DG schemes for hyperbolic systems with source terms, enhanced by neural networks

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Outline

Introduction

DG scheme with prior on the equilibrium

Prior and PINNs

Results

Future works and extension
Introduction
Nonlinear conservation laws and WB schemes

- We consider the following type of models (like everybody here):

\[ \partial_t U + \partial_x F(U) = S(U) \]

- We are interested by the simulation of flows such as:

\[ \partial_x F(U) = S(U) + \varepsilon P(t, x) \]

**Numerical difficulties**

We consider a scheme of order \( q \). For a equilibrium \( \partial_x F(U) = S(U) \) we have

\[ \partial_x F(U_h) = S(U_h) + C \Delta x^q Q_h(t, x). \]

If \( \varepsilon < C \Delta x^q \) our scheme will not correctly capture perturbed flows.

**WB and A-WB schemes**

For a equilibrium \( \partial_x F(U) = S(U) \), a Well-Balanced scheme is such that \( \partial_x F(U_h) = S(U_h) \), and an Approximately Well-Balanced scheme is such that

\[ \partial_x F(U_h) = S(U_h) + C_2 \Delta x^{q_2} Q_h(t, x) \]

with \( q_2 > q \) or \( C_2 \ll C \).

- WB et A-WB make it possible to capture these perturbed flows.
Non-exhaustive state of the art

Many people have been working on approximately and exactly well-balanced schemes, including many in the audience!

For instance, we mention:

- Exactly or approximately well-balanced schemes for the shallow water equations:
  - Audusse, Bouchut, …
  - Bermúdez, Vázquez, …
  - Berthon, Chalons, Desveaux, Michel-Dansac,…
  - Clain, Figueiredo, …
  - the Málaga group: Castro, Parés, …
  - Noelle, Shu, Xing, …

- Exactly or approximately well-balanced schemes for the Euler equations:
  - Franck, Mendoza, …
  - Käppeli, Mishra, …
  - Thomann, Klingenberg, Puppo, …

- Exactly or approximately well-balanced schemes for other systems:
  - Busto, Dumbser, Gaburro, …
  - Chertock, Kurganov, …
DG schemes

- We recall quickly the Discontinuous Galerkin method.

\[
\partial_t U + \partial_x F(U) = S(U)
\]

\[
\int_{\Omega_j} \partial_t U \phi \, dx + \int_{\Omega_j} \partial_x F(U) \phi \, dx = \int_{\Omega_j} S(U) \phi \, dx
\]

- In each cell we consider a discrete vectorial polynomial space: 
  \( V_h = \text{Span}(\phi_1(x), \ldots, \phi_q(x)) \) and we use

\[
U|_{\Omega_j}(t, x) = \sum_{i=1}^{q} \alpha_i(t) \phi_i(x) \in V_h
\]

and

\[
\phi = \phi_1, \ldots, \phi = \phi_q
\]

- We obtain a matrix-vector system of size \( q \times q \)

\[
\mathcal{M} \partial_t \alpha(t) + \mathcal{K}(\alpha(t)) = S(\alpha(t))
\]

with \( S, \mathcal{K} \in \mathbb{R}^q \) and \( \mathcal{M} \in \mathbb{R}^{q \times q} \)
DG scheme with prior on the equilibrium
We consider a family of equilibria
\[ U_{eq}(x; \mu) \]
indexed by some parameters \( \mu \).

We assuming that we are able to produce an approximation of this equilibrium family, called the prior:
\[ U_\theta(x; \mu) \]

Idea
Incorporate this prior in the local basis to obtain an A-WB scheme with a much higher accuracy around the equilibrium.

Questions
- What is the potential new basis (next slide)?
- Can we ensure the convergence of the new scheme (this section)?
- How to construct this prior (next section)?
Proposed basis

Idea
Introduce the prior on the equilibrium into the DG basis, to generate non-polynomial basis.

Basis with multiplicative prior

\[ V^1_h = \text{Span} \left( U_\theta(x; \mu), U_\theta(x; \mu)(x - x_j), \ldots, U_\theta(x; \mu) \frac{(x - x_j)^k}{k!} \right) \]

Basis with additive prior

- Solution 1:

\[ V^2_h = \text{Span} \left( U_\theta(x; \mu), 1, \ldots, \frac{(x - x_j)^{k-1}}{(k-1)!} \right) \]

- Solution 2:

\[ V^3_h = \text{Span} \left( U_\theta(x; \mu), (x - x_j), \ldots, \frac{(x - x_j)^k}{k!} \right) \]

- Does DG converge with non-polynomial bases?
Main result I of [YuanShu06]

