Using deep learning to overcome algorithmic bottlenecks

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NumHyp19
Malaga, 22 June 2019

École
polytecnique
fédérale
de Lausanne

In collaboration with ...

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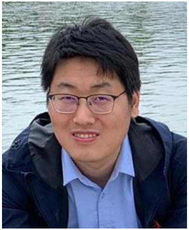
Director MCSS
EPFL



Qian Wang
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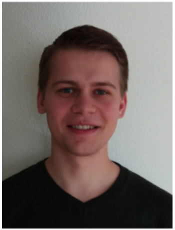
Niccolò Discacciati
Doctoral student
EPFL



Lukas Schwander
Master student
ETH Zürich

Deep learning in action

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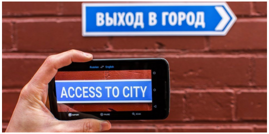

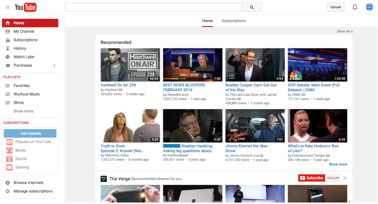

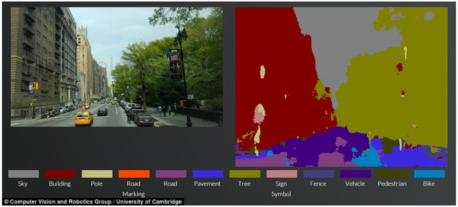

Blending deep learning and numerics

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- 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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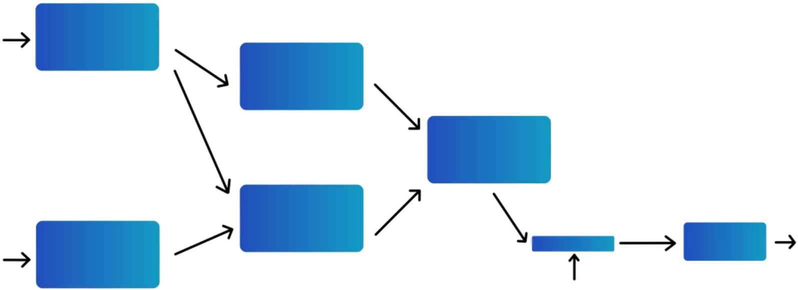

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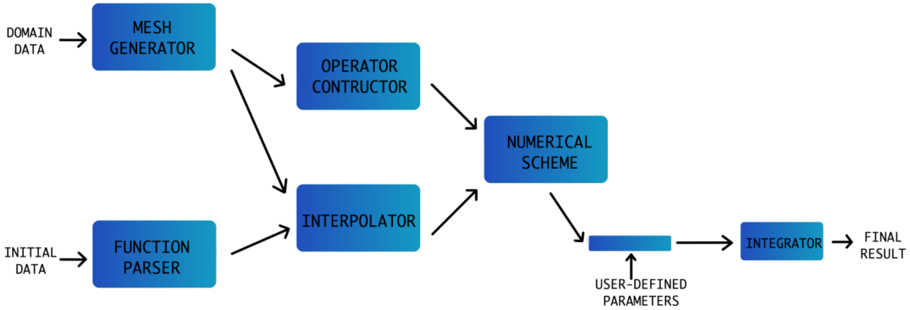

DOMAIN DATA
MESH GENERATOR
OPERATOR CONTRUCTOR
INITIAL DATA
FUNCTION PARSER
INTERPOLATOR
NUMERICAL SCHEME
USER-DEFINED PARAMETERS
INTEGRATOR
FINAL RESULT

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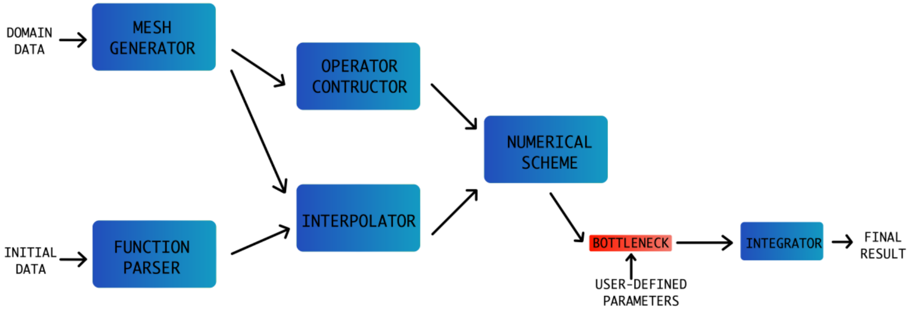
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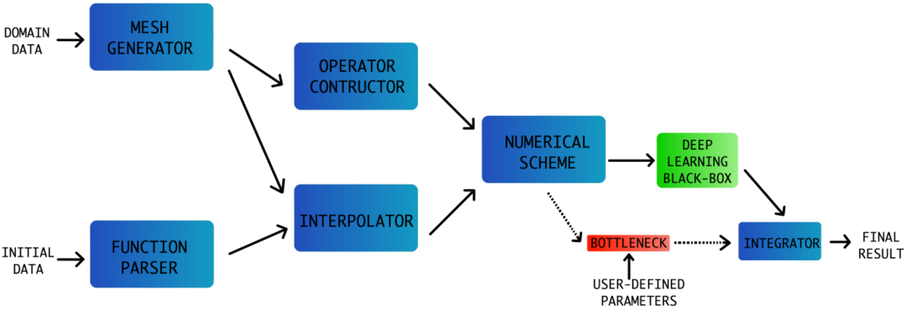
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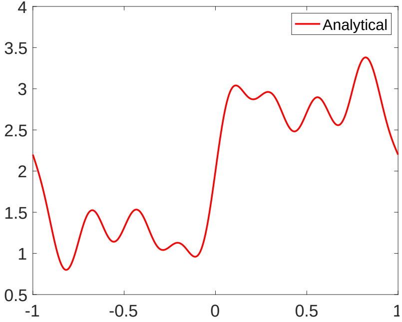
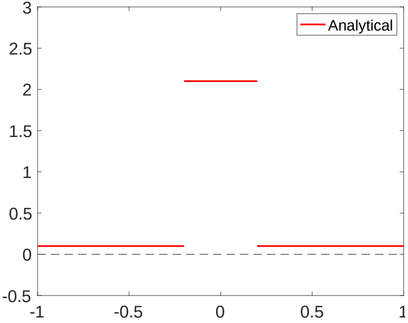
Today's bottleneck – controlling spurious oscillations!

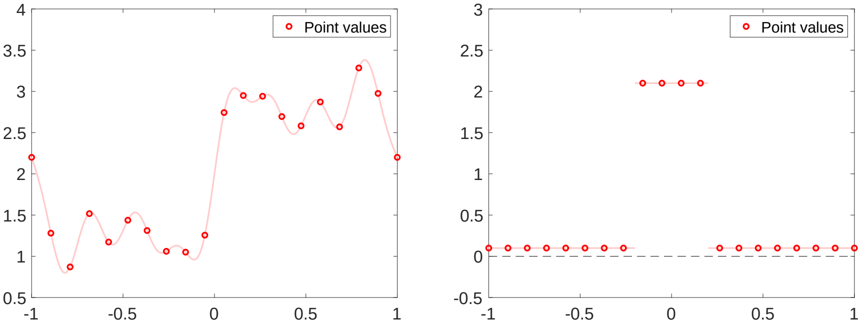




Today’s bottleneck – controlling spurious oscillations!

