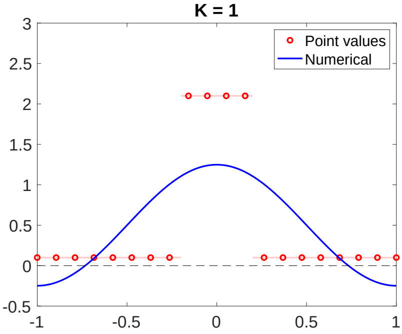




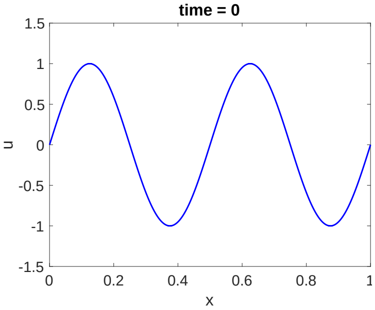
Consider

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

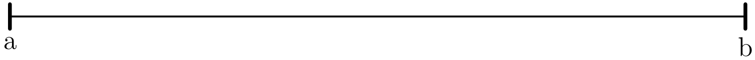
Non-linearity

$\Longrightarrow$

Discontinuities in finite time

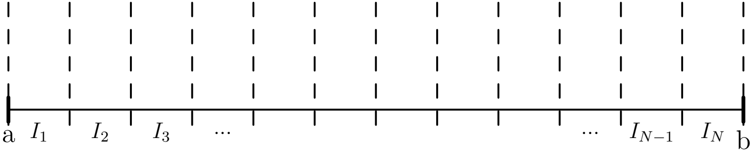


$$0 \leq t \leq T_f \qquad\qquad a \leq x \leq b$$



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

- Discretize spatial domain $[a, b]$ into N cells

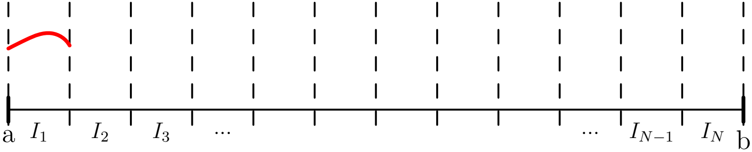


Solving conservation laws numerically

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

- Discretize spatial domain $[a, b]$ into N cells
- At time t approximate solution in each cell

$$u_i(x) = \sum_{p=1}^{K} u_p^i \phi_p^i(x), \quad x \in I_i, \quad 1 \leq i \leq N$$



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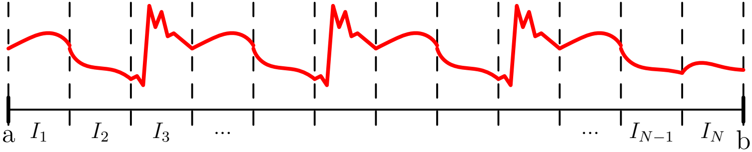

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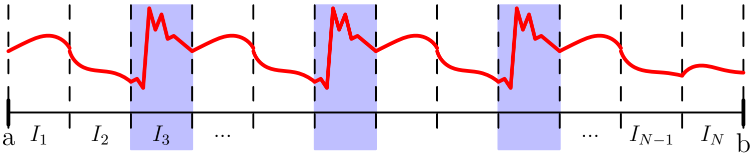
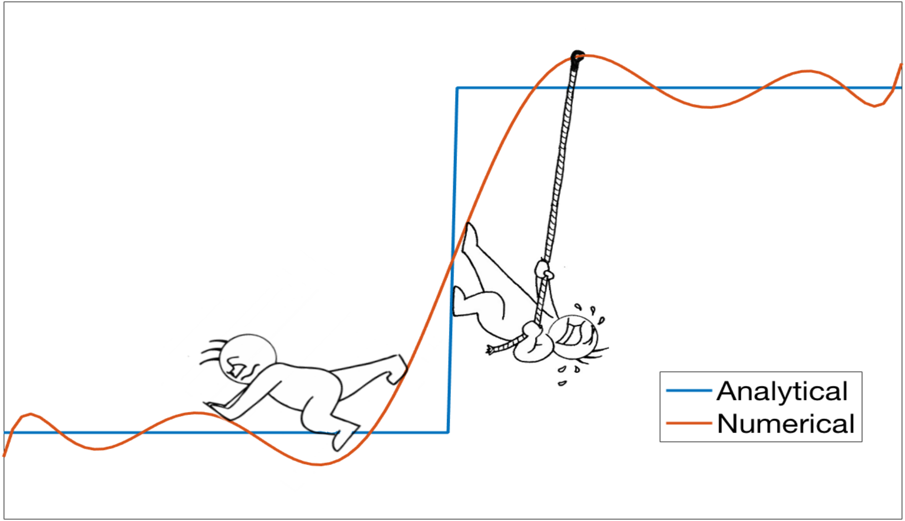
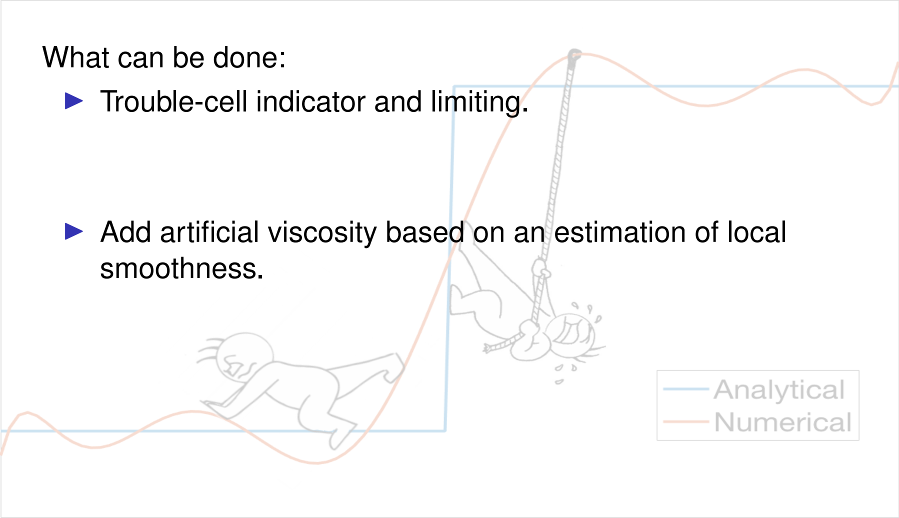


The menace of Gibbs oscillations



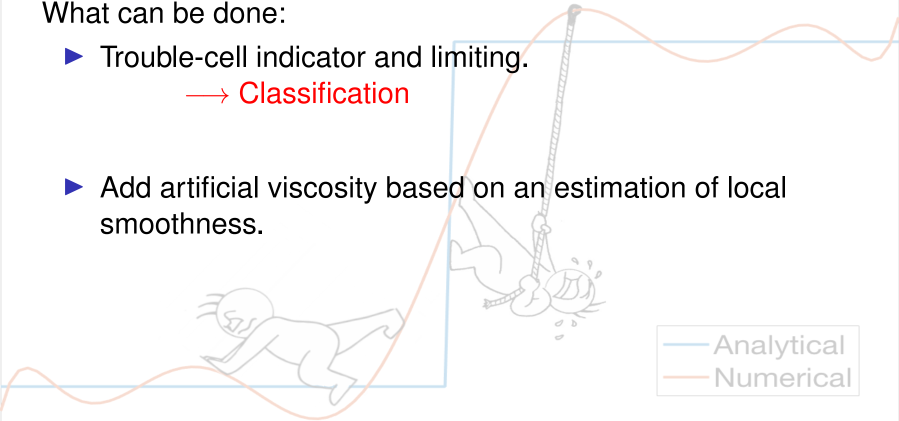
What can be done:

- Trouble-cell indicator and limiting.
- Add artificial viscosity based on an estimation of local smoothness.



What can be done:

- Trouble-cell indicator and limiting.
  $\longrightarrow$ Classification
- Add artificial viscosity based on an estimation of local smoothness.