We consider a basis \((v_1, .., v_K)\) of the space \(V_h\). If there are constant \(a_{ik}\) and \(b_i\) indépendant of the size of the cell \(\Delta x_j\), and if we have

\[
|v_i(x) - \sum_{k=1}^{K} a_{ik}(x - x_i)^k| \leq b_i(\Delta x_j)^{K+1} \tag{1}
\]

then for any function \(u \in H^{K+1}(\Omega_j)\), there exists \(v_h \in V_h\) and

\[
|v_h - u_h| \leq C|u|_{H^{K+1}(\Omega_j)}(\Delta x_j)^{K+\frac{1}{2}}
\]

Main result II of [YuanShu06]

With the first result, we can prove the convergence (with additional steps) of the DG scheme using the \(V_h\) basis.
Convergence with the Yuan-Shu framework II

Result in the scalar case

We assume that \( u_\theta(x; \mu) \in C^p(\Omega) \) with \( p \geq K + 1 \). Then, the previously proposed bases satisfy the assumption of [YuanShu06], and the DG scheme converges.

- Example of proof for \( V^1_h \).
- Since the neural network is \( C^{K+1}(\mathbb{R}) \), we can write a Taylor series, to obtain:

\[
    u_\theta(x) = u(x_j) + (x - x_j) u'_\theta + \ldots + \frac{u^{(K)}(x_j)}{K!} (x - x_j)^K + \frac{u^{(K+1)}(c)}{(K+1)!}
\]

with \( c \in [x_j, x] \). We then get:

\[
    \begin{pmatrix}
        u_\theta(x) \\
        u_\theta(x)(x - x_j) \\
        \vdots \\
        u_\theta(x)(x - x_j)^K
    \end{pmatrix} = 
    \begin{pmatrix}
        u_\theta(x_j) & u'_\theta(x_j) & \ldots & \frac{u^{(K)}(x_j)}{K!} \\
        0 & u_\theta(x_j) & \ldots & \frac{u^{(K-1)}(x_j)}{(K-1)!} \\
        \vdots & \vdots & \ldots & \frac{u^{(K)}(x_j)}{(K-1)!} \\
        0 & 0 & \ldots & u_\theta(x_j)
    \end{pmatrix} \begin{pmatrix}
        1 \\
        (x - x_j) \\
        \vdots \\
        (x - x_j)^K
    \end{pmatrix} + 
    \begin{pmatrix}
        \frac{u^{(K+1)}(c)}{(K+1)!} \\
        \frac{u^{(K)}(c)}{(K)!} \\
        \vdots \\
        1
    \end{pmatrix}
\]

- It easy to see that the matrix \( A \), its inverse \( A^{-1} \), and the vector \( b \) are independent from \( \Delta x_j \). Therefore, the assumption is verified.
Specific estimate I

- **Problem**: the previous approach does not give the expected gain associated with these bases.
- We propose to compute a specific estimate using these bases.
- **Current work**: we obtained the projector estimate for the basis $V_1^h$.
- **Following**: finish the global proof (we do not expect complications) and do the same for other bases.

**First lemma**

We consider a basis $(v_1, \ldots, v_K)$ of the space $V_1^h$ and assume that $u_\theta(x; \mu) \in C^p(\Omega)$

$$u_\theta(x; \mu)^2 > \alpha_0, \quad \forall x \in \Omega$$

For any function $u \in H^{K+1}(\Omega_j)$, the $L^2$ projector on $V_1^h$, $P_h(u) \in V_1^h$, satisfies

$$|u - P_h(u)| \leq C \left| \frac{u(x)}{u_\theta(x, \mu)} \right|_{H^{K+1}(\Omega_j)} (\Delta x_j)^{K+\frac{1}{2}} |u_\theta(x, \mu)|$$

- **Key point**: the pointwise interpolation and $L^2$ projector associated with this basis can be rewritten as the classical one applied at $\frac{u(x)}{u_\theta(x, \mu)}$ and multiplied by $u_\theta(x, \mu)$
Specific estimate II

Second lemma

Under the same assumptions than the previous lemma, for the basis $V_h^{\text{mod},3}$, we obtain that for any function $u \in H^{K+1}(\Omega)$

$$|u - P_h(u)|_{L^2(\Omega)} \leq C \left| \frac{u(x)}{u_\theta(x, \mu)} \right|_{H^{K+\frac{1}{2}}(\Delta x)^{K+1}} \| u_\theta(x, \mu) \|_\infty$$

- **Idea of proof**:
  1. sum the previous result on the cells
  2. use that the prior is $C^p(\Omega)$ to bound $|u_\theta(x, \mu)|$ locally in each cell
  3. use the assumption $C_1 \Delta x \leq \Delta x_j \leq C_2 \Delta x$