Approximating the function using a smooth basis

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



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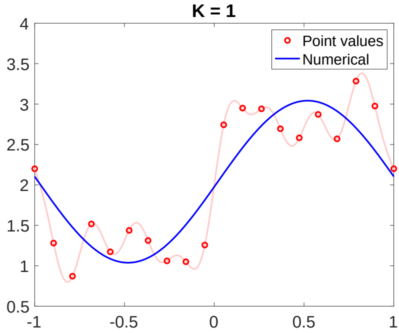

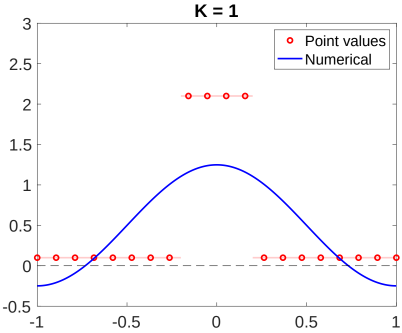

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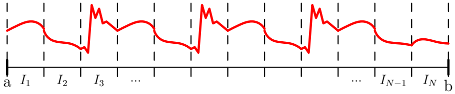
Mechanism to detect discontinuity/smoothness



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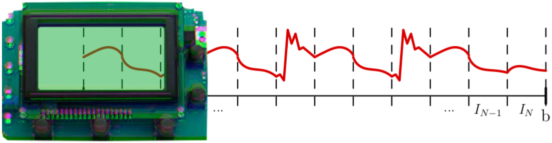

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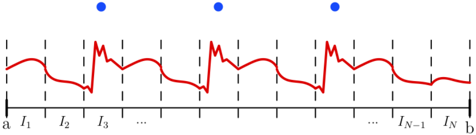

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- Limit the local solution
- Adapt the local polynomial/basis order
- Add artificial viscosity

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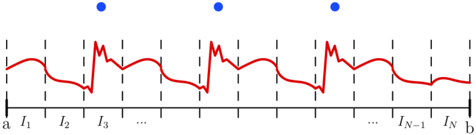

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Problems with existing methods

- Specification of problem-dependent parameters
- Computationally-expensive
- Too conservative

Overcome bottlenecks using deep learning

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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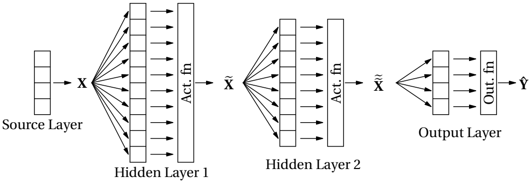
We train a suitable multilayer perceptron



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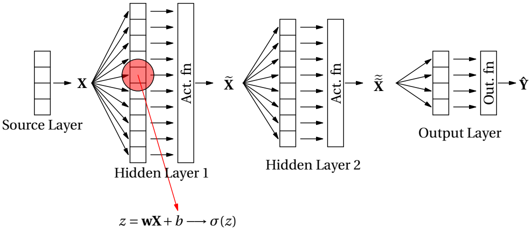

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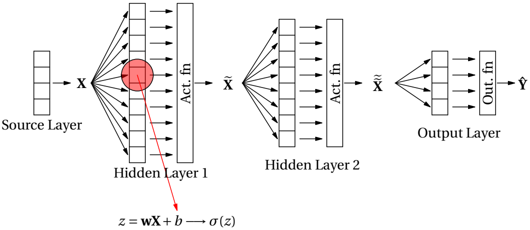

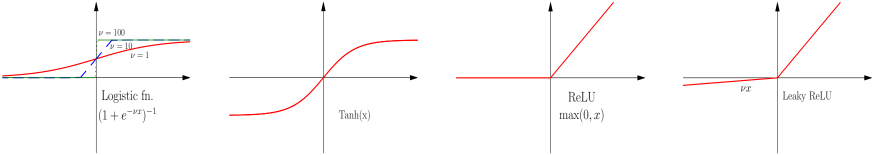

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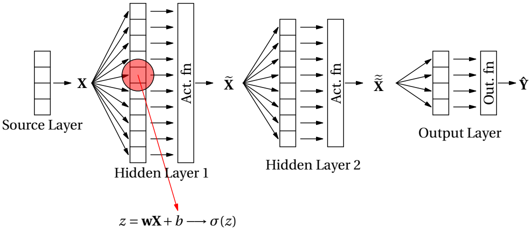

$$\hat{\mathbf{Y}} = \mathcal{O} \circ \sigma \circ H^L \circ \sigma \circ H^{L-1} \circ \ldots \circ \sigma \circ H^1(\mathbf{X}), \quad H^l(\tilde{\mathbf{X}}) = \mathbf{W}^l \tilde{\mathbf{X}} + \mathbf{b}^l$$

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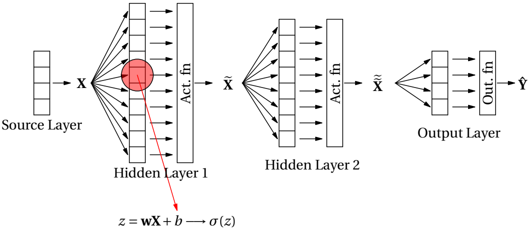

Find parameters $\theta = \{\mathbf{W}^l, \mathbf{b}^l\}$ that minimizes the loss function

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

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
- Your expectation from the network!

Some applications we will see today

- Troubled-cell detection (Hesthaven and R.)
- Artificial viscosity (Discacciati, Hesthaven and R.)
- p-adaption (Wang, Hesthaven and R.)
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The network is always trained offline!

Troubled-cell detector

Conservation laws

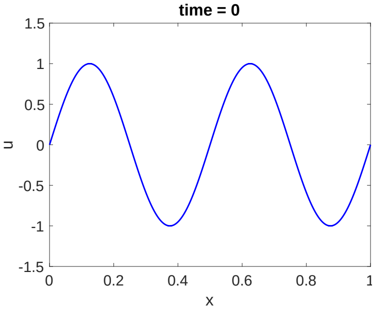
Consider

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

Non-linearity

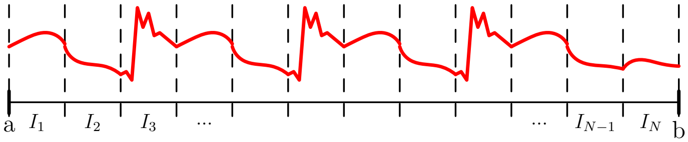
$\Longrightarrow$

Discontinuities in finite time



Detecting and limiting

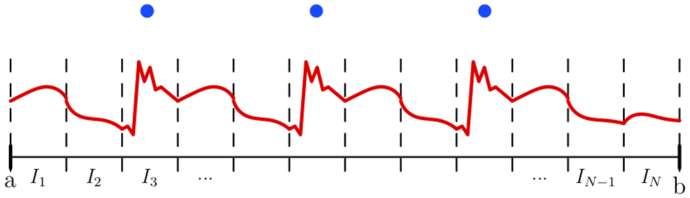
Strategy in the context of RKDG schemes:



Detecting and limiting

Strategy in the context of RKDG schemes:

