A data-driven approach to predict artificial viscosity in high-order solvers

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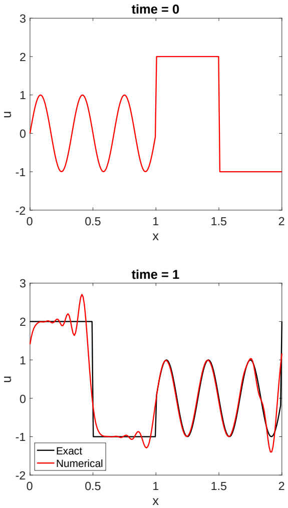
Conservation laws and Gibbs oscillations



Consider the conservation law

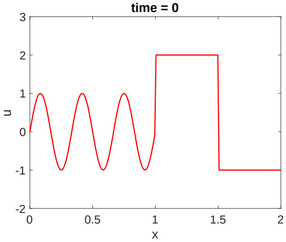
$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = 0$$

Discontinuity + high-order solver

$\Downarrow$

Spurious oscillations

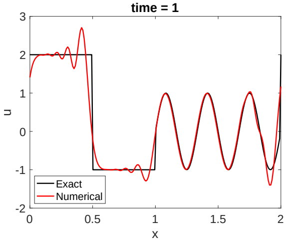
Conservation laws and Gibbs oscillations



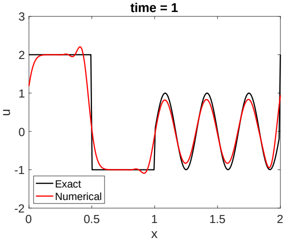
Consider the modified PDE

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

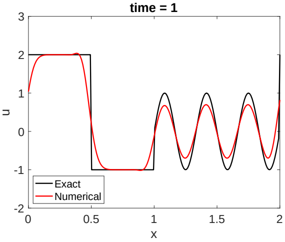
- Where to introduce viscosity?
- How much viscosity?
- Prescription without tuneable parameters?



$\mu = 0$



$\mu = 5e-4$



$\mu = 1e-3$

Outline

- Deep neural networks
- Artificial viscosity for DG schemes – regression networks
- Artificial viscosity for global schemes – classification networks
- Conclusion

Deep neural networks

Deep neural networks: supervised learning

- Consider an unknown function

$$\boldsymbol{F} : \boldsymbol{x} \in \Omega_x \mapsto \boldsymbol{y} \in \Omega_y$$

and a given 'labelled' dataset $\mathcal{S} = \{(\boldsymbol{x}_i, \boldsymbol{y}_i)\}_{i=1}^{N}$.

- A neural network is a parametrized mapping

$$\boldsymbol{F}_{\boldsymbol{\theta}} : \Omega_x \to \Omega_y$$

typically formed by alternating composition

$$\boldsymbol{F}_{\boldsymbol{\theta}} := \mathcal{A}^{(L+1)}_{\boldsymbol{\theta}_{L+1}} \circ \rho \circ \mathcal{A}^{(L)}_{\boldsymbol{\theta}_{L}} \circ \rho \circ \mathcal{A}^{(L-1)}_{\boldsymbol{\theta}_{L-1}} \circ \cdots \circ \rho \circ \mathcal{A}^{(1)}_{\boldsymbol{\theta}_{1}}$$

where

$$\begin{aligned} \boldsymbol{\theta} = \{\boldsymbol{\theta}_k\}_{k=1}^{L} &\longrightarrow \text{ trainable weights and biases of the network} \\ \mathcal{A}^{(k)}_{\boldsymbol{\theta}_k} &\longrightarrow \text{ parametrized affine transformation} \\ \rho &\longrightarrow \text{ non-linear activation function} \end{aligned}$$

AIM: Determine $\boldsymbol{\theta}$ such that $\boldsymbol{F}_{\boldsymbol{\theta}} \approx \boldsymbol{F}$.

Deep neural networks: supervised learning

- Consider a suitable measure

$$\mu : \Omega_y \times \Omega_y \to \mathbb{R}$$

s.t. $\mu(\boldsymbol{y}, \boldsymbol{F}_{\boldsymbol{\theta}}(\boldsymbol{x}))$ is the prediction error/discrepancy for $(\boldsymbol{x}, \boldsymbol{y}) \in \mathcal{S}$.