- **Following**: use this estimation to prove the convergence
- do the same for the other bases

Key point

- If the prior is good, then $\left| \frac{u(x)}{u_\theta(x, \mu)} \right|_{H^{K+\frac{1}{2}}(\Omega)}$ is small, and so is the error.
- For other bases, we expect an error in $\left| u(x) - u_\theta(x, \mu) \right|_{H^{K+\frac{1}{2}}(\Omega)}$
Prior and PINNs
Supervised machine learning and classical models

- **Supervised learning**: construct models $f : \mathbb{R}^d \rightarrow \mathbb{R}^m$ like

  $$y = f(x) + \varepsilon, \text{ or } \mathbb{P}(y|x)$$

  with $\varepsilon$ some noise, using inputs and outputs examples. We solve the optimization problem:

  $$\min_\theta \sum_{i=1}^{n} L(f(x_i), y_i),$$

  with $L$ a loss (cost) function.

- **Linear regression**: We choose

  $$f_\theta = Ax + b$$

  with $\theta = (A, b), \ A \in \mathbb{R}^{m,d}$ and $b \in \mathbb{R}^m$.

- **Polynomial regression**: We choose

  $$f_\theta = \sum_{i=1}^{dq} \theta_i P_i(x)$$

  with $q$ the order of the polynomial. Huge number of coefficients for large dimensions.

- **Kernel regression**: theory using Hilbert space with reproducing kernel.

  In all the case, we obtain convex optimization.
Deep learning: neural networks

- Current choice: kernel approximation or neural network.

### Layer
A layer is a function $L_l(x_l) : \mathbb{R}^{d_l} \rightarrow \mathbb{R}^{d_{l+1}}$ given by

$$L_l(x_l) = \sigma(A_l x_l + b_l),$$

where $A_l \in \mathbb{R}^{d_{l+1} \times d_l}$, $b \in \mathbb{R}^{d_{l+1}}$ and $\sigma(\cdot)$ a nonlinear function applied component by component.

### Neural network
A neural network is a parametric function obtained by composition of layers:

$$f_\theta(x) = L_n \circ \ldots \circ L_1(x)$$

with $\theta$ the trainable parameters composed of all the matrices $A_{l,l+1}$ and biases $b_l$.

- Fully connected neural network (FCNN): the matrices $A_{l,l+1}$ are dense.
Activation functions and gradients

- The local nonlinear functions are called activation functions.
- Exemple (site MonCoachdata):

  - Sigmoid: \( \sigma(x) = \frac{1}{1 + e^{-x}} \)
  - tanh: \( \tanh(x) \)
  - ReLU: \( \max(0, x) \)
  - Leaky ReLU: \( \max(0, 1x, x) \)
  - Maxout: \( \max(w_1^T x + b_1, w_2^T x + b_2) \)
  - ELU: \( \begin{cases} x & x \geq 0 \\ \alpha(e^x - 1) & x < 0 \end{cases} \)

- It is possible to use adaptive activation functions (whose parameters are also learned).

Key point

According to the activation function, the neural network are \( C^p(\mathbb{R}^d) \) functions

- We train the Neural network with a gradient-type approach. This generates non-convex optimization problems.
Neural network vs Polynomial

- We compare over-parametrized NN and polynomial regression on the Runge function.
- 120 data and approximately 800 parameters in each model.
We compare over-parametrized NN and polynomial regression on the Runge function.

- 120 data and approximately 800 parameters in each model.
Neural network vs Polynomial

- We compare over-parametrized NN and polynomial regression on the Runge function.
- 120 data and approximately 800 parameters in each model.

The polynomial model tends to oscillate in the over parameterized regime. Problematic for overfitting.
We compare over-parametrized NN and polynomial regression on the Runge function.

- 120 data and approximately 800 parameters in each model.
Neural network vs Polynomial

- We compare over-parametrized NN and polynomial regression on the Runge function.
- 120 data and approximately 800 parameters in each model.

- The ANN generates very smooth/low frequency approximations.
- It is related to the spectral bias. The low frequencies are learned before the high frequencies. This property seems to be very helpful for the generalization.
PINN’s I

- We solve PDEs of the form:

\[
\begin{align*}
\frac{\partial_t U}{\partial U} &= \mathcal{N}(U, \partial_x U, \partial_{xx} U, \beta) \\
U_h(t, x) &= g(x), \quad \forall x \in \partial \Omega \\
U(0, x) &= U_0(x, \alpha),
\end{align*}
\]

with the parameters

\[\mu = (\alpha, \beta)\]

- The first idea comes from the remark that neural networks are smooth functions of the inputs. Since their derivatives are easily computable by automatic differentiation, ANNs are possible objects to approximate PDE solution.