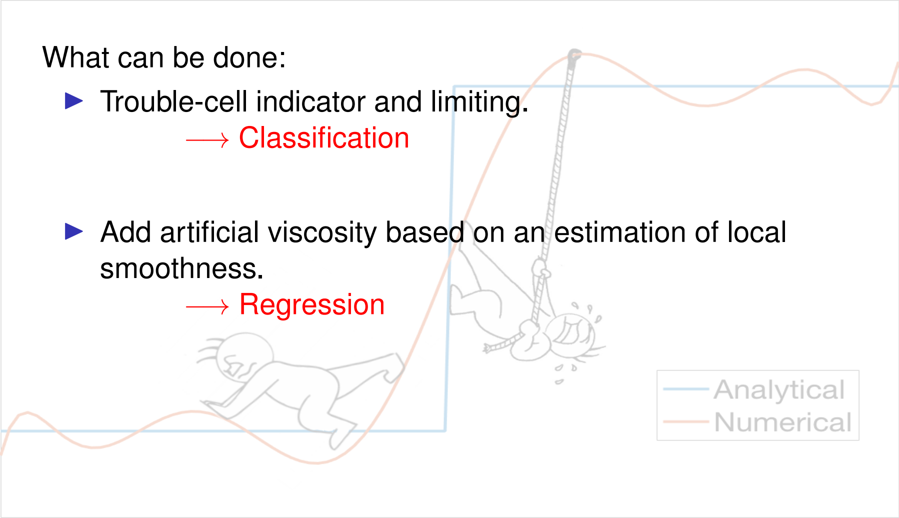
What can be done:

- Trouble-cell indicator and limiting.

  $\longrightarrow$ Classification

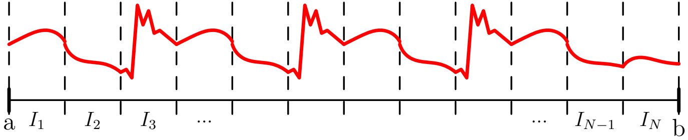
- Add artificial viscosity based on an estimation of local smoothness.

  $\longrightarrow$ Regression



Detecting and limiting

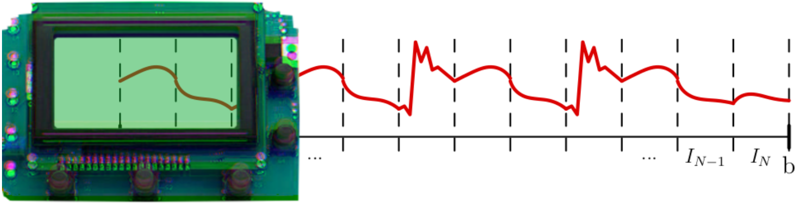
Strategy:



Detecting and limiting

Strategy:

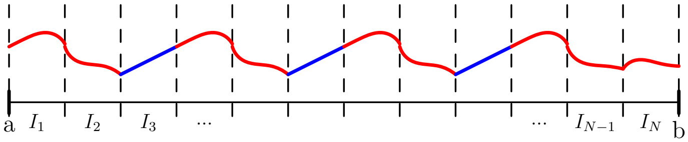
1. Find troubled-cells.



Detecting and limiting

Strategy:

1. Find troubled-cells.
2. Limit solution in flagged cells.



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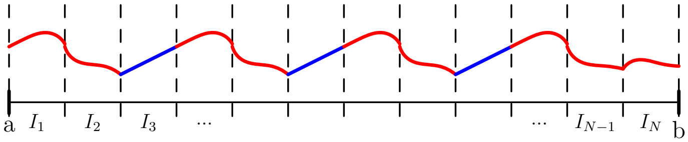


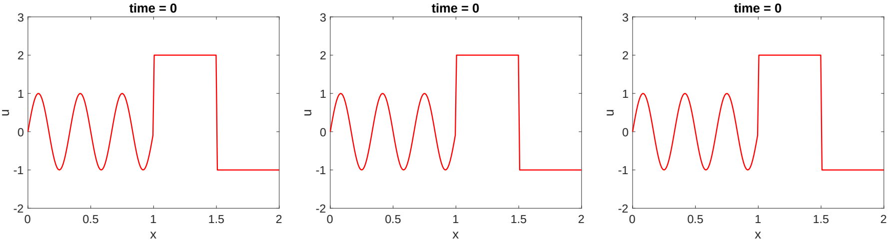
Issues:

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

Adding artificial viscosity

Consider the following modified PDE

$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = \frac{\partial}{\partial x}\left(\mu \frac{\partial u}{\partial x}\right)$$



$\mu = 0$ $\qquad$ $\mu = 5.0e-4$ $\qquad$ $\mu = 1.0e-3$

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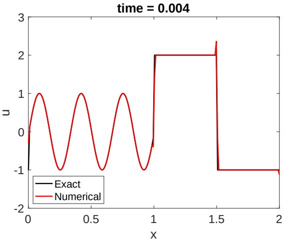

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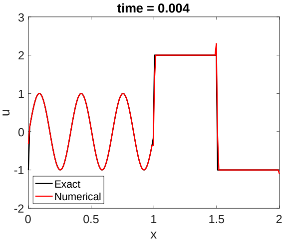

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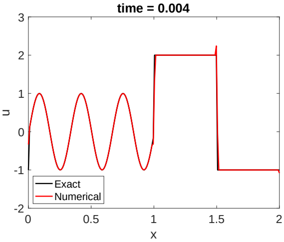

$\mu = 1.0e-3$

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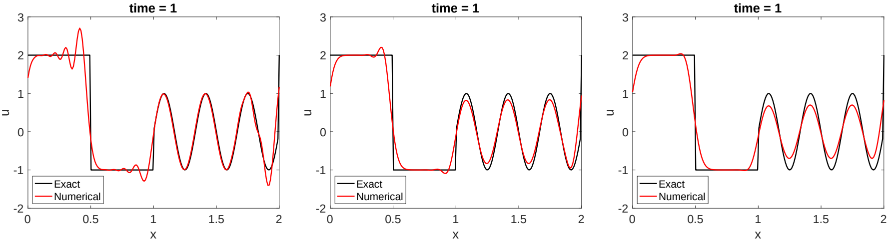

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Issues:

- Where to introduce viscosity?
- How much viscosity?

AIM: To develop a method that

1. Detects troubled-cells/predicts the viscosity μ.
2. Is free of problem-dependent parameters.
3. Is computationally efficient.

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Accomplish this using neural networks.

We wish to approximate the function

$$\mathbf{F} : \mathbf{X} \mapsto \mathbf{Y}, \quad \mathbf{X} \in \mathbb{R}^n,\ \mathbf{Y} \in \mathbb{R}^m$$

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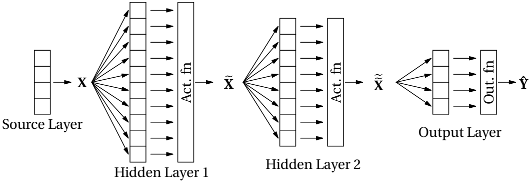
We train a suitable multilayer perceptron (MLP)



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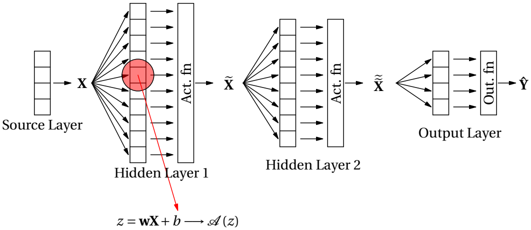

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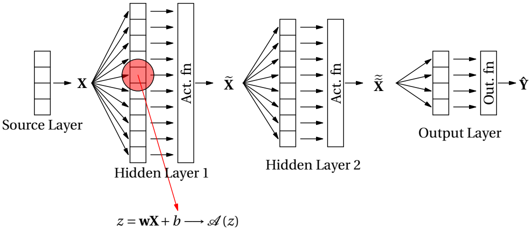

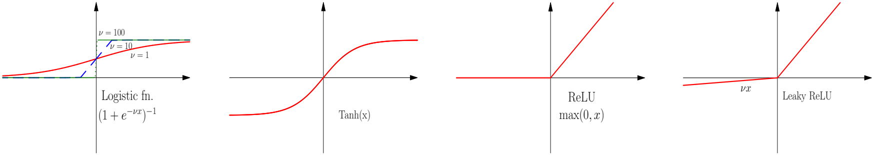

Neural networks

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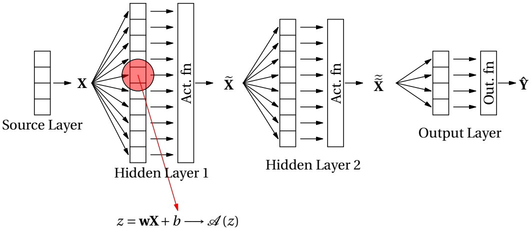

$$\hat{\mathbf{Y}} = \mathcal{O} \circ \mathcal{A} \circ H^L \circ \mathcal{A} \circ H^{L-1} \circ \ldots \circ \mathcal{A} \circ H^1(\mathbf{X}), \quad H^l(\tilde{\mathbf{X}}) = \mathbf{W}^l\tilde{\mathbf{X}} + \mathbf{b}^l$$

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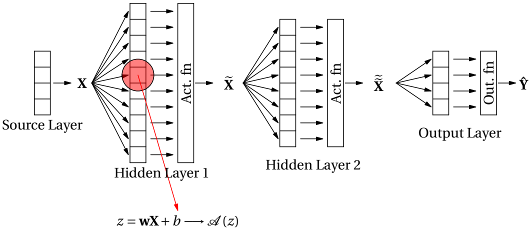

Find parameters $\theta = \{\mathbf{W}^l, \mathbf{b}^l\}$ that minimizes the loss function

$$\mathcal{L}(\mathbf{Y}_i, \hat{\mathbf{Y}}_i), \qquad (\mathbf{X}_i, \mathbf{Y}_i) \in \mathbb{T}.$$

Then $\hat{\mathbf{F}}(\theta) \approx \mathbf{F}$.