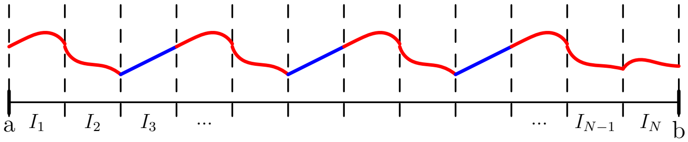
1. Find troubled-cells



Detecting and limiting

Strategy in the context of RKDG schemes:

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



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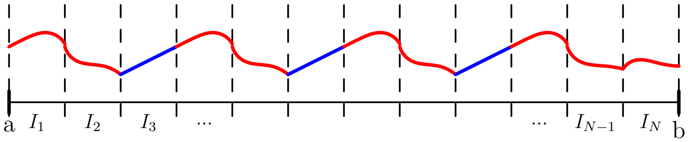

Issues:

- 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

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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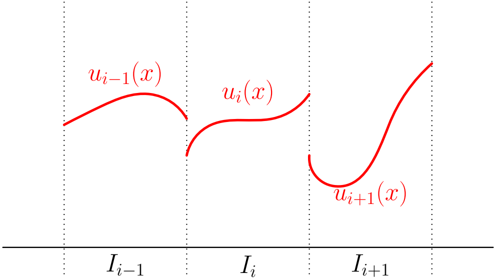
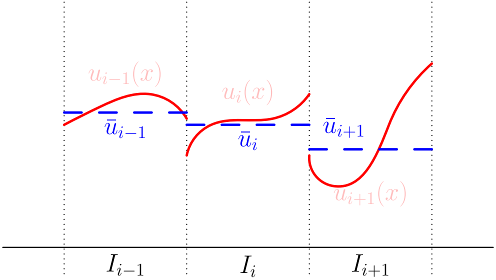


An MLP-based detector

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



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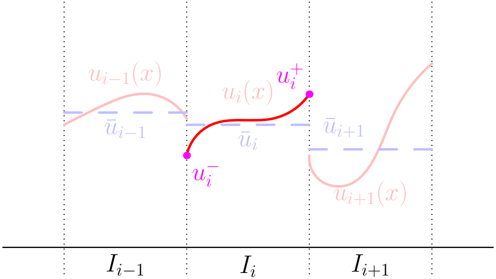
- Input $\mathbf{X} = [\overline{u}_{i-1}, \overline{u}_i, \overline{u}_{i+1}, u_i^-, u_i^+] \in \mathbb{R}^5$



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

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

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- 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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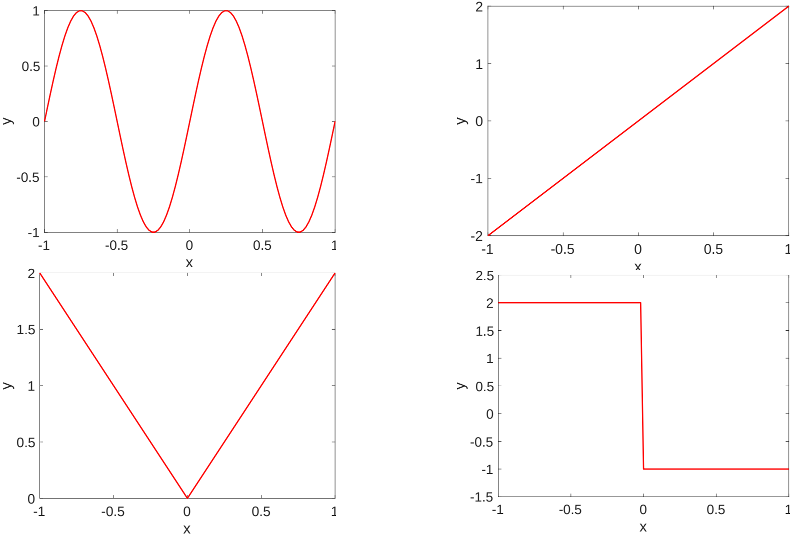
- Cost functional: L2 regularized cross-entropy

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

Generating training data

Types of functions used:



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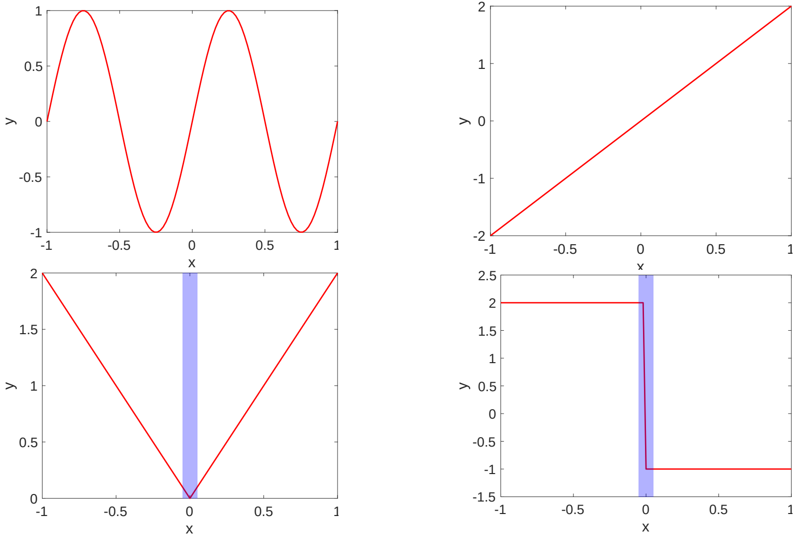

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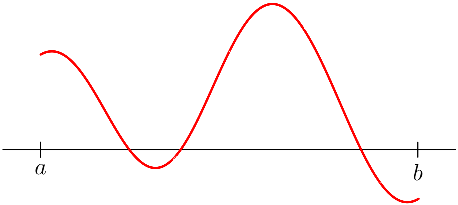
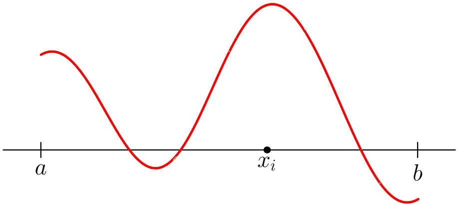


Data sampling is achieved by

- Choose a known function $u(x)$

Generating training data



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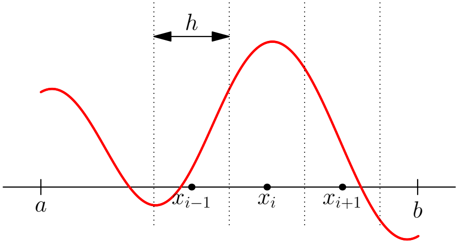

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- Choose a known function $u(x)$
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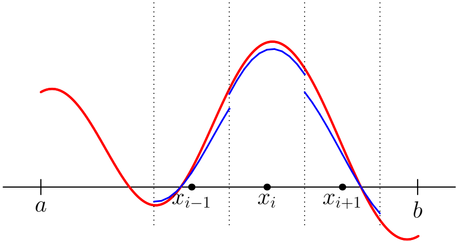
- Pick a cell size h and make stencil

Generating training data



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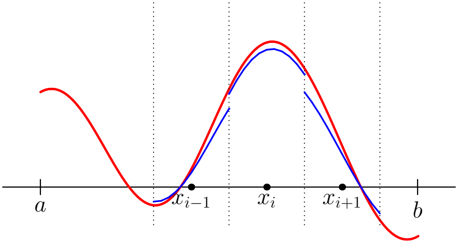