- A PINN is a neural network with inputs \((t, x)\), denoted by \(U_\theta(t, x)\).

## Basic approach

If we have data \(U^n_i\) approximating the solution at the points \((x_i, t_n)\), we will learn the weights of the NN by minimizing the loss:

\[
\min_\theta J_{\text{data}}(\theta) = \min_\theta \sum_{n=1}^{N_{\text{data}}} \sum_{i=1}^{N_{\text{data}}} |U_\theta(t_n, x_i) - U^n_i|^2
\]

How can we do that without data or with few data??
PINN's II

**PINNs approach**

Since we can differentiate the NN, we compute the PDE residual and check to what extent it is a solution of the PDE. **Main idea:** Learn using this property.

- We define the residual:
  \[ R(t, x) = |\partial_t U_\theta - \mathcal{N}(U_\theta, \partial_x U_\theta, \partial_{xx} U_\theta, \beta)| \]

- To learn \( U_\theta(t, x) \), we minimize:
  \[
  \min_{\theta} J_{\text{data}}(\theta) + J_r(\theta) + J_b(\theta) + J_i(\theta)
  \]
  with
  \[
  J_r(\theta) = \int_0^T \int_\Omega |R(t, x)|^2_2 dxdt
  \]
  and
  \[
  J_b(\theta) = \int_0^T \int_{\partial\Omega} |U_\theta(t, x) - g(x)|^2_2 dxdt, \quad J_i(\theta) = \int_\Omega |U_\theta(0, x) - U_0(x, \alpha)|^2_2 dx
  \]

**Question**

How to compute the integrals of the residuals?
Monte Carlo

How to compute the integrals of the residuals?

- Quadrature rule. Limited for large domains and small dimension.
- Quadrature rule + mesh. Requires a grid and limited to small dimensions.
- **Monte-Carlo approach**. Slow convergence but no mesh and no dimension issues.

- The Monte-Carlo method stems from the **Law of large numbers**.
- We consider a function $g : \mathbb{R}^d \to \mathbb{R}$. We define $X$ a random variable with the law $\mu$.
- The method comes from:

$$\frac{\text{Var}(\mu)}{\sqrt{N}} \left( \frac{1}{N} \sum_{i=1}^{N} f(X_i) - \mathbb{E}_\mu[f(X)] \right) \to \mathcal{N}(0, 1)$$

with $X_i$ an random example sampled with the law $\mu$.

- It allows to compute integrals. Indeed:

$$\int_{\Omega} f(x) dx = \int_{\mathbb{R}^d} f(x) U_\Omega dx = \mathbb{E}[f(X)]$$

with $U_\Omega$ the density of the uniform law $\Omega$ and $X$ random variable following this law.

- So we have

$$\left| \frac{1}{N} \sum_{i=1}^{N} f(x_i) - \int_{\Omega} f(x) dx \right| = O \left( \frac{\text{Var}(U_\Omega)}{\sqrt{N}} \right)$$

with $x_i$ points sampled uniformly on $\Omega$. 

E. Franck
Applying the MC method to the PINNs loss, we obtain the following minimization problem:

\[
\min_\theta J_{\text{data}}(\theta) + J_r(\theta) + J_b(\theta) + J_i(\theta),
\]

with

\[
J_r(\theta) = \sum_{n=1}^{N} \sum_{i=1}^{N} |R(t_n, x_i)|_2^2
\]

with \((t_n, x_i)\) sampled uniformly and

\[
J_b(\theta) = \sum_{n=1}^{N_b} \sum_{i=1}^{N_b} |U_\theta(t_n, x_i) - g(x_i)|_2^2, \quad J_i(\theta) = \sum_{i=1}^{N_i} |U_\theta(0, x_i) - U_0(x_i)|_2^2
\]

These loss functions can be interpreted as a regularization of classical learning which uses data.

To avoid loss for the BC and initial condition, we use:

\[
\bar{u}_\theta(t, x) = u_0(x) + t(\phi(x) * u_\theta(x))
\]

with \(\phi(x) = g(x)\) on the boundary and some value within the domain.
Example: Burgers equation

- Application: Burgers equation $\partial_t \rho + \partial_x \left( \frac{\rho^2}{2} \right) = \nu \partial_{xx} \rho$.