The hyperparameters

Based on some theory and prior experience, choose

- Network size – depth and width
- Activation function
- Loss function
- Regularization technique – to avoid overfitting
- Training and validation datasets
- Stopping criteria for training
- Optimizer

Troubled-cell detector

Available troubled-cell indicators

- Minmod-based TVB limiter [Cockburn and Shu; Math. Comp. '98]
- Moment limiter [Biswas et al.; Appl. Numer. Math. '94]
- Modified moment limiter [Burbeau; JCP '01]
- Monotonicity preserving limiter [Suresh and Huynh; JCP '97]
- Modified MP limiter [Rider and Margolin; JCP '01]
- KXRCF indicator [Krivodonova et al.; App. Numer. Math. '04]
- Polynomial degree based limiter [Fu and Shu; JCP '17]
- Outlier detection using Tukey's boxplot method [Vuik and Ryan; J. Sci. Comp. '16]
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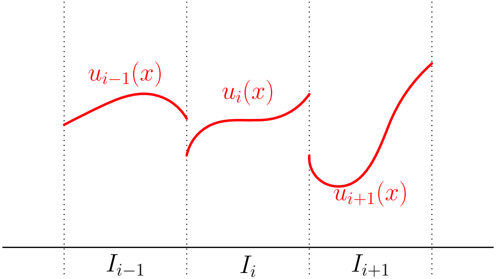
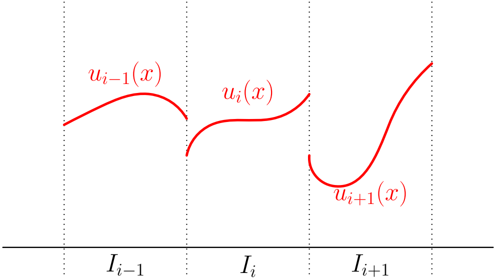
TVB Indicator: Search for the elusive M



- For each cell I_i, get

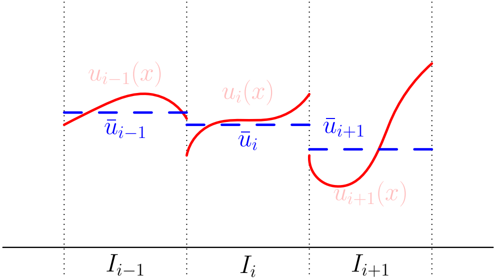
TVB Indicator: Search for the elusive M

$$\overline{u}_i = \frac{1}{|I_i|} \int_{I_i} u_i(x) \mathrm{d}x$$

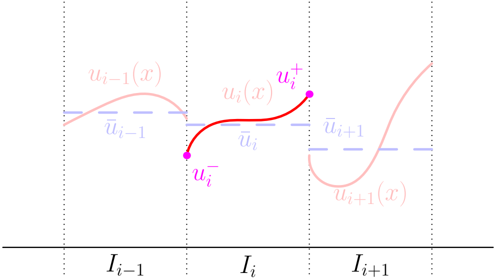


- For each cell I_i, get

TVB Indicator: Search for the elusive M

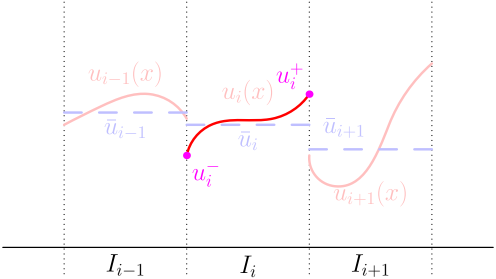


- For each cell I_i, get $[\overline{u}_{i-1}, \overline{u}_i, \overline{u}_{i+1} \quad\quad\quad]$



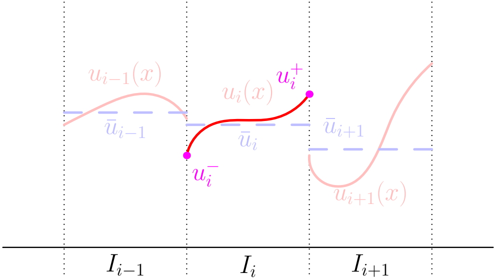
- For each cell I_i, get $[\overline{u}_{i-1}, \overline{u}_i, \overline{u}_{i+1}, u_i^-, u_i^+] \in \mathbb{R}^5$

TVB Indicator: Search for the elusive M



- For each cell I_i, get $[\overline{u}_{i-1}, \overline{u}_i, \overline{u}_{i+1}, u_i^-, u_i^+] \in \mathbb{R}^5$
- Evaluate divided difference $\longrightarrow$ estimate the local gradient.

TVB Indicator: Search for the elusive *M*



- For each cell I_i, get $[\overline{u}_{i-1}, \overline{u}_i, \overline{u}_{i+1}, u_i^-, u_i^+] \in \mathbb{R}^5$
- Evaluate divided difference $\longrightarrow$ estimate the local gradient.
- Choose M $\longrightarrow$ problem dependent!!

An MLP-based detector

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

An MLP-based detector

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

- Input $\mathbf{X} = [\overline{u}_{i-1}, \overline{u}_i, \overline{u}_{i+1}, u_i^-, u_i^+] \in \mathbb{R}^5$ (Scaled)
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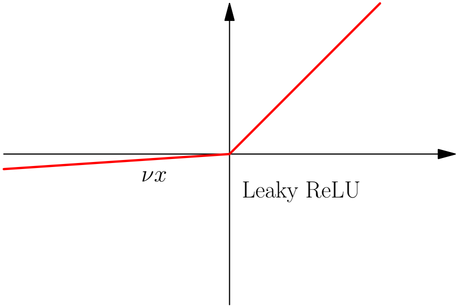
- Leaky ReLU activation function with $\nu = 10^{-3}$



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- 5 Hidden Layers with width 256, 128, 64, 32, 16
- Leaky ReLU activation function with $\nu = 10^{-3}$
- Softmax output function

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

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

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

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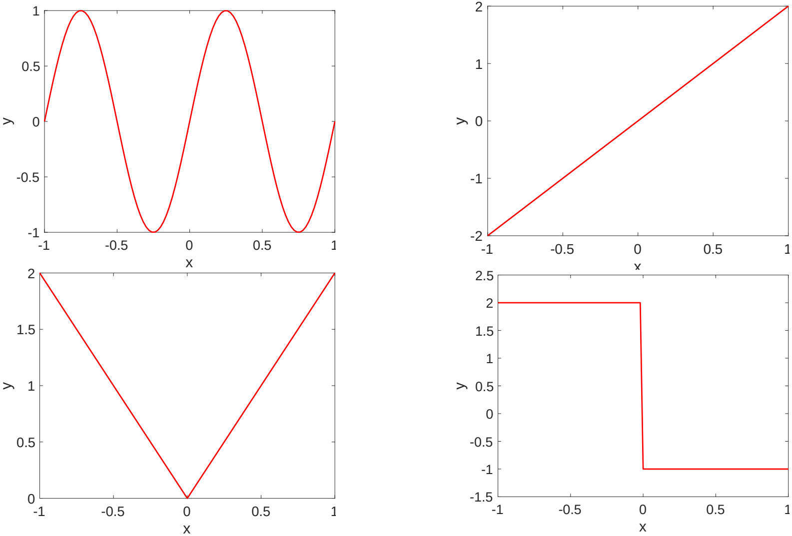
Troubled-cell if $\hat{Y}^{(0)} > 0.5$