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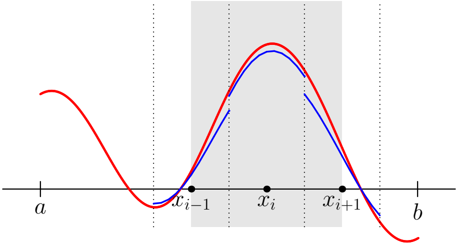
- Choose a known function $u(x)$
- Pick a point x_i
- Pick a cell size h and make stencil
- Pick a degree r and approximate
- Extract needed data $[\overline{u}_{i-1}, \overline{u}_i, \overline{u}_{i+1}, u^+_{i-\frac{1}{2}}, u^-_{i+\frac{1}{2}}]$

Generating training data



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

Numerical setup

- Comparison with TVB limiter by setting parameter M
- 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

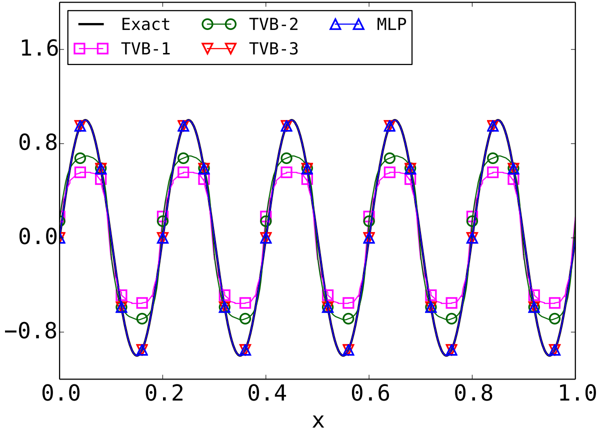
An artificial neural network as a troubled-cell indicator, by R. and Hesthaven; JCP vol. 367, pp. 166–191, 2018.

Detecting troubled-cells on two-dimensional unstructured grids using a neural network, by R. and Hesthaven, 2019 (submitted).

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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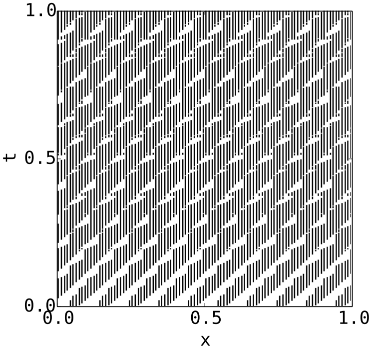
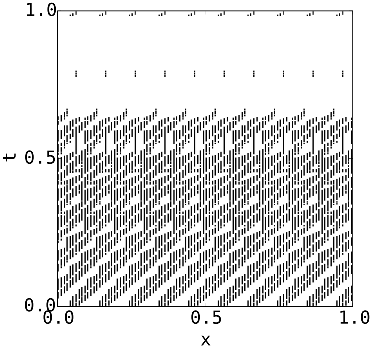


TVB-1

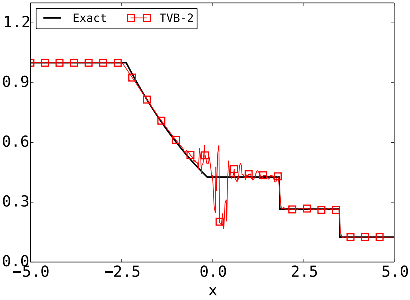


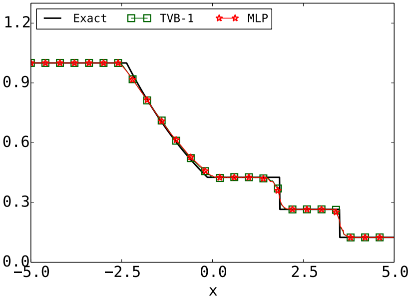
TVB-2

MLP and TVB-3 do not flag any cell

Euler equations: Sod shock tube

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

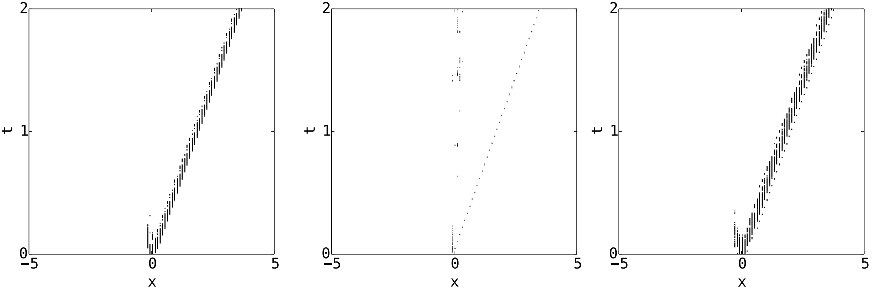




Loss of positivity with TVB-3

Euler equations: Sod shock tube

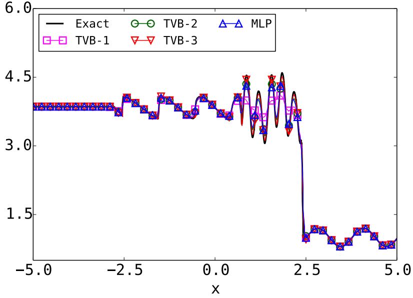
$$T_f = 2, \quad N = 100, \quad r = 4$$

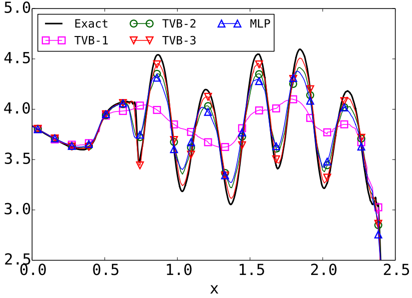


TVB-1 **TVB-2** **MLP**

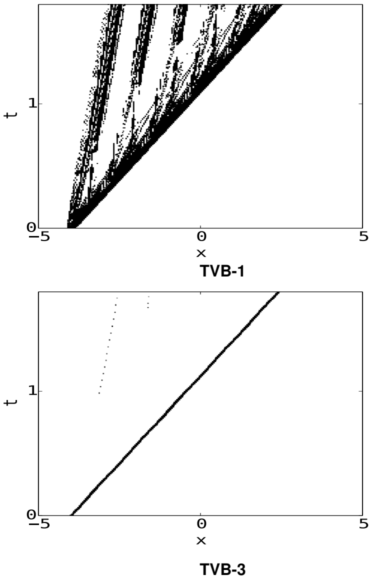
1D Euler equations: Shu-Osher problem

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



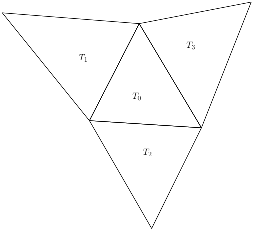


1D Euler equations: Shu-Osher problem



Extension to 2D

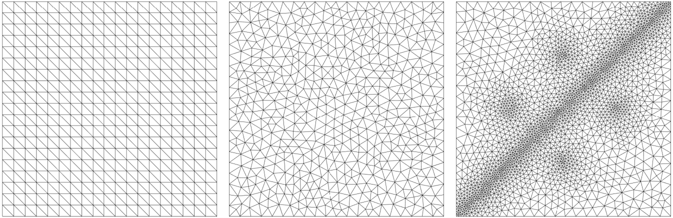
We consider unstructured triangular grids