- Solving for different values of the $\mu$ parameters:
  - $\nu = \frac{0.1}{\pi}$. 10000 pts, medium-sized NN.
  - beginning of training

```
iter = 200
loss = 0.0774
L2 error: 4.7142e-01
```

```
iter = 400
loss = 0.0318
L2 error: 4.0850e-01
```
Example: Burgers equation

- Application: Burgers equation \( \partial_t \rho + \partial_x \left( \frac{\rho^2}{2} \right) = \nu \partial_{xx} \rho. \)

- Solving for different values of the \( \mu \) parameters:
  - \( \nu = \frac{0.1}{\pi} \). 10000 pts, medium-sized NN.
  - middle of training

    iter = 2000
    loss = 0.0000
    L2 error: 9.0829e-03

![Graphs for different times and iter](image.png)

  iter = 2200
  loss = 0.0000
  L2 error: 8.2614e-03

![Graphs for different times and iter](image.png)
Example: Burgers equation

- Application: Burgers equation $\partial_t \rho + \partial_x \left( \frac{\rho^2}{2} \right) = \nu \partial_{xx} \rho$.
- Solving for different values of the $\mu$ parameters:
- $\nu = \frac{0.1}{\pi}$. 10000 pts, medium-sized NN.
- end of training

```
iter = 4800
loss = 0.0000
L2 error: 4.6718e-03
```

```
iter = 5000
loss = 0.0000
L2 error: 4.7307e-03
```
**Example: Burgers equation**

- **Application:** Burgers equation \( \partial_t \rho + \partial_x \left( \frac{\rho^2}{2} \right) = \nu \partial_{xx} \rho. \)

- **Solving for different values of the \( \mu \) parameters:**
  - \( \nu = \frac{0.01}{\pi} \). 10000 pts, medium NN.

- **Beginning of training**
  
  iter = 600  
  loss = 0.0885  
  L2 error: 4.3601e-01

- **Iter = 800**
  
  loss = 0.0233  
  L2 error: 2.0901e-01
Example: Burgers equation

- Application: Burgers equation $\partial_t \rho + \partial_x \left( \frac{\rho^2}{2} \right) = \nu \partial_{xx} \rho$.
- Solving for different values of the $\mu$ parameters:
  - $\nu = \frac{0.01}{\pi}$. 10000 pts, medium NN.
  - middle of training

```
iter = 2000
loss = 0.0003
L2 error: 1.8053e-02
```

![Graphs showing solutions at different times](image)

```
iter = 2200
loss = 0.0002
L2 error: 1.7773e-02
```

![Graphs showing solutions at different times](image)
Example: Burgers equation

- Application: Burgers equation $\partial_t \rho + \partial_x \left( \frac{\rho^2}{2} \right) = \nu \partial_{xx} \rho$.
- Solving for different values of the $\mu$ parameters:
  - $\nu = \frac{0.01}{\pi}$. 10000 pts, medium NN.
- end of training
  - iter = 4800
  - loss = 0.0001
  - L2 error: 5.9728e-03

- iter = 5000
- loss = 0.0001
- L2 error: 5.2593e-03
Example: Burgers equation

- Application: Burgers equation \( \partial_t \rho + \partial_x \left( \frac{\rho^2}{2} \right) = \nu \partial_{xx} \rho. \)

- Solving for different values of the \( \mu \) parameters:
  - \( \nu = \frac{0.002}{\pi} \). 10000 pts, medium NN.

- beginning of training

  iter = 200
  loss = 0.0774
  L2 error: 4.7142e-01

- end of training

  iter = 400
  loss = 0.0318
  L2 error: 4.0850e-01
Example: Burgers equation

- Application: Burgers equation $\partial_t \rho + \partial_x \left( \frac{\rho^2}{2} \right) = \nu \partial_{xx} \rho$.

- Solving for different values of the $\mu$ parameters:
  - $\nu = 0.002 \cdot \frac{\pi}{\pi}$. 10000 pts, medium NN.
  - middle of training

```
iter = 2000
loss = 0.2076
L2 error: 6.2666e-01
```

```
iter = 2200
loss = 0.1361
L2 error: 6.0138e-01
```
Example: Burgers equation

- Application: Burgers equation $\partial_t \rho + \partial_x \left( \frac{\rho^2}{2} \right) = \nu \partial_{xx} \rho$.
- Solving for different values of the $\mu$ parameters:
  - $\nu = \frac{0.002}{\pi}$. 10000 pts, medium NN.
- end of training

iter = 4800
loss = 0.0272
L2 error: 4.0909e-01

![Graphs showing different solutions at t=0.24, t=0.80, t=1.35](image)

iter = 5000
loss = 0.0212
L2 error: 4.0300e-01

![Graphs showing different solutions at t=0.24, t=0.80, t=1.35](image)
Example: Burgers equation

- Application: Burgers equation $\partial_t \rho + \partial_x \left( \frac{\rho^2}{2} \right) = \nu \partial_{xx} \rho$.
- Solving for different values of the $\mu$ parameters:
  - $\nu = \frac{0.002}{\pi}$. 20000 pts, medium NN.
  - beginning of training
    