- Define the loss/objective function

$$\Pi(\boldsymbol{\theta}) = \frac{1}{N} \sum_{i=1}^{N} \mu(\boldsymbol{y}_i, \boldsymbol{F}_{\boldsymbol{\theta}}(\boldsymbol{x}_i))$$

Solve the non-convex optimization problem

$$\boldsymbol{\theta}^* = \arg\min_{\boldsymbol{\theta}} \Pi(\boldsymbol{\theta})$$

Then $\boldsymbol{F}_{\boldsymbol{\theta}^*} \approx \boldsymbol{F}$

- Also need to tune network hyper-parameters, such as:
  • Width • Depth (L) • Activation function ρ • Optimizer • Loss function
- Regression vs classification.

Artificial viscosity for DG schemes

Artificial viscosity for DG schemes

For the modified conservation law

$$\frac{\partial u}{\partial t} + \nabla \cdot \boldsymbol{f} = \nabla \cdot \boldsymbol{g}, \quad \boldsymbol{g} = \mu \boldsymbol{q}, \quad \boldsymbol{q} = \nabla u$$

Solution approximated on each element D_k, $\Omega = \bigcup_{k=1}^{K} D_k$

$$u(\boldsymbol{x}, t) \approx u_h(\boldsymbol{x}, t) = \bigoplus_{k=1}^{K} u_h^k(\boldsymbol{x}, t), \quad u_h^k(\boldsymbol{x}, t) = \sum_{i=1}^{N} u_i^k(t) \phi_i^k(\boldsymbol{x})$$

where $\{\phi_i^k\}_{i=0}^N$ is a basis of order m.

Solve ODE for nodal/modal coefficient vector $\boldsymbol{u}^k = [u_1^k, ..., u_N^k]^\top$

$$\frac{\mathrm{d}\boldsymbol{u}^k}{\mathrm{d}t} = \boldsymbol{L}(\boldsymbol{u}, \mu), \quad 1 \leq k \leq K$$

Artificial viscosity for DG schemes

Popular viscosity models:

- Highest modal decay (MDH) model [Persson and Peraire, 2006]
- Averaged modal decay (MDA) model [Klökner et al., 2011]
- Entropy viscosity (EV) model [Guermond et al., 2011]

Require prescription of problem-dependent parameters!

If parameters are not appropriately selected:

- Re-appearance of spurious oscillations.
- Excessive smearing in smooth regions.

Idea: Let a neural network analyse the local solution and estimate a local μ .

Network-based viscosity estimator

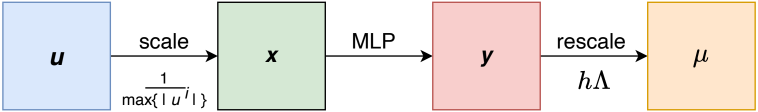
$$\text{Target function } \boldsymbol{F} : \text{solution in } D_k \xrightarrow{\text{regression}} \mu \text{ in } D_k$$

Network architecture:

- Input $\boldsymbol{x} \in \mathbb{R}^N$: nodal values of u in D_k, $N = N(m)$.
- Architecture: MLP with 5 hidden layers and Leaky ReLU activation.
- Output $\boldsymbol{y} \in \mathbb{R}^N$: nodal values of μ in D_k.

MLP: Multilayer perceptron / fully-connected neural network.

Scaling is important for generalization:



h : local mesh size $\qquad \Lambda = \max\{ |\boldsymbol{f}'(u)| \}$

Network-based viscosity estimator

What about the training set?

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

Note:

- The network for a given m is trained offline.
- Same network for any conservation law.
- No further tuning required after training.

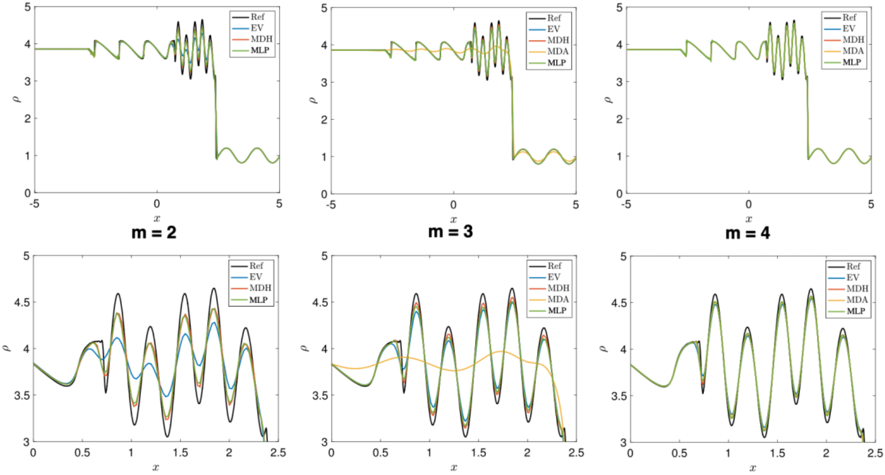
The trained network can be interpreted as an automatic, dynamic and local adaptor between MDH, MDA and EV.