- Cost functional: L2 regularized cross-entropy

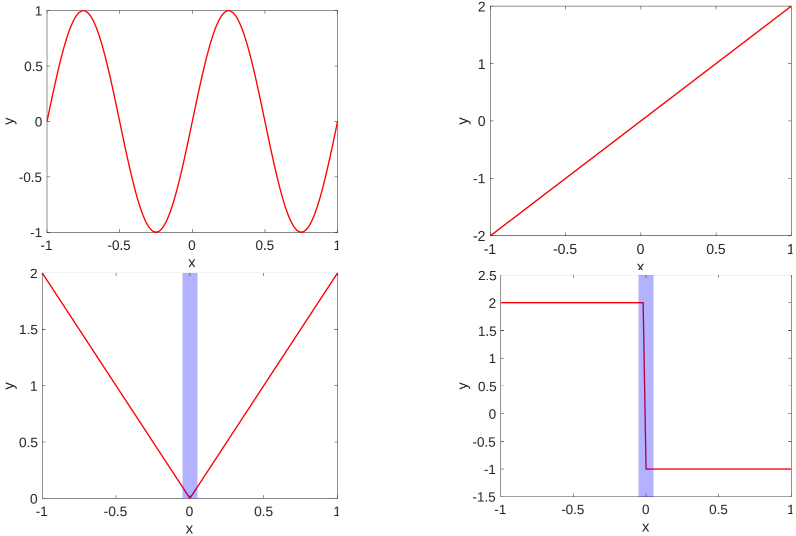
$$\mathcal{L} = -\sum_{i=1}^{K} \sum_{j=0}^{1} Y_i^{(j)} \log(\hat{Y}_i^{(j)}) \; + \; \lambda \|\mathbf{W}\|_2^2$$

Types of functions used:



Generating training data

Types of functions used:



Numerical setup

- Discontinuous Galerkin scheme.
- In flagged cells, perform limited linear reconstruction with MUSCL limiter.
- Legendre basis (Jacobi polynomials in 2D) with degree r.
- Local Lax-Friedrich numerical flux.
- Time integration with SSP-RK3.
- Comparison with TVB indicator by setting parameter M.

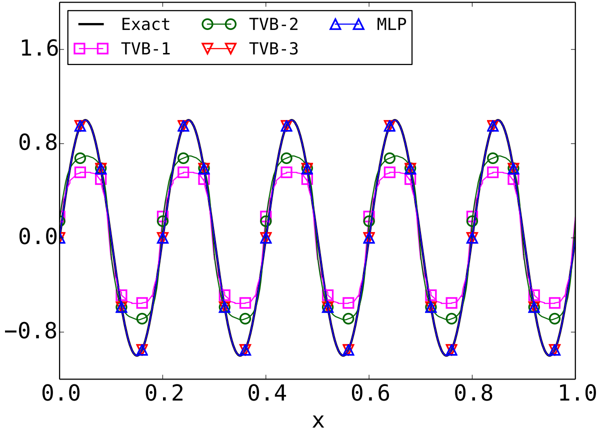
An artificial neural network as a troubled-cell indicator, by R. and Hesthaven; JCP vol. 367, 2018.

Detecting troubled-cells on two-dimensional unstructured grids using a neural network, by R. and Hesthaven, JCP vol. 397, 2019.

Linear advection: $u_t + u_x = 0$

$$u_0(x) = \sin(10\pi x), \quad x \in [0,1], \quad T_f = 1, \quad N = 100, \quad r = 4$$

TVB-1 $\longrightarrow$ M=10
TVB-2 $\longrightarrow$ M=100
TVB-3 $\longrightarrow$ M=1000



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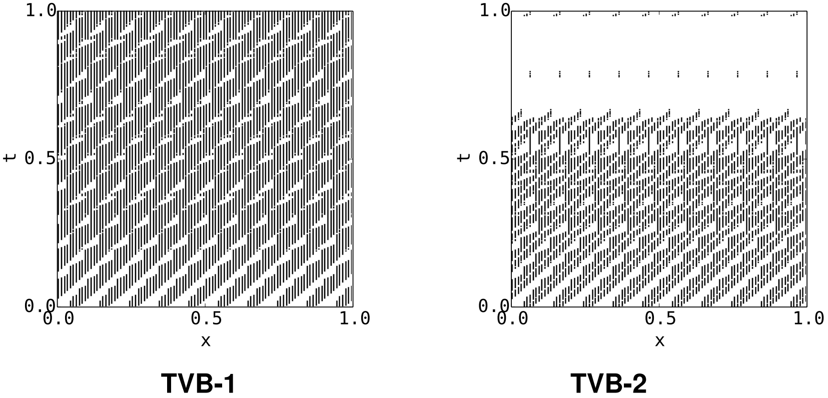
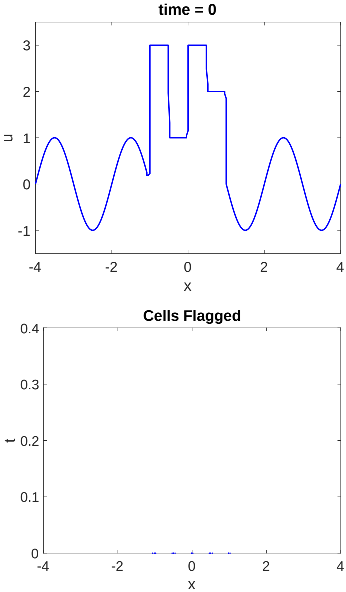


MLP and TVB-3 do not flag any cell

Burgers equation: $u_t + (u^2/2)_x = 0$

$N = 200$,
$r = 4$,
$T_f = 0.4$



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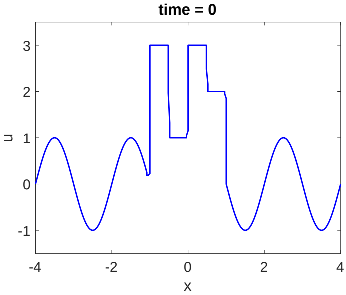

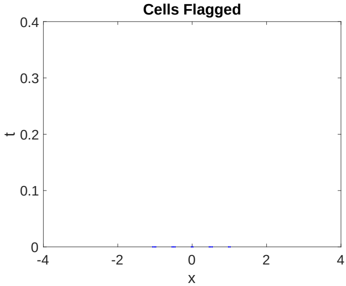

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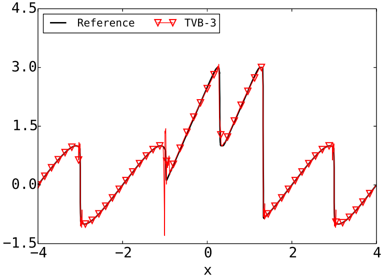
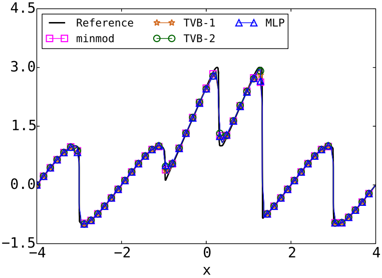




Euler equations

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

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

$\rho \longrightarrow$ fluid density

$v \longrightarrow$ velocity

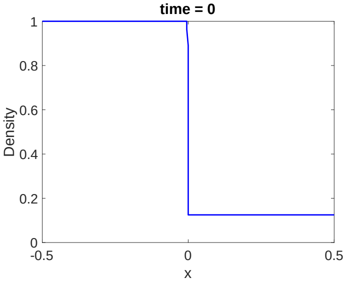
$p \longrightarrow$ pressure

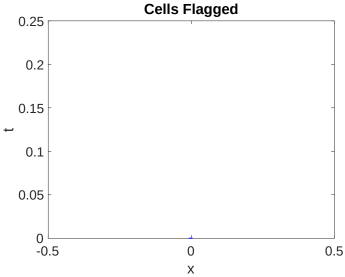
$E \longrightarrow$ total energy

$e \longrightarrow$ internal energy

Euler equations: Sod shock tube

$N = 100$,
$r = 4$,
$T_f = 2$





Euler equations: Sod shock tube

$N = 100,$
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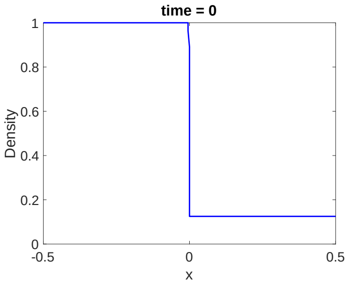
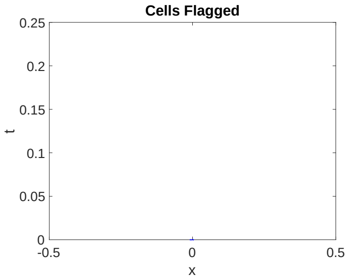
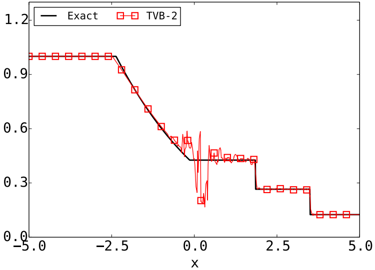
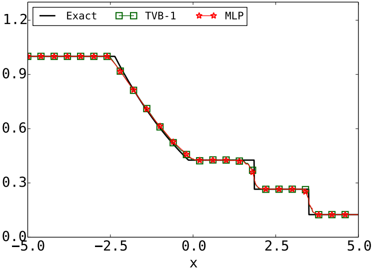