MLP network with 5 hidden layers of width 20 each

Extension to 2D

We consider unstructured triangular grids

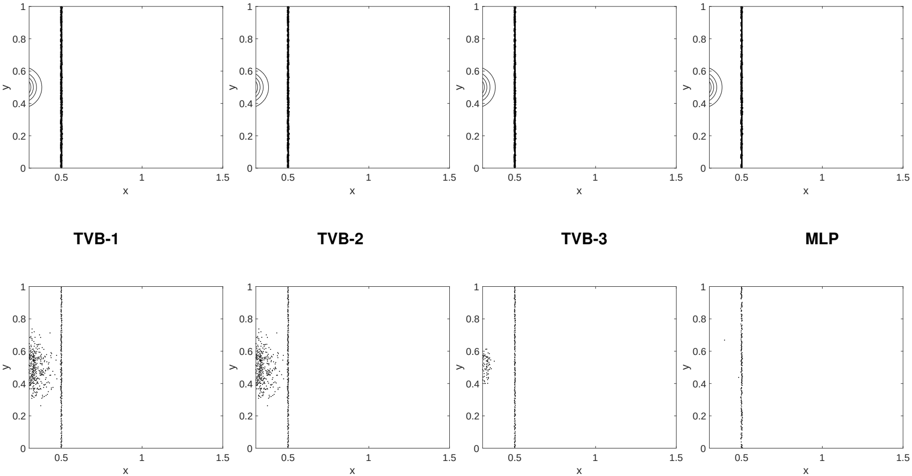


MLP network with 5 hidden layers of width 20 each
Training data constructed by:

- 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.

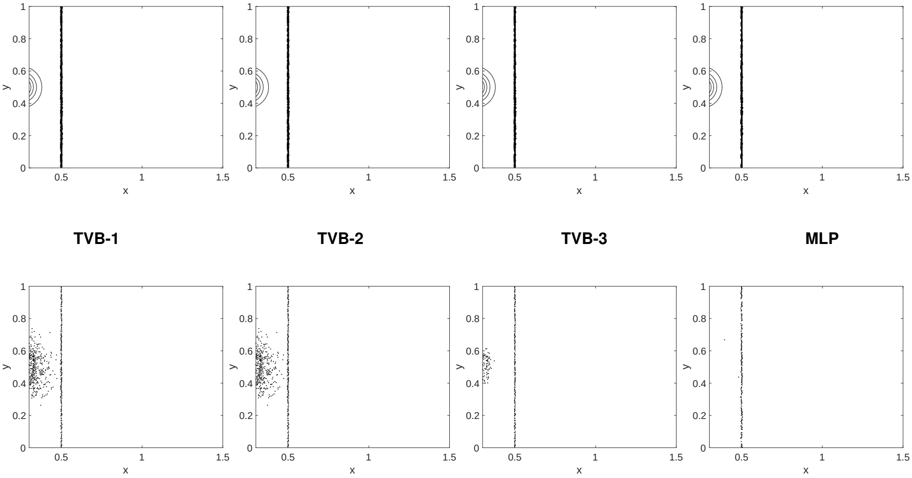
2D Euler equations: Shock-vortex

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



2D Euler equations: Shock-vortex

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



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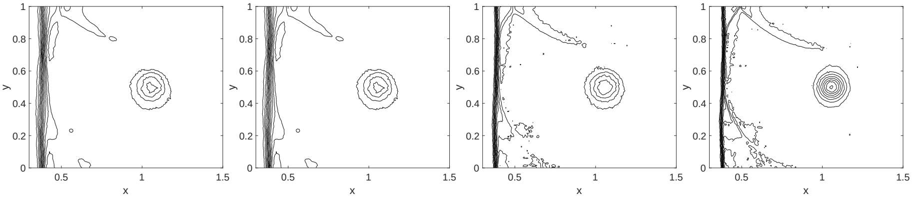
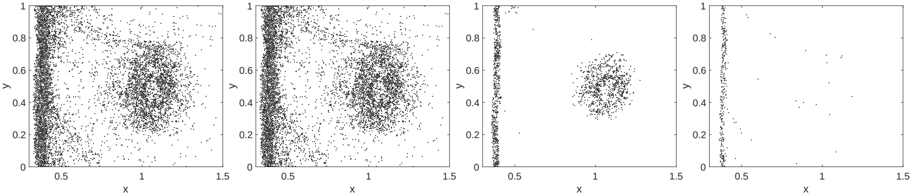


TVB-1 **TVB-2** **TVB-3** **MLP**



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

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- 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

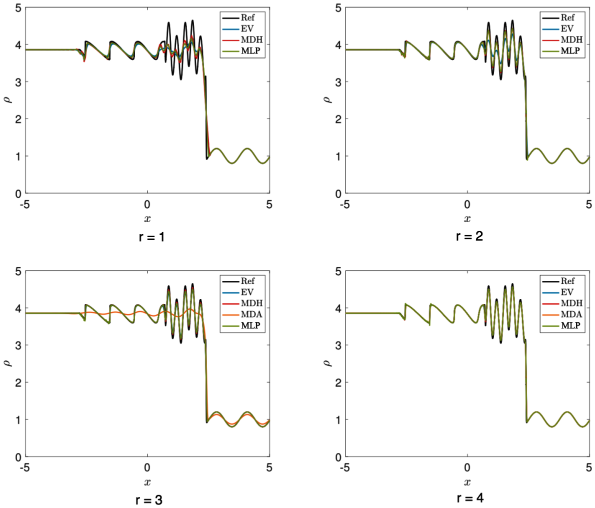
Training/validation sets:

- 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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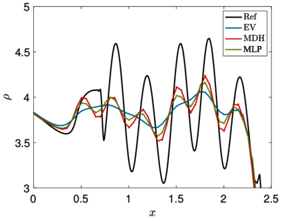
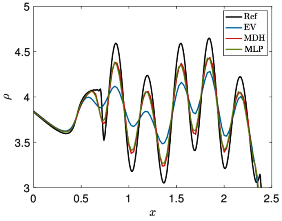
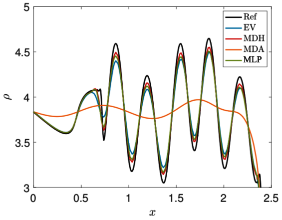