Controlling oscillations in high-order Discontinuous Galerkin schemes using artificial viscosity tuned by neural networks, by Discacciati, Hesthaven and R.; JCP, 2020.

Numerical setup

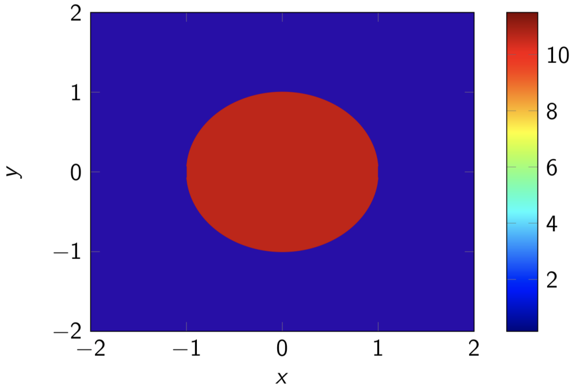
- DG scheme with Legendre basis (Jacobi polynomials in 2D).
- Triangular mesh in 2D.
- Local Lax-Friedrich numerical flux.
- Appropriate proxy variable for systems (ρ for Euler eqns.)
- Time integration with 5 stage 4th-order low-storage explicit Runge-Kutta scheme.
- Parameters for standard methods are fixed.

1D Euler equations: Shu-Osher (density based μ prediction)



2D KPP equations: Rotating wave

$$\boldsymbol{f}(u) = (\sin u, \cos u), \quad m = 4$$



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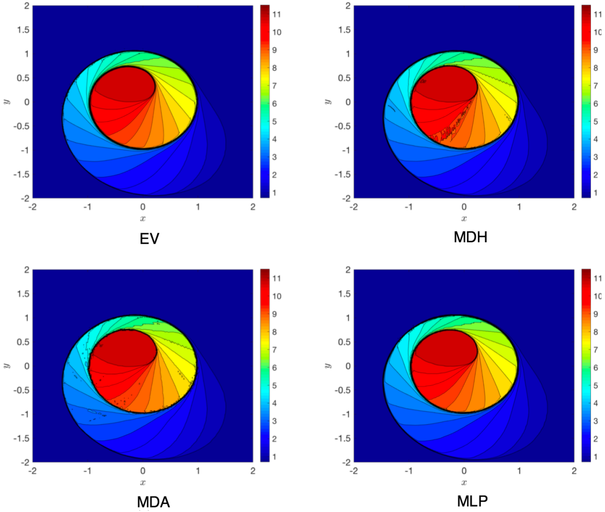
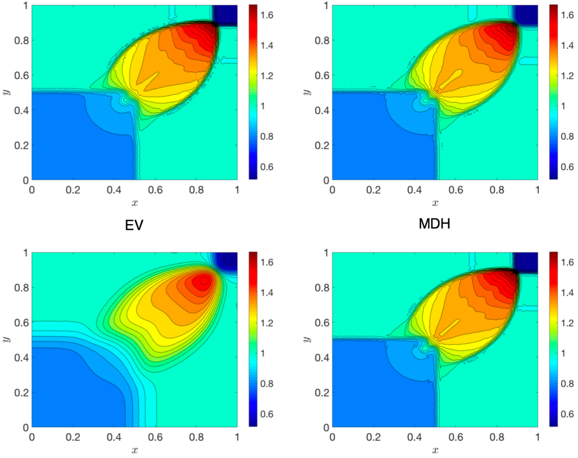


2D Euler equations: Riemann Problem config. 12

$m = 3$



EV MDH

MDA MLP

Artificial viscosity for global schemes

Consider the conservation law (periodic)

$$\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = 0, \quad x \in [0, 2\pi]$$

Define N collocation points (uniform mesh) $x_j = \frac{2\pi}{N} j, \;\; j = 0, ...N-1$.