    ```
    iter = 200
    loss = 0.1495
    L2 error: 6.1471e-01
    ```

- Iteration details:
  - $t=0.24$, $t=0.80$, $t=1.35$

- Iteration details:
  - $t=0.24$, $t=0.80$, $t=1.35$

  ```
  iter = 400
  loss = 0.1170
  L2 error: 5.2688e-01
  ```
Example: Burgers equation

- Application: Burgers equation $\partial_t \rho + \partial_x \left( \frac{\rho^2}{2} \right) = \nu \partial_{xx} \rho$.
- Solving for different values of the $\mu$ parameters:
  - $\nu = \frac{0.002}{\pi}$. 20000 pts, medium NN.
  - middle of training
    
    iter = 2000
    loss = 0.0040
    L2 error: 1.7457e-01

![Graphs showing solution at different times t=0.24, t=0.80, t=1.35](image)

- iter = 2200
- loss = 0.0024
- L2 error: 1.6838e-01

![Graphs showing solution at different times t=0.24, t=0.80, t=1.35](image)
Example: Burgers equation

- Application: Burgers equation \( \partial_t \rho + \partial_x \left( \frac{\rho^2}{2} \right) = \nu \partial_{xx} \rho \).

- Solving for different values of the \( \mu \) parameters:
  - \( \nu = \frac{0.002}{\pi} \). 20000 pts, medium NN.

- end of training
  - iter = 4800
  - loss = 0.0395
  - L2 error: 3.9314e-01

- iter = 5000
  - loss = 0.0133
  - L2 error: 3.6761e-01
Example: Burgers equation

- Application: Burgers equation $\partial_t \rho + \partial_x \left( \frac{\rho^2}{2} \right) = \nu \partial_{xx} \rho$.
- Solving for different values of the $\mu$ parameters:
  - $\nu = \frac{0.002}{\pi}$. 40000 pts, larger NN.
- end of training

```
iter = 4800
loss = 0.0006
L2 error: 2.3011e-01
```

```
iter = 5000
loss = 0.0004
L2 error: 2.2456e-01
```
PINN’s and parametric PDEs

- **Advantages of PINNs**: mesh-less approach, not too sensitive to the dimension.
- **Drawbacks of PINNs**: they are not competitive with classical methods.
- **Interesting possibility**: use the strengths of PINNs to solve parametric PDEs.
- The neural network becomes \( U_\theta(t, x, \alpha, \beta) \).

**New Optimization problem for parametric PINN’s**

\[
\min_\theta J_r(\theta) + \ldots
\]

with

\[
J_r(\theta) = \int_V \int_0^T \int_\Omega \left| \frac{\partial t}{\partial t} U_\theta(t, x) - \mathcal{L}(U_\theta, \partial_x U_\theta, \partial_{xx} U_\theta, \mu)(t, x) \right|^2 dx \, dt
\]

with \( V \) a subspace of the parameters \((\alpha, \beta)\).

- Application to the Burgers equations with many viscosities \([10^{-2}, 10^{-4}]\) (training: 2h). Same time for the smaller viscosity.
Numerical results
In all the numerical experiments, we use the $V_h^3$ basis. Results are similar with the other bases.

We first consider the first-order advection equation

$$\begin{cases}
\partial_t u + \partial_x u = s(u; \mu), \\
u(t = 0, x) = u_0(x),
\end{cases}$$

with the following parameterized source term and initial condition

- $s(u; \alpha, \beta) = \alpha u + \beta u^2$;
- $u_0(x) = \varepsilon + u_{eq}(x; \alpha, \beta, \nu)$, with the steady solution $u_{eq}$ depending on $\alpha$, $\beta$ and an additional parameter $\nu$.

Hence, we have three parameters: $0.5 \leq \alpha \leq 1$, $0.5 \leq \beta \leq 1$, $0.1 \leq \nu \leq 0.2$

We propose three experiments: approximate

- a steady solution,
- a perturbed steady solution,
- an unsteady solution.

Training the PINN takes about 10 minutes on an old GPU, with no data, only the PINN loss.

**Last minute remark:** the errors are not well computed. Perhaps constant change (for all methods) and a little bit the order.
In this case, $\varepsilon = 0$ in the initial condition, so we approximate the steady solution itself.

We compute the error between the exact and approximate solutions, for polynomial bases with $n_G \in \{1, 2, 3, 4\}$ elements, and with or without PINN prior.

We take a quadrature of degree $n_Q = \max(3, n_G + 1)$.