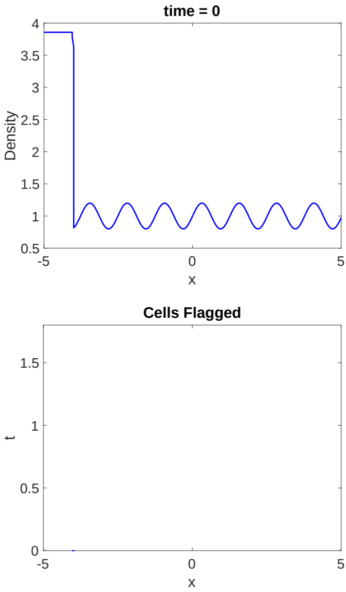




Loss of positivity with TVB-3

1D Euler equations: Shu-Osher problem

$N = 256,$
$r = 4,$
$T_f = 1.8$



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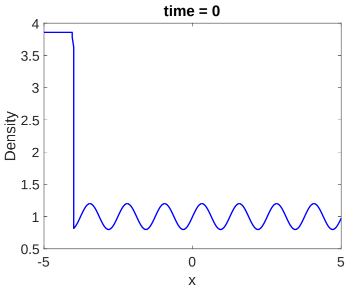
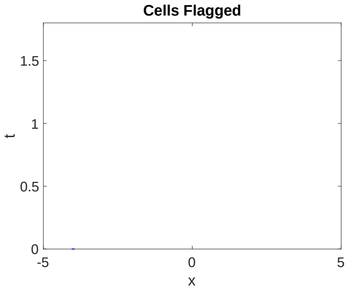
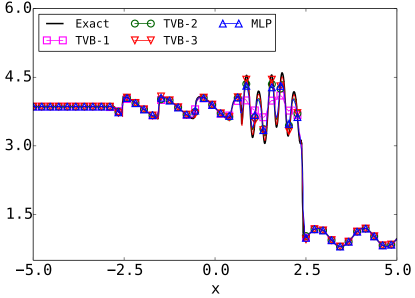
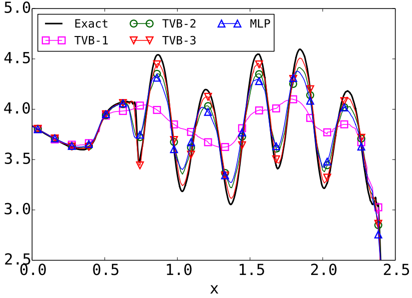




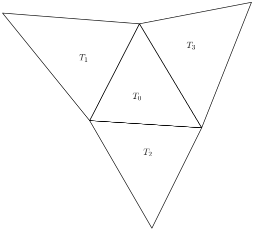
1D Euler equations: Shu-Osher problem





Extension to 2D

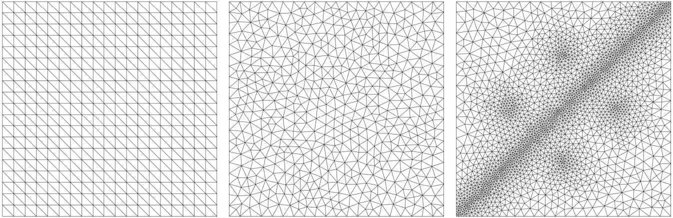
We consider unstructured triangular grids



MLP network with 5 hidden layers of width 20 each

Extension to 2D

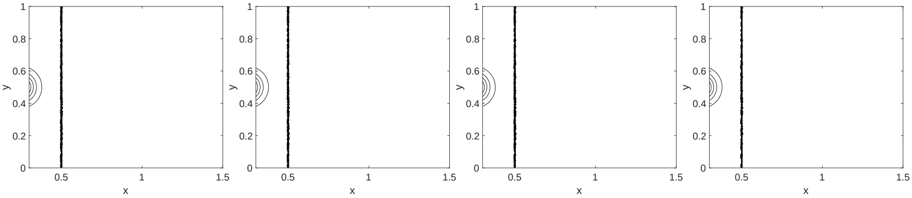
We consider unstructured triangular grids



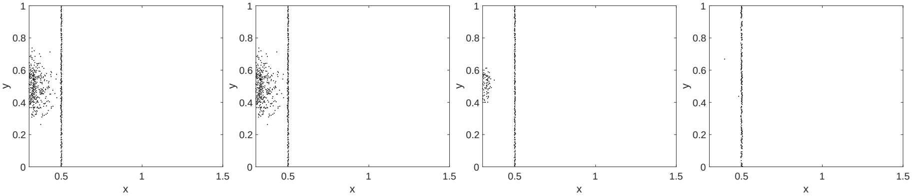
MLP network with 5 hidden layers of width 20 each
Training data constructed by:

- Interpolating functions to patch of 4 triangles.
- Extracting linear components, with $\mathbf{X} \in \mathbb{R}^{12}$.
- Label cell as troubled-cell if discontinuity present within circumscribed circle.

$$T_f = 0.8, \quad h = 0.01, \quad r = 3, \quad \text{Barth-Jesperson limiter}$$

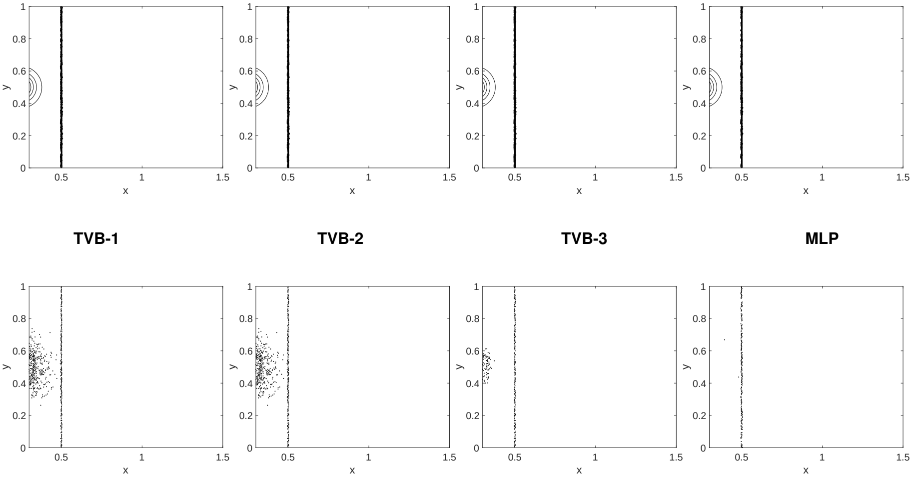


TVB-1 **TVB-2** **TVB-3** **MLP**



2D Euler equations: Shock-vortex

$T_f = 0.8, \quad h = 0.01, \quad r = 3,$ Barth-Jesperson limiter



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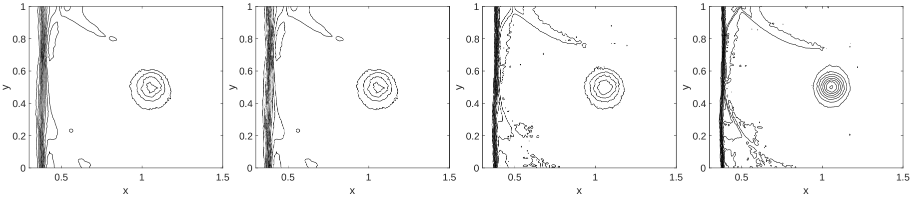
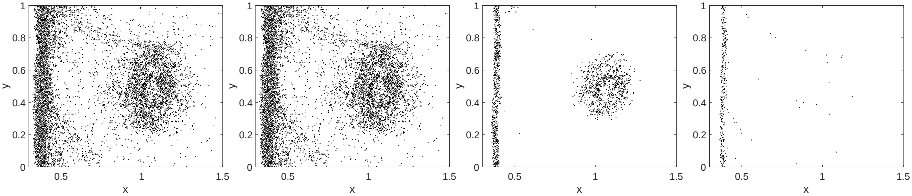