Using DFT, approximate the solution using the interpolant

$$u(x,t) \approx u_h(x,t) = \frac{1}{2\pi} \sum_{k=-N/2}^{N/2} \hat{u}_k(t) e^{ikx}, \quad \hat{u}_k(t) = \frac{2\pi}{N} \sum_{j=0}^{N-1} u_h(x_j, t) e^{-ikx_j}$$

Solve for the coefficients

$$\begin{aligned} \frac{\mathrm{d}\boldsymbol{u}_h(t)}{\mathrm{d}t} + \boldsymbol{D}\boldsymbol{f}_h(t) &= 0 \\ \boldsymbol{u}_h(t) &= [u_h(x_0,t), ..., u_h(x_{N-1},t)]^\top \\ \boldsymbol{f}_h(t) &= [f(u_h(x_0,t)), ..., f(u_h(x_{N-1},t))]^\top \end{aligned}$$

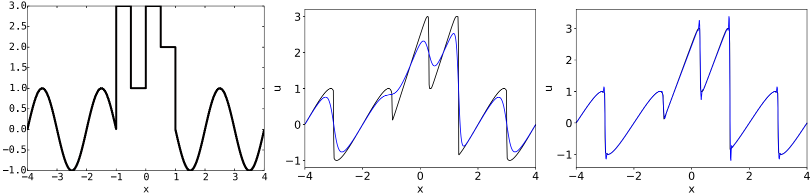
Define the filter of order p

$$\sigma(x) = \begin{cases} e^{(-\beta x^p)} & \text{if } 0 \leq x \leq 1, \\ 0, & \text{if } x > 1 \end{cases} \qquad (\text{fix } \beta = 10)$$

Modify the Fourier coefficients as

$$\hat{u}_k \rightarrow \sigma_p\left(\frac{|k|}{N/2}\right) \quad \forall -\frac{N}{2} \leq k \leq \frac{N}{2}.$$

For example, solving the Burgers equation (N=600)



(a) Init. cond.　(b) p=2　(c) p=4

Handling Gibbs oscillations: artificial viscosity

Modify scheme as

$$\begin{aligned} \frac{\mathrm{d}\boldsymbol{u}_h(t)}{\mathrm{d}t} + \boldsymbol{D}\boldsymbol{f}_h(t) &= \boldsymbol{D}(\boldsymbol{\mu}_h(t) \odot \boldsymbol{D}\boldsymbol{u}_h(t)) \\ \boldsymbol{\mu}_h(t) &= [\mu_h(x_0, t), ..., \mu_h(x_{N-1}, t)]^\top \end{aligned}$$

Issue: Determining $\mu_h(x_j, t)$ in the absence of local regularity estimates.

One approach: Estimate $\mu_h(x_j, t)$ based on entropy production (EV)

- Existence of an entropy pair
- Parameter tuning

Handling Gibbs oscillations: artificial viscosity + filtering

Proposed approach:

1. Train a network to classify the "local" regularity τ_j on a stencil S_j^7

$$\tau_j = \begin{cases} 1 & \text{if } u \text{ is discontinuous} \\ 2 & \text{if } u \in C^0 \setminus C^1 \\ 3 & \text{if } u \in C^1 \setminus C^2 \\ 4 & \text{if } u \in C^2 \end{cases}$$

2. Apply a high order exponential filter of order $p = 14$
3. Estimate artificial viscosity (inspired by MDA)

$$\mu_j = \mathcal{Q}(\tau_j) h \max_{x \in \mathcal{S}_7^r} |f'(u)|, \quad \mathcal{Q}(\tau_j) = \begin{cases} 0.5, & \text{if } \tau_j = 1, \\ 0.25, & \text{if } \tau_j = 2, \\ 0.0, & \text{if } \tau_j \geq 3 \end{cases}$$

Handling Gibbs oscillations: artificial viscosity + filtering

Proposed approach:

Input stencil S_j^7 with 7 points.