<table>
<thead>
<tr>
<th>pts</th>
<th>$\text{error}_\phi$</th>
<th>order</th>
<th>$\text{error}_{\bar{\phi}}$</th>
<th>order</th>
<th>gain</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
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<td>3.89e-04</td>
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<td>190.66</td>
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<td>1.47</td>
<td>6.95e-06</td>
<td>1.45</td>
<td>170.09</td>
</tr>
</tbody>
</table>

(a) errors with a one-element basis, $n_G = 1$
In this case, $\varepsilon = 0$ in the initial condition, so we approximate the steady solution itself.

We compute the error between the exact and approximate solutions, for polynomial bases with $n_G \in \{1, 2, 3, 4\}$ elements, and with or without PINN prior.

We take a quadrature of degree $n_Q = \max(3, n_G + 1)$.

<table>
<thead>
<tr>
<th>pts</th>
<th>error$_{\phi}$</th>
<th>order</th>
<th>error$\bar{\phi}$</th>
<th>order</th>
<th>gain</th>
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<td>1.08e-08</td>
<td>2.38</td>
<td>166.83</td>
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</tbody>
</table>

(b) errors with a two-element basis, $n_G = 2$
In this case, $\varepsilon = 0$ in the initial condition, so we approximate the steady solution itself.

We compute the error between the exact and approximate solutions, for polynomial bases with $n_G \in \{1, 2, 3, 4\}$ elements, and with or without PINN prior.

We take a quadrature of degree $n_Q = \max(3, n_G + 1)$.

\[
\begin{array}{|c|c|c|c|c|c|}
\hline
\text{pts} & \text{error}_\phi & \text{order} & \text{error}_\bar{\phi} & \text{order} & \text{gain} \\
\hline
10 & 2.23e-05 & \text{---} & 9.34e-07 & \text{---} & 23.94 \\
20 & 2.02e-06 & 3.46 & 8.80e-08 & 3.41 & 23.01 \\
40 & 1.75e-07 & 3.53 & 7.41e-09 & 3.57 & 23.60 \\
80 & 1.45e-08 & 3.59 & 6.29e-10 & 3.56 & 23.14 \\
160 & 1.46e-09 & 3.32 & 6.35e-11 & 3.31 & 22.99 \\
\hline
\end{array}
\]

(c) errors with a three-element basis, $n_G = 3$
In this case, $\varepsilon = 0$ in the initial condition, so we approximate the steady solution itself.

We compute the error between the exact and approximate solutions, for polynomial bases with $n_G \in \{1, 2, 3, 4\}$ elements, and with or without PINN prior.

We take a quadrature of degree $n_Q = \max(3, n_G + 1)$.

<table>
<thead>
<tr>
<th>pts</th>
<th>$\text{error}_{\phi}$</th>
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<th>$\text{error}_{\bar{\phi}}$</th>
<th>order</th>
<th>gain</th>
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<td>1.32e-10</td>
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<td>2.77e-13</td>
<td>4.29</td>
<td>4.40</td>
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</table>

(d) errors with a four-element basis, $n_G = 4$
We now study the effect of nonzero values of $\varepsilon$ in the initial condition: we take $\varepsilon \in \{10^{-4}, 10^{-2}, 10^{-1}, 1\}$ and 20 discretization cells.

We represent the error, over time, between the approximate and exact solutions.

(a) errors with a one-element basis, $n_G = 1$
Linear advection equation: perturbed steady solution

We now study the effect of nonzero values of $\varepsilon$ in the initial condition: we take $\varepsilon \in \{10^{-4}, 10^{-2}, 10^{-1}, 1\}$ and 20 discretization cells.

We represent the error, over time, between the approximate and exact solutions.

(b) errors with a two-element basis, $n_G = 2$
We now study the effect of nonzero values of $\varepsilon$ in the initial condition: we take $\varepsilon \in \{10^{-4}, 10^{-2}, 10^{-1}, 1\}$ and 20 discretization cells.

We represent the error, over time, between the approximate and exact solutions.

(c) errors with a three-element basis, $n_G = 3$
Lastly, we perform the approximation of an unsteady solution with the two bases (with and without prior), to show that using the enhanced basis does not decrease approximation performance on unsteady solutions. The source term is zero in this case.

In this case, we take $n_G = 3$ and 20 discretization cells.

(a) without prior; error is $8.874 \times 10^{-3}$
Lastly, we perform the approximation of an unsteady solution with the two bases (with and without prior), to show that using the enhanced basis does not decrease approximation performance on unsteady solutions. The source term is zero in this case.

In this case, we take $n_G = 3$ and 20 discretization cells.