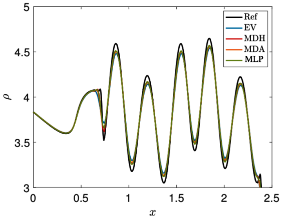
r = 1



r = 2



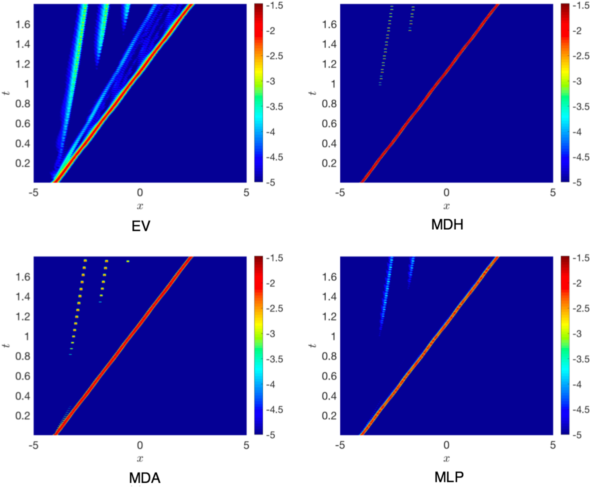
r = 3



r = 4

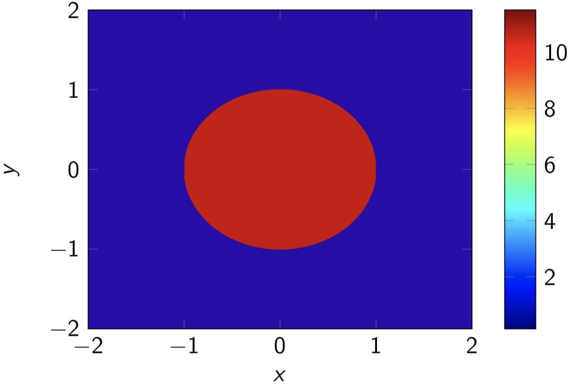
1D Euler equations: Shu-Osher

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



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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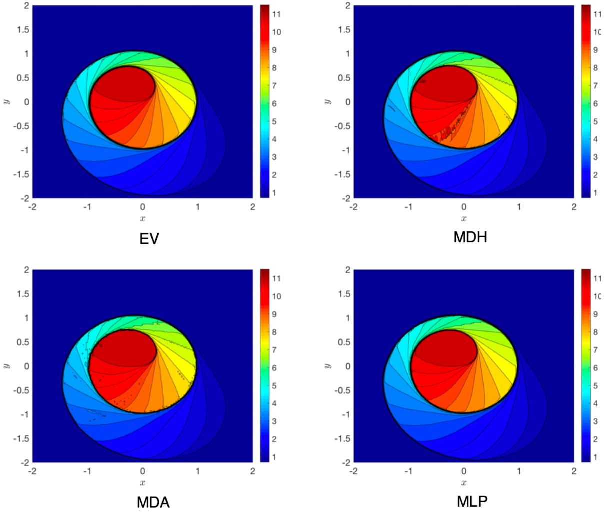
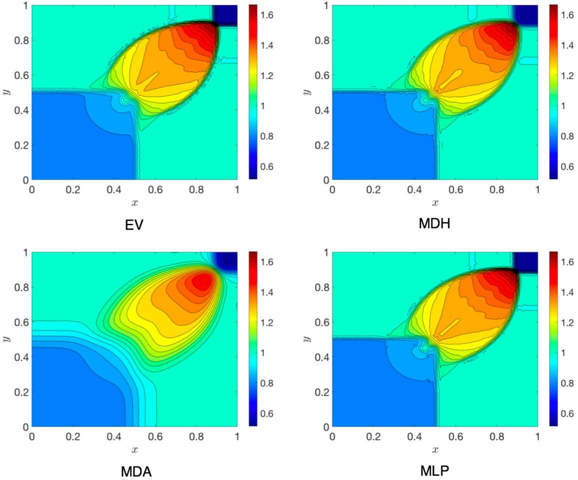
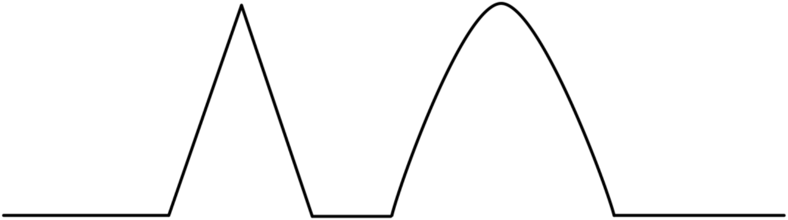


2D Euler equations: Riemann Problem config. 12 ($r = 3$)

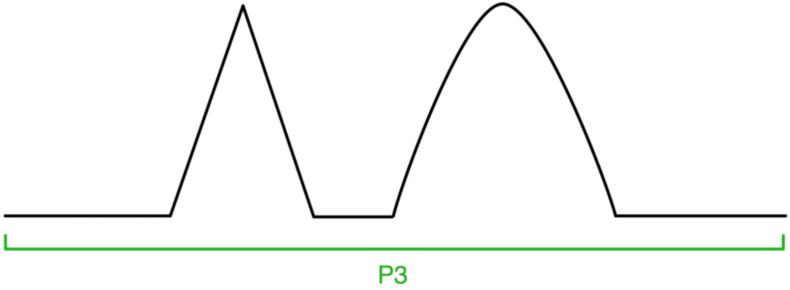


Learning p-adaption

Idea of p-adaption

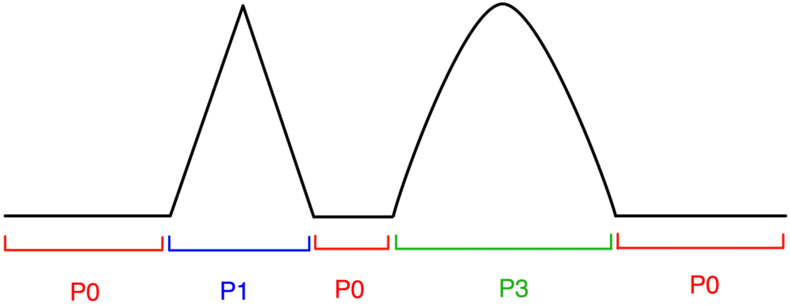


Idea of p-adaption



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

Idea of p-adaption



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

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

How to choose p?

Existing methods:

- p-refinement indicator based on a posteriori estimator [Naddei et al., JCP, 2019]
- Dynamic p-adaption based on flow gradients [Burbeau and Sagaut, Comp. Fluids, 2005; Kubatko et al., Comp. Meth. App. Mech. Engg., 2009]

Dependent on problem specific parameters

How to choose p?

MLP based p refinement for a pre-defined p_{max}:

- **Input:** Full modal coefficients of 3-cell patch

$$\mathbf{X} = [\hat{u}_0^{i-1}, ..., \hat{u}_{p_{max}}^{i-1},\ \ \hat{u}_0^{i}, ..., \hat{u}_{p_{max}}^{i},\ \ \hat{u}_0^{i+1}, ..., \hat{u}_{p_{max}}^{i+1}] \in \mathbb{R}^{3(p_{max}+1)}$$

- **Output:** $\hat{\mathbf{Y}} \in \mathbb{R}^{p_{max}+2}$, where

$$\begin{aligned} \hat{\mathbf{Y}}_j,\ 0 \le j \le p_{max} \quad &\longrightarrow \quad \text{order } p_j \ \ \text{(smooth)} \\ \hat{\mathbf{Y}}_{p_{max}+1} \quad &\longrightarrow \quad \text{discontinuity} \end{aligned}$$

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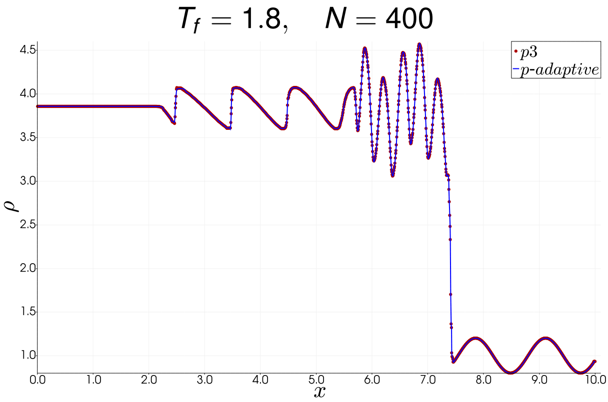
For $p_{max} = 3$:

- MLP with 5 hidden layers of width 20 each.
- Trained on samples generated from polynomials and generalized (linear) Riemann data.