Training data sampled from the following periodic functions on $[0, 2\pi]$

$$f_1(x) = \begin{cases} a_1 & \text{if } |x-\pi| \le a_3, \\ a_2 & \text{if } |x-\pi| > a_3, \end{cases}$$

$$f_2(x) = \begin{cases} a_1|x-\pi| - a_1 a_3 & \text{if } |x-\pi| \le a_3, \\ a_2|x-\pi| - a_2 a_3 & \text{if } |x-\pi| > a_3, \end{cases}$$

$$f_3(x) = \begin{cases} 0.5 a_1 |x-\pi|^2 - a_1 a_3 & \text{if } |x-\pi| \le a_3, \\ a_2|x-\pi|^2 - a_2 a_3 - 0.5 a_3^2 (a_1 - a_2) & \text{if } |x-\pi| > a_3 \end{cases}$$

$$f_4(x) = \sin(2xa)$$

We don't use solutions to conservation laws!

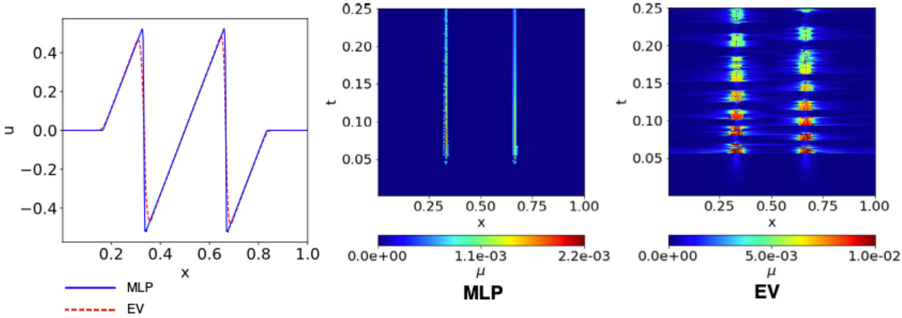
Numerical setup

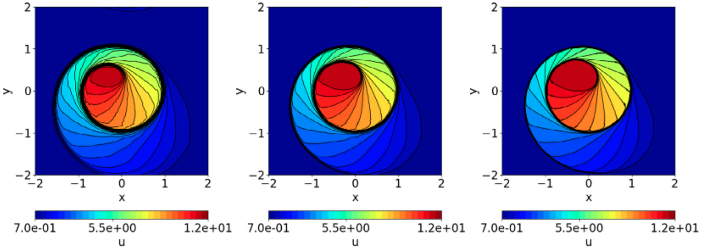
- Same network for all problems.
- Time-marching using SSPRK-4.
- In multi-D, network applied in a dimension-by-dimension manner + nodal minimum.

Controlling oscillations in spectral methods by local artificial viscosity governed by neural networks, by Schwander, Hesthaven and R.; JCP, 2021.

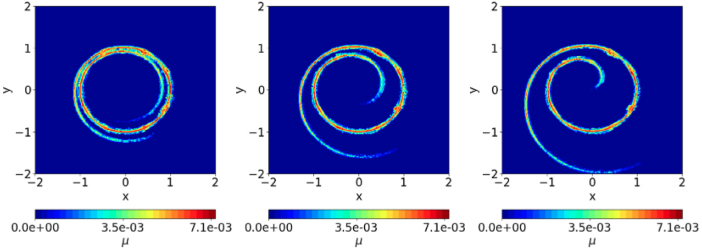
Burgers equation: EV vs. MLP

$$u_0(x) = \begin{cases} -\sin(6\pi x) & \text{if } \frac{1}{6} \le x \le \frac{5}{6}, \\ 0 & \text{otherwise} \end{cases}$$

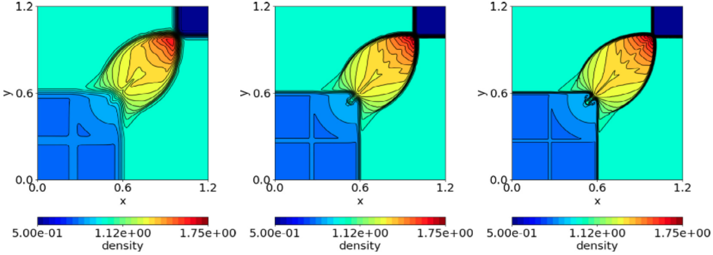




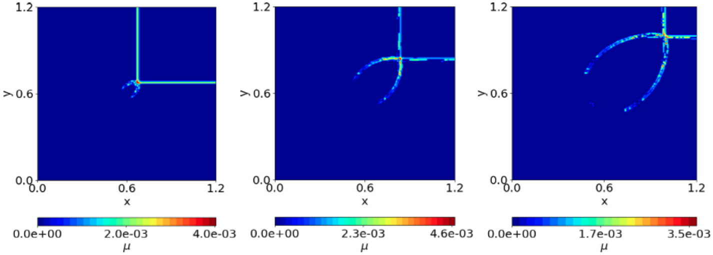
(a) 100×100. (b) 200×200. (c) 400×400.