TVB-1 **TVB-2** **TVB-3** **MLP**



Predicting artificial viscosity

Adding artificial viscosity

Now consider the problem

$$\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot \mathbf{f}(\mathbf{u}) = \nabla \cdot \mathbf{g}, \quad \mathbf{g} = \mu \mathbf{w}, \quad \mathbf{w} = \nabla \mathbf{u}$$

Viscosity depends on **u** and locally controls oscillations.

$$\mu \sim h|\mathbf{f}'(\mathbf{u})|$$

Several artificial viscosity models exist

- MDH: Highest Modal Decay [Persson and Peraire; 14th AIAA meet, 2016]
- MDA: Averaged Modal Decay [Klöckner et al.; Math. Mod. Nat. Phen., 2011]
- EV: Entropy Viscosity [Guermond et al.; JCP, 2011]

Dependent on problem specific parameters

Training an MLP

Network architecture:

- Input: Full data from each element (no neighbours).
- 5 hidden layers of width 10 each with Leaky ReLU.
- Softplus output function, i.e., $f(x) = \log(1 + e^x)$.
- Mean Squared Error cost function.

Training an MLP

Network architecture:

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- 5 hidden layers of width 10 each with Leaky ReLU.
- Softplus output function, i.e., $f(x) = \log(1 + e^x)$.
- Mean Squared Error cost function.

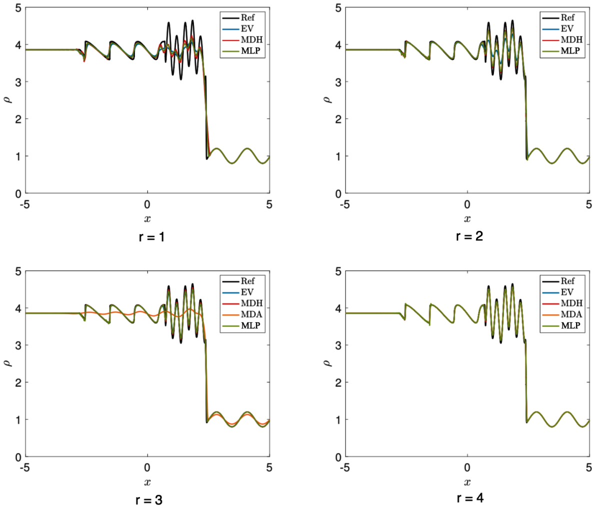
Training/validation sets:

- Using numerical solution of conservation laws (only linear adv. and Burgers).
- Target viscosity: viscosity corresponding to "best" model.
- Different network for each degree r.

Controlling oscillations in high-order Discontinuous Galerkin schemes using artificial viscosity tuned by neural networks, by Discacciti, Hesthaven and R.; 2019 (submitted).

1D Euler equations: Shu-Osher

$T_f = 1.8, \quad h = 10/200$



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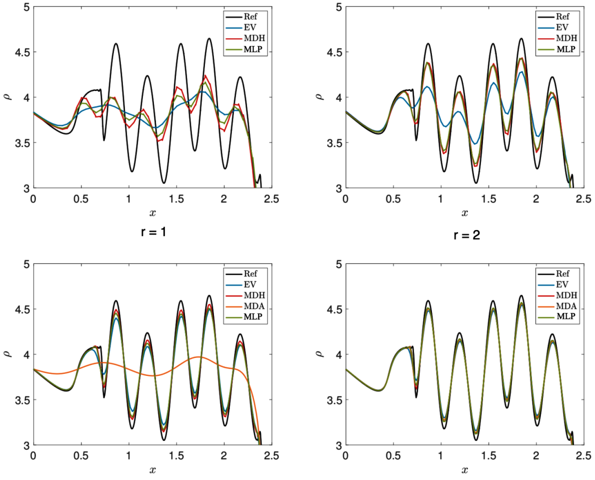
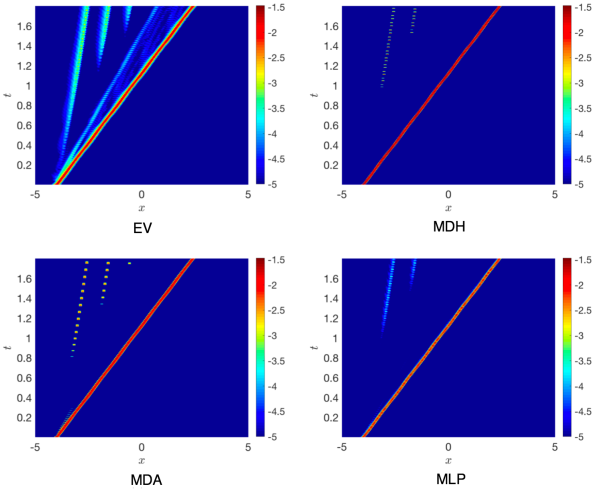


r = 1 r = 2

r = 3 r = 4

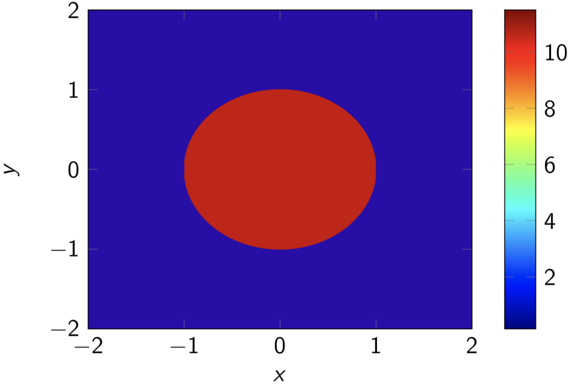
1D Euler equations: Shu-Osher

$$T_f = 1.8, \quad h = 10/200, \quad r = 4$$



2D KPP equations: Rotating wave

$$\mathbf{f}(u) = (\sin u, \cos u), \quad T_f = 1, \quad h = 4\sqrt{2}/120, \quad r = 4$$



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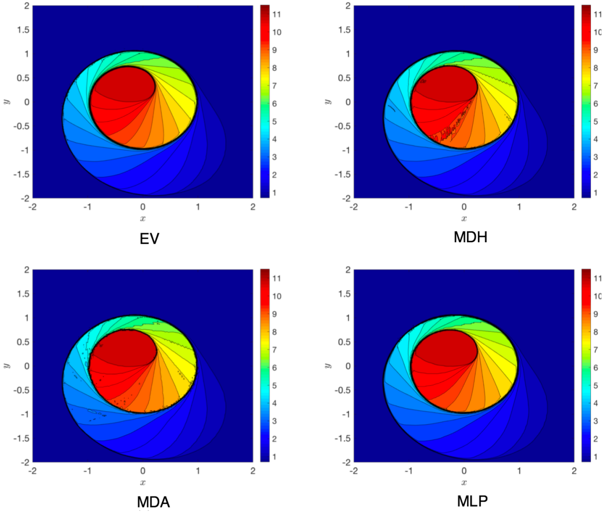
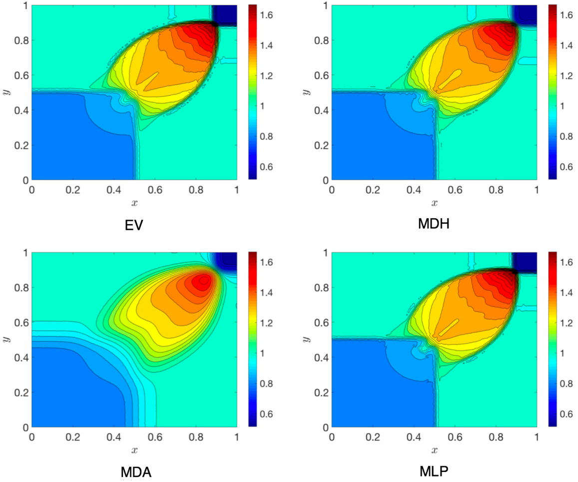
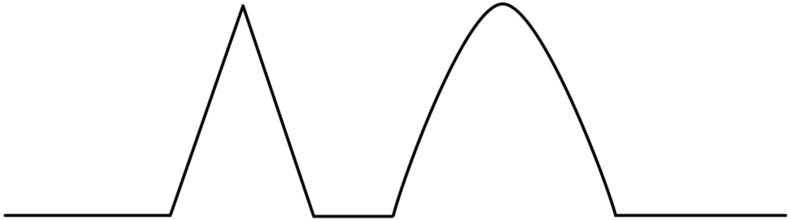