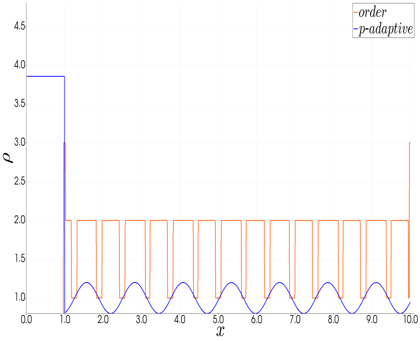
Euler equations: Shu-Osher

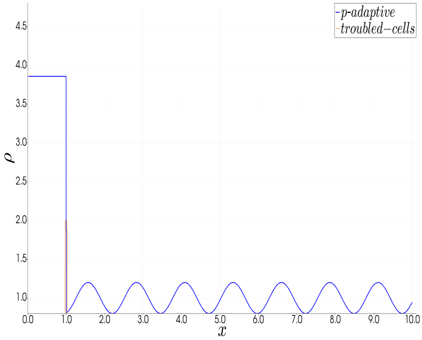


Multi-dimensional WBAP limiter [Li et al., JCP, 2011] used near discontinuities.

Euler equations: Shu-Osher

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





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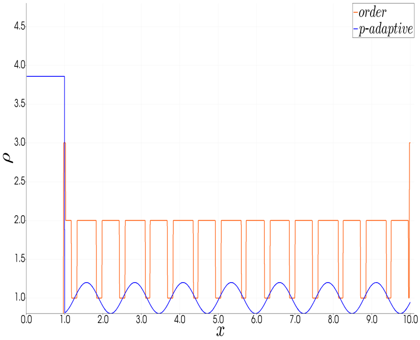

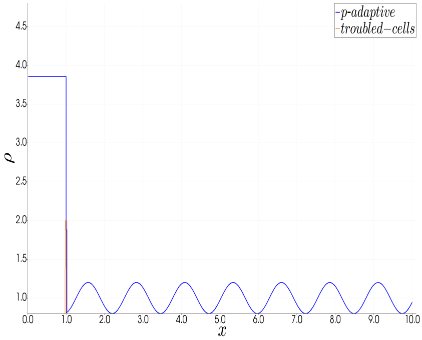

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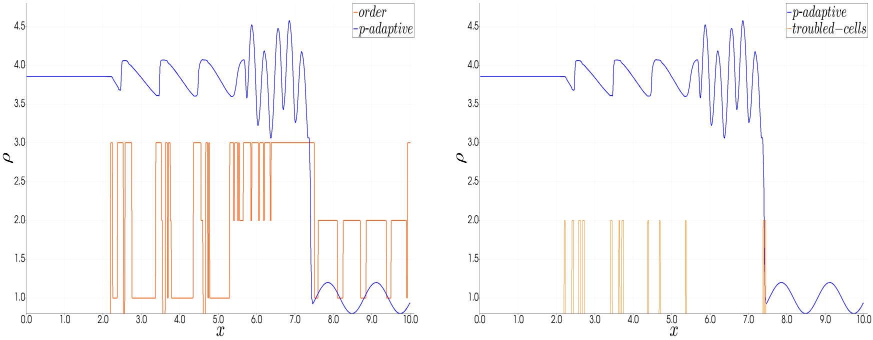

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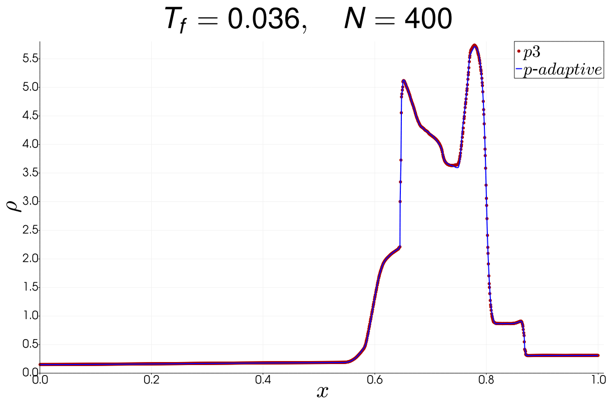
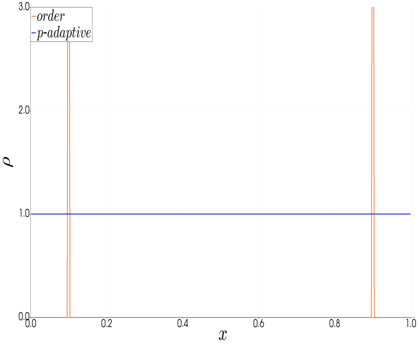
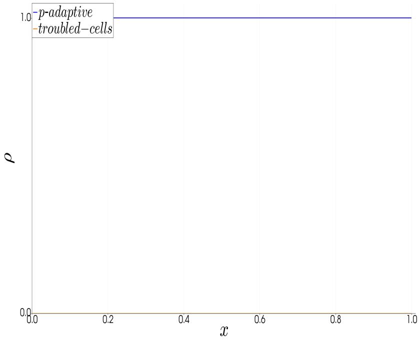
Euler equations: Blastwave



Euler equations: Blastwave

$$T_f = 0.036, \quad N = 400$$





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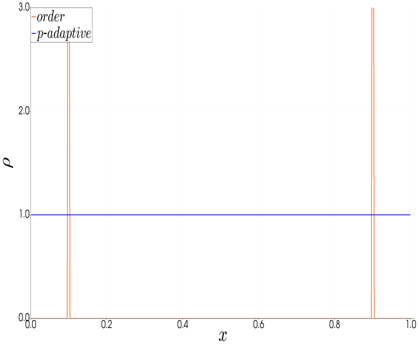

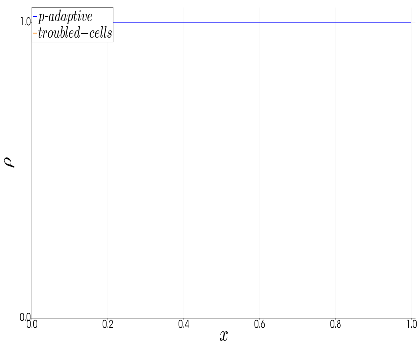

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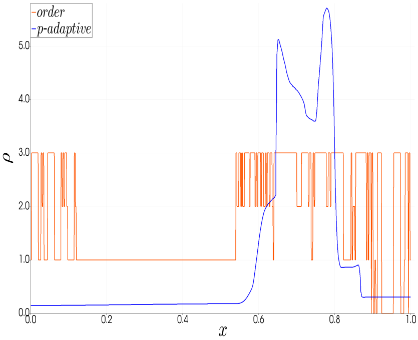

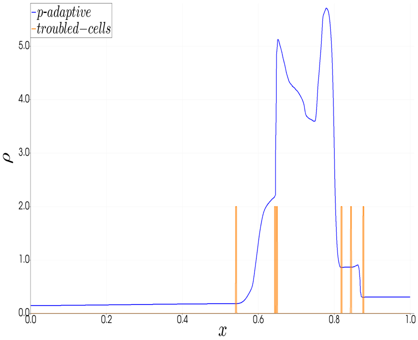

Computational cost

Table: Computational cost for the Blast Waves problem. Unit of cost: second (s).