(d) 400×400, $t = 0.2$ (e) 400×400, $t = 0.6$ (f) 400×400, $t = 1$



(a) 100×100. (b) 200×200. (c) 300×300.



(d) 300×300, $t = 0.05$ (e) 300×300, $t = 0.15$ (f) 300×300, $t = 0.25$

Conclusion

- Neural networks are useful for shock-capturing.
  - Estimate viscosity
  - Detect troubled-cells (R. and Hesthaven, 2019)
- Deep learning can be used to enhance numerical algorithms.
- Neural networks are great at detecting patterns.
- Domain knowledge is valuable in constructing datasets.

Questions?

Popular viscosity models for DG schemes

Highest modal decay (MDH) model [Persson and Peraire, 2006]:

Based on the decay of modal coefficients in each element

$$S_k = \frac{\|u_h^k - \tilde{u}_h^k\|^2_{L^2(D_k)}}{\|u_h^k\|^2_{L^2(D_k)}} \quad \to \quad \text{fraction of energy in highest modes}$$

For $s_k = \log_{10}(S_k)$

$$\mu = \mu_{\max} \begin{cases} 0 & \text{if } s_k < s_0 - c_k, \\ \frac{1}{2}\left(1 + \sin\left(\frac{\pi(s_k - s_0)}{2c_k}\right)\right) & \text{if } s_0 - c_k \leq s_k \leq s_0 + c_k, \\ 1 & \text{if } s_0 + c_k \leq s_k \end{cases}$$

where $s_0 = -c_A - 4\log_{10}(m)$.

Highest modal decay (MDH) model [Persson and Peraire, 2006]:

Based on the decay of modal coefficients in each element

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where $s_0 = -c_A - 4\log_{10}(m)$.

Problem-dependent parameters

Popular viscosity models for DG schemes

Averaged modal decay (MDA) model [Klökner et al., 2011]:

Can be seen as an improvement over MDH.

$$\mu = \mu_{\text{max}} \begin{cases} 1 & \text{if } \tau < 1; , \\ 1 - \dfrac{\tau - 1}{2} & \text{if } 1 \leq \tau < 3, \\ 0 & \text{if } 3 \leq \tau \end{cases}$$

where the "local" smoothness estimator τ is obtained by solving local optimization problems.

Problem-dependent parameter

Popular viscosity models for DG schemes

Entropy viscosity (EV) model [Guermond et al., 2011]:

Based on the entropy residual for the pair $(\eta(u), \mathcal{F}(u))$

$$\mu = \min\{\mu_\eta, \mu_{\max}\}, \quad \mu_\eta = \frac{C_\eta}{A}\left(\frac{h}{m}\right)^2 \max\left(\max_{D_k}|R(u)|, \max_{D_k}|H(u)|\right)$$

where

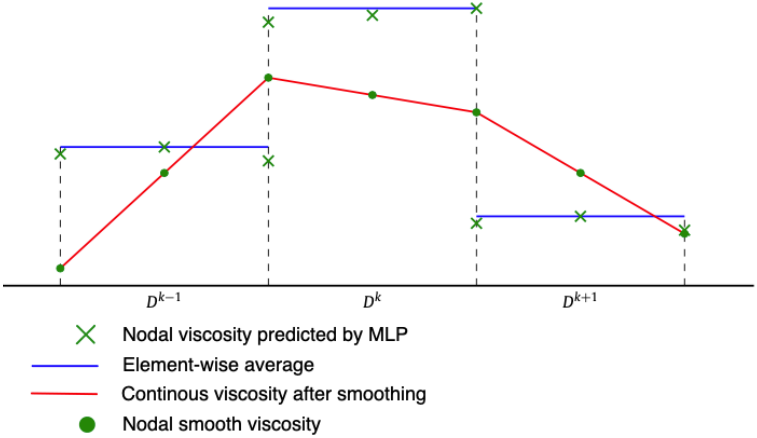
$$R = \frac{\eta^n - \eta^{n-1}}{\Delta t} + \frac{\nabla \cdot \mathcal{F}^n + \nabla \cdot \mathcal{F}^{n-1}}{2}$$