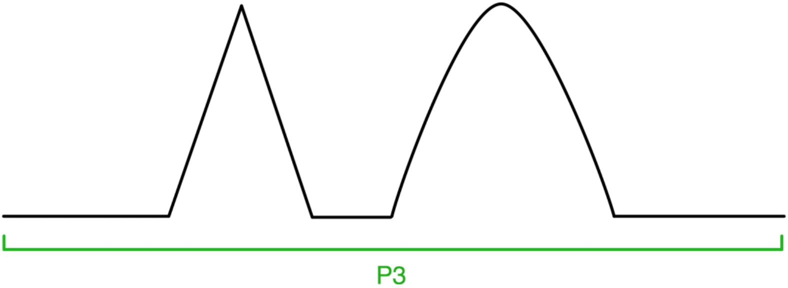
2D Euler equations: Riemann Problem config. 12 ($r = 3$)



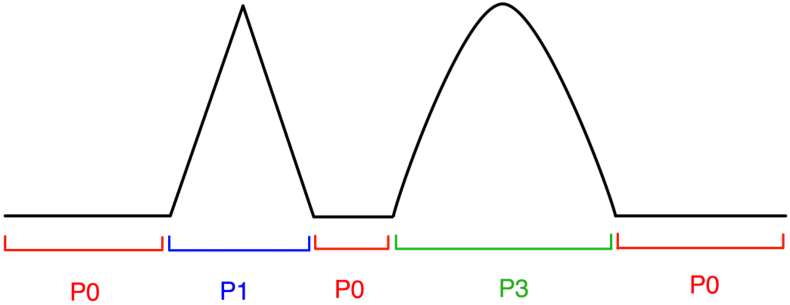
What else can we do?



p-adaption



In each element: $u_i^h(x) = \sum_{l=0}^{p_{max}} \hat{u}_l^i \phi_l(x)$

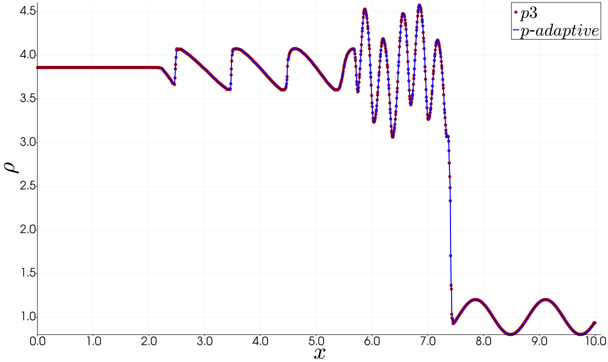


In each element: $u_i^h(x) = \sum_{l=0}^{p_{max}} \hat{u}_l^i \phi_l(x)$

Adapt P**:** $u_i^h(x) = \sum_{l=0}^{p_i} \hat{u}_l^i \phi_l(x), \;\; 0 \leq p_i \leq p_{max}$

Euler equations: Shu-Osher

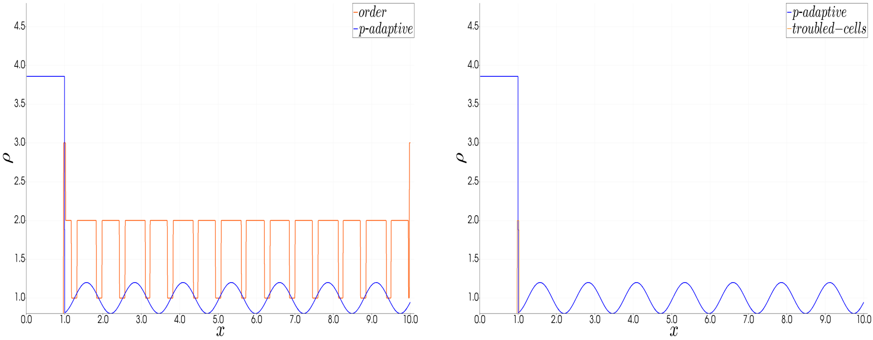
$T_f = 1.8, \quad N = 400$



Multi-dimensional WBAP limiter [Li et al., JCP, 2011] used near discontinuities.

Euler equations: Shu-Osher

$$T_f = 1.8, \quad N = 400$$



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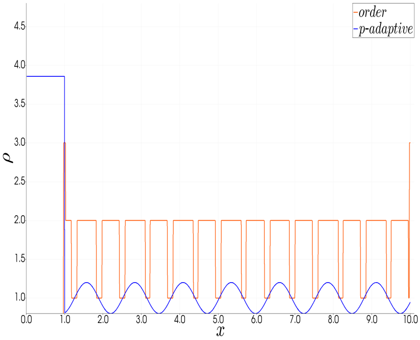

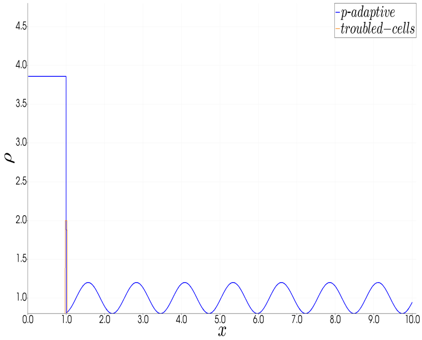

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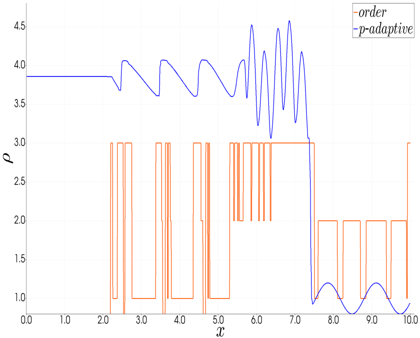


Multi-dimensional WBAP limiter [Li et al., JCP, 2011] used near discontinuities.

Assuming periodic boundary conditions on $[0, L]$

$$u(x,t) \approx u_h(x,t) = \sum_{n=-N}^{N} \tilde{u}_n(t) \exp\left(i\, n\, 2\pi \frac{x}{L}\right) \quad \longrightarrow \quad \text{global}$$

Define $2N+1$ collocation points (uniform mesh)

$$x_j = \frac{L}{2N+1} j, \quad j = 0, \ldots 2N$$

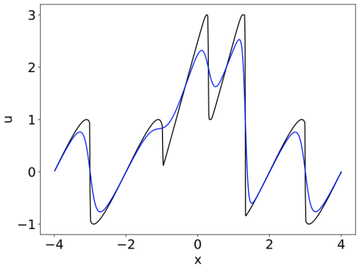
Solve for

$$\frac{\mathrm{d}\mathbf{u}(t)}{\mathrm{d}t} + \mathbf{D}\mathbf{u}(t) = 0$$

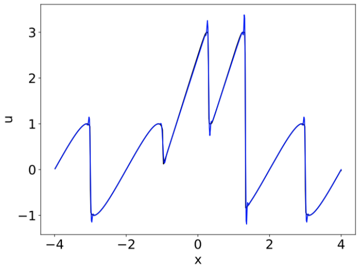
where $\mathbf{u}(t) = [u_h(x_0, t), \ldots, u_h(x_{2N}, t)]^\top$.

Handling Gibbs oscillations:

- Add hyper-viscosity
  - Second-order: cures oscillations but smears solution.
  - High-order: better accuracy but local oscillations remain.
- Post-processing exponential filter – same issue as above.
- Use Fourier-Padé reconstruction – oscillations still persist.



Filter order 2



Filter order 4

Handling Gibbs oscillations:

- Add hyper-viscosity
  - Second-order: cures oscillations but smears solution.
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- Post-processing exponential filter – same issue as above.
- Use Fourier-Padé reconstruction – oscillations still persist.