	total	p-adaption	residual	limiter	time-stepping
p3	155.17	0	31.68	116.26	6.44
p-adaptive	246.12	113.98	14.69	113.52	3.34

Table: Computational cost for the Shu-Osher problem. Unit of cost: second (s).

	total	p-adaption	residual	limiter	time-stepping
p3	101.76	0	21.00	76.20	4.05
p-adaptive	165.72	75.57	11.10	75.88	2.71

Local smoothening for global schemes

Fourier spectral methods

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

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

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

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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

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

Local viscosity with an MLP

Network architecture:

- Input: $\mathbf{X} \in \mathbb{R}^7$; Output: $\hat{\mathbf{Y}} \in \mathbb{R}^4$
- 3 hidden layers of width 16 each
- A dropout layer is used for regularization

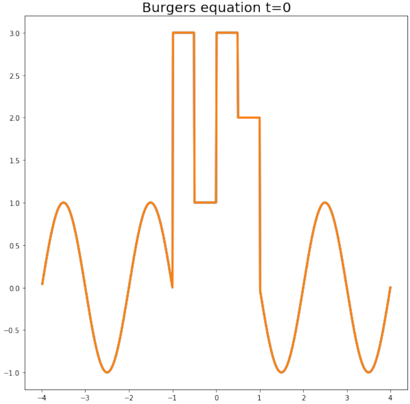
Training/validation data sets created used functions of varying regularity.

Viscosity used along with a high-order exponential filter

- order 12 if $\tau = 1, 2, 3$
- order 14 if $\tau = 4$

Burgers equation

$$N = 600, \quad T_f = 0.4$$



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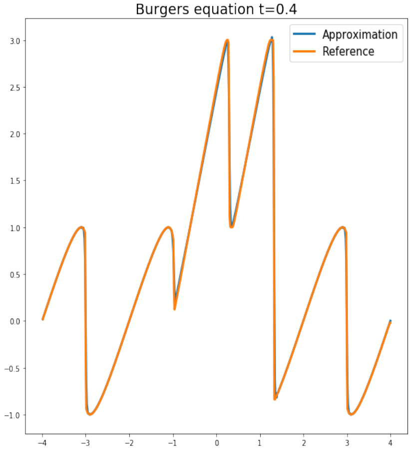
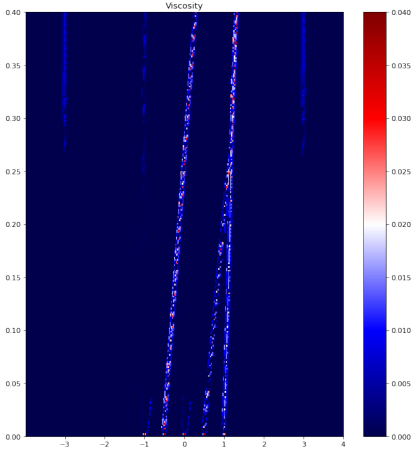
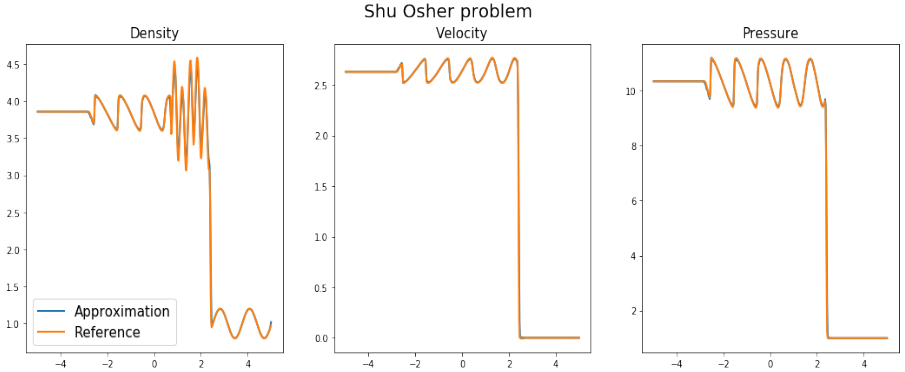




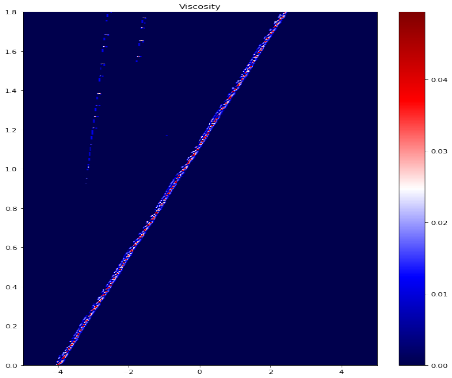
Euler equations: Shu-Osher

$$N = 600, \quad T_f = 1.8$$



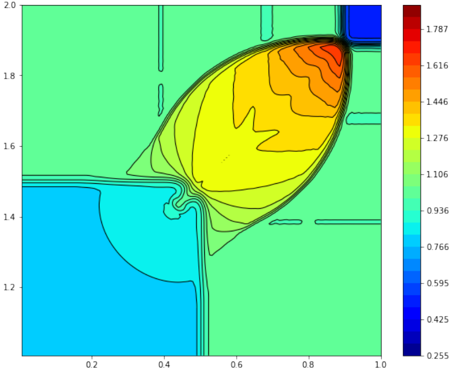
Euler equations: Shu-Osher

$$N = 600, \quad T_f = 1.8$$



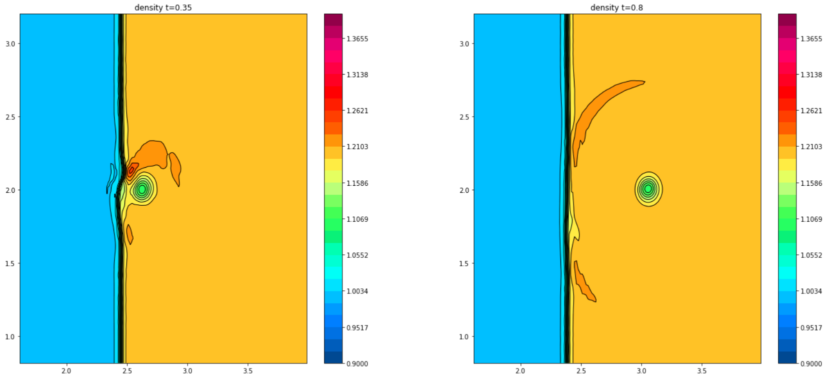
2D Euler equations: Riemann problem config. 12

$$N_x = N_y = 100$$



2D Euler equations: Shock-vortex

$$N_x = N_y = 200$$



Conclusions and future scope

- Demonstrated that deep learning can be used as a surrogate – both for classification and regression
- Networks trained (once) offline and then used for any conservation law
- Useful in constructing methods free of problem-dependent parameters
- Need to use domain-knowledge to construct training sets

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Troubled-cell detector: what next?

- Extension to 3D
- Network for general hybrid meshes – how to handle variable input size?
- Possible to estimate angle of discontinuity?

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Artificial viscosity: what next?

- Extension to 3D and hybrid grids
- Explore more sophisticated subcell resolution based on network prediction
- Automate learning – perhaps using reinforcement learning

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p-**adaption:** what next?

- Extension to higher-dimensions and hybrid grids
- Use network for *hp*-adaption

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Local viscosity for global methods: what next?

- Test on non-uniform grids
- Explore similar ideas for ROM.

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

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*if possible