$$H = \left(\frac{m}{h}\right)[\![\mathcal{F}]\!] \cdot \boldsymbol{n}$$

$$A = \max_{\Omega}\left|\eta - \frac{1}{|\Omega|}\int_\Omega \eta \, d\Omega\right|$$

Problem-dependent parameters

DG viscosity smoothing

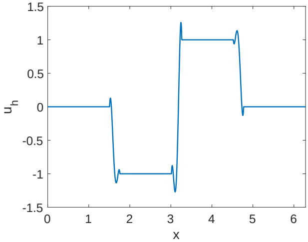


DG scheme

- Local basis in each element.
- For smooth solutions

$$\textit{Error} \sim \mathcal{O}(h^{m+1/2})$$

- Local Gibbs oscillations

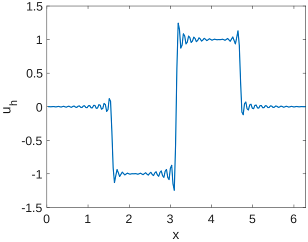


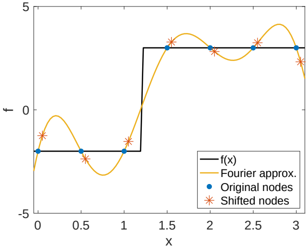
Fourier spectral scheme

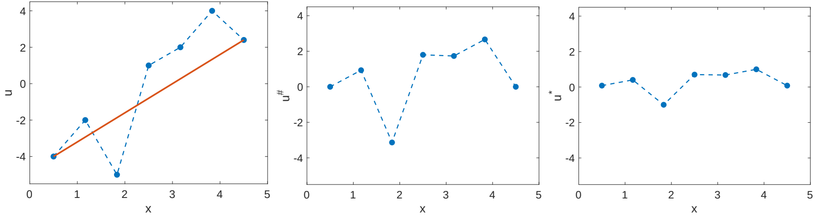
- Global basis.
- For smooth solutions

$$\textit{Error} \sim \mathcal{O}(h^p) \ \forall \ p \geq 0$$

- Global Gibbs oscillations



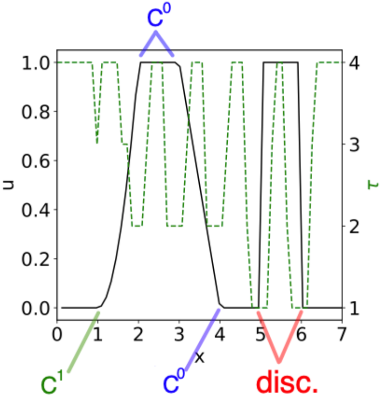




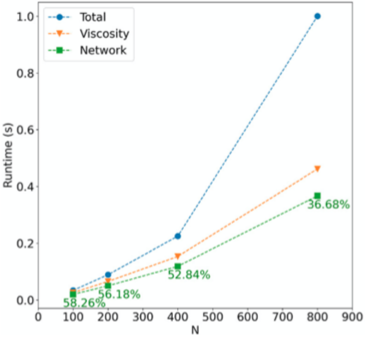
(a) Find line (b) Rotate (c) Scale

Proposed approach:

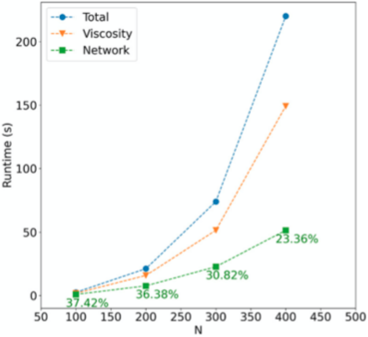
- Input $\boldsymbol{x} \in \mathbb{R}^7$.
- Output $\boldsymbol{y} \in \mathbb{R}^4$ – class probability.
- MLP with 3 hidden layers and ELU activation function.



SVANN: Computational cost



(a) 1D Burgers' problem



(b) 2D KPP problem