A simpler approach using MLPs

$$\frac{\mathrm{d}\mathbf{u}(t)}{\mathrm{d}t} + \mathbf{D}\mathbf{u}(t) = \mathbf{D}[\mu \otimes \mathbf{D}\mathbf{u}]$$

where μ varies locally based on local-regularity

Local viscosity with an MLP

Evaluate viscosity as a classification problem [Klöckner et al., 2011; Yu et al., 2018]

The network predicts the local regularity τ based on a seven-point stencil

τ	1	2	3	4
Reg.	Disc.	C0/C1	C1/C2	C2

Local viscosity with an MLP

Evaluate viscosity as a classification problem [Klöckner et al., 2011; Yu et al., 2018]

The network predicts the local regularity τ based on a seven-point stencil

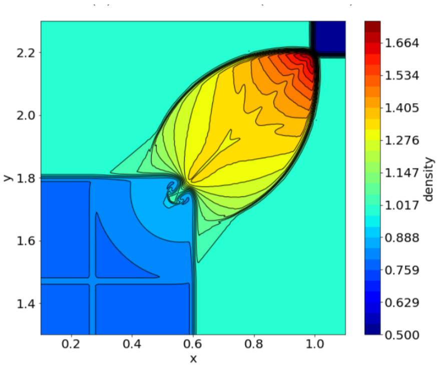
τ	1	2	3	4
Reg.	Disc.	C0/C1	C1/C2	C2

$$\mu = \mu_{max} \begin{cases} 1 - (\tau - 1)/2 & \text{if } 1 \leq \tau \leq 3 \\ 0 & \text{if } \tau = 4 \end{cases}$$

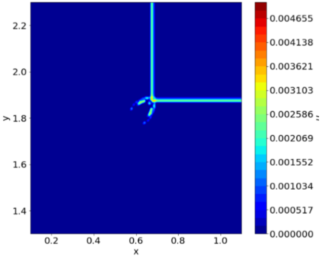
where $\mu_{max} = \frac{h}{2} \max(|f'(u)|)$.

2D Euler equations: Riemann problem config. 12

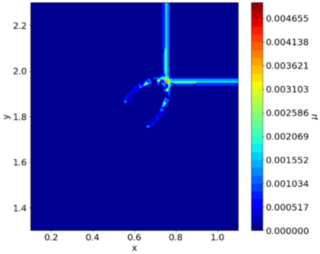
$$N_x = N_y = 250$$



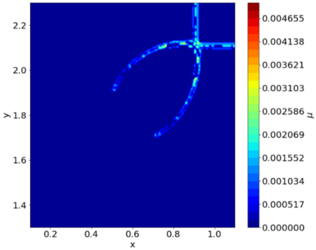
2D Euler equations: Riemann problem config. 12



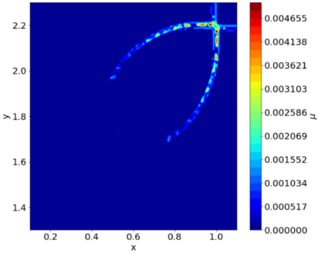
t=0.05



t = 0.1

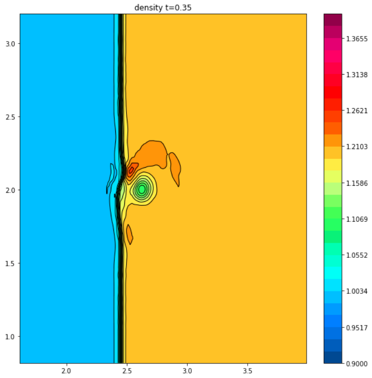


t=0.2



t = 0.25

$$N_x = N_y = 200$$


density t=0.35
3.0
2.5
2.0
1.5
1.0
2.0
2.5
3.0
3.5
1.3655
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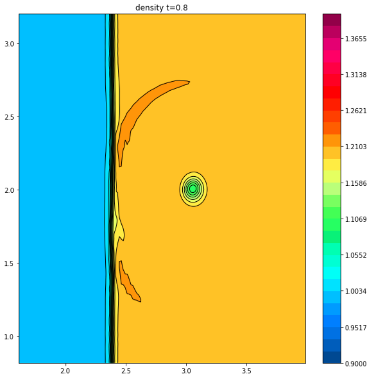
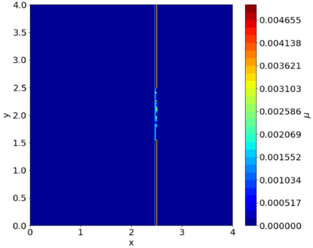
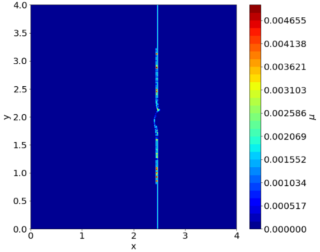
1.2621
1.2103
1.1586
1.1069
1.0552
1.0034
0.9517
0.9000


density t=0.8
3.0
2.5
2.0
1.5
1.0
2.0
2.5
3.0
3.5
1.3655
1.3138
1.2621
1.2103
1.1586
1.1069
1.0552
1.0034
0.9517
0.9000

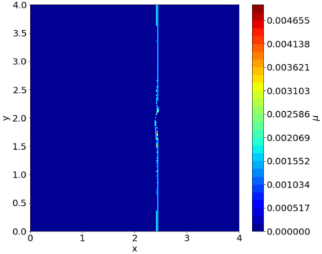
2D Euler equations: Shock-vortex



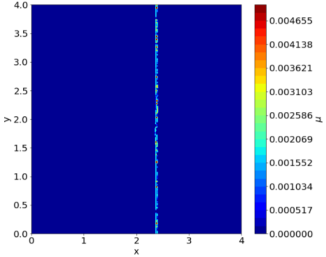
t=0.1



t = 0.35



t=0.5



t = 0.8

Conclusions

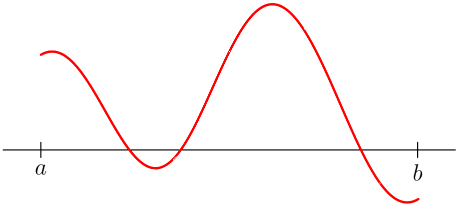
- Demonstrated that deep learning can be used as a surrogate – both for classification and regression.
- Networks trained (once) offline and then used for any model (conservation law).
- Useful in constructing methods free of problem-dependent parameters.
- Need to use domain-knowledge to construct training sets.
- Must have reasonable expectations from networks – cannot solve every problem!

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

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

*if possible

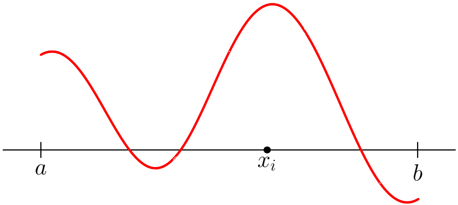
Generating training data



Data sampling is achieved by

- Choose a known function $u(x)$

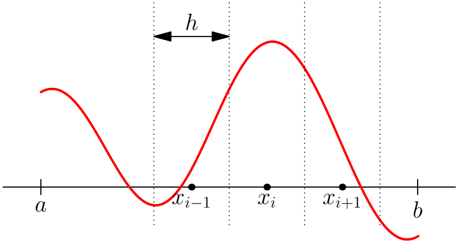
Generating training data



Data sampling is achieved by

- Choose a known function $u(x)$
- Pick a point x_i

Generating training data



Data sampling is achieved by

- Choose a known function $u(x)$
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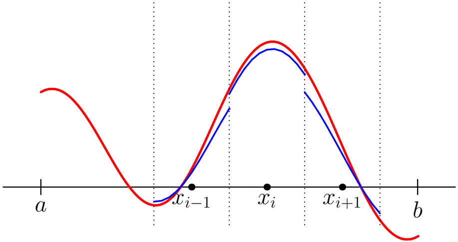
- Pick a cell size h and make stencil

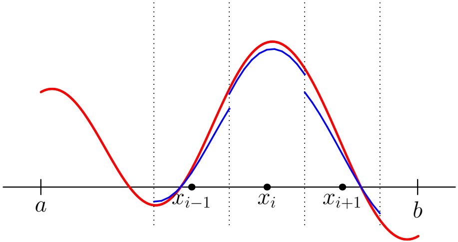
Generating training data



Data sampling is achieved by

- Choose a known function $u(x)$
- Pick a point x_i
- Pick a cell size h and make stencil
- Pick a degree r and approximate

Generating training data



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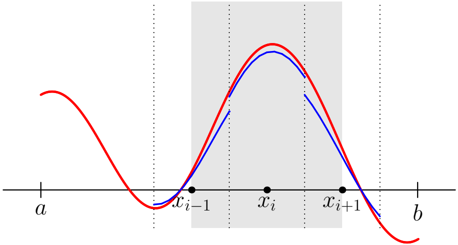
- Extract needed data $[\overline{u}_{i-1}, \overline{u}_i, \overline{u}_{i+1}, u^+_{i-\frac{1}{2}}, u^-_{i+\frac{1}{2}}]$

Generating training data



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