(b) with prior; error is $8.874 \times 10^{-3}$, the same as without prior
Shallow water equations

We consider the shallow water system with topography

\[
\begin{align*}
\partial_t h + \partial_x q &= 0, \\
\partial_t q + \partial_x \left( \frac{q^2}{h} + \frac{1}{2}gh^2 \right) &= -gh\partial_x Z.
\end{align*}
\]

The smooth moving steady solutions are given by

\[
q = \text{cst} = q_0; \quad \frac{q^2}{2h^2} + g(h + Z) = \text{cst} = B_0.
\]

The space domain is \((0, 1)\).

We consider two topography functions, which depend on two parameters \(\alpha\) and \(\beta\):

- \(Z_g(x; \alpha, \beta) = \beta \omega(\alpha x)\), with \(\omega\) a Gaussian bump function;
- \(Z_c(x; \alpha, \beta) = \beta \omega_0(\alpha x)\), with \(\omega_c\) a compactly supported Gaussian bump function.

Then, the steady solution \(h(x; \alpha, \beta, h_0, B_0)\) depends on the two topography parameters \(\alpha\) and \(\beta\), as well as on the two steady flow parameters \(B_0\) and \(q_0\).
Shallow water equations: steady solution

Training takes about 10 minutes on an old GPU, with no data, only the PINN loss.

Results for the non-compactly-supported topography $Z_g$.

We use a quadrature of degree $n_Q = n_G + 2$.

<table>
<thead>
<tr>
<th>pts</th>
<th>error$_h^\phi$</th>
<th>order</th>
<th>error$_q^\phi$</th>
<th>order</th>
<th>error$_h^\bar{\phi}$</th>
<th>order</th>
<th>gain</th>
<th>error$_q^\bar{\phi}$</th>
<th>order</th>
<th>gain</th>
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<td>4.18e-02</td>
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<td>2.64e-05</td>
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<td>463.99</td>
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<td>439.97</td>
</tr>
</tbody>
</table>

(a) errors with a one-element basis, $n_G = 1$
Training takes about 10 minutes on an old GPU, with **no data**, only the PINN loss.

Results for the non-compactly-supported topography $Z_g$.

We use a quadrature of degree $n_Q = n_G + 2$.

<table>
<thead>
<tr>
<th>pts</th>
<th>error$_h^\phi$ order</th>
<th>error$_q^\phi$ order</th>
<th>error$_h^\bar{\phi}$ order</th>
<th>gain</th>
<th>error$_q^\bar{\phi}$ order</th>
<th>gain</th>
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<td>139.46</td>
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<td>2.99e-07 2.53</td>
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</tbody>
</table>

(b) errors with a two-element basis, $n_G = 2$
Shallow water equations: steady solution

Training takes about 10 minutes on an old GPU, with no data, only the PINN loss.

Results for the non-compactly-supported topography $Z_g$.

We use a quadrature of degree $n_Q = n_G + 2$.

<table>
<thead>
<tr>
<th>pts</th>
<th>error$^h_{\phi}$ order</th>
<th>error$^q_{\phi}$ order</th>
<th>error$^h_{\phi}$ order gain</th>
<th>error$^q_{\phi}$ order gain</th>
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</thead>
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<td>9.04e-05 — 68.79</td>
</tr>
<tr>
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<td>2.90e-09 3.53 66.39</td>
<td>1.03e-08 3.41 66.94</td>
</tr>
</tbody>
</table>

(c) errors with a three-element basis, $n_G = 3$
Training takes about 10 minutes on an old GPU, with no data, only the PINN loss.

Results for the compactly-supported topography $Z_c$.

We use a quadrature of degree $n_Q = n_G + 7$. This is needed because of the large values of the derivatives of the topography (and therefore of the steady solution).

(a) errors with a one-element basis, $n_G = 1$
Training takes about 10 minutes on an old GPU, with no data, only the PINN loss.

Results for the compactly-supported topography $Z_c$.

We use a quadrature of degree $n_Q = n_G + 7$. This is needed because of the large values of the derivatives of the topography (and therefore of the steady solution).

<table>
<thead>
<tr>
<th>pts</th>
<th>error$_h^\phi$</th>
<th>order</th>
<th>error$_q^\phi$</th>
<th>order</th>
<th>error$_h^\phi$</th>
<th>order</th>
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<th>error$_q^\phi$</th>
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</table>

(b) errors with a two-element basis, $n_G = 2$
Training takes about 10 minutes on an old GPU, with no data, only the PINN loss.

Results for the compactly-supported topography $Z_c$.

We use a quadrature of degree $n_Q = n_G + 7$. This is needed because of the large values of the derivatives of the topography (and therefore of the steady solution).

<table>
<thead>
<tr>
<th>pts</th>
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<th>$q$ error of $\phi$</th>
<th>order</th>
<th>$h$ error of $\bar{\phi}$</th>
<th>order</th>
<th>gain</th>
<th>$q$ error of $\bar{\phi}$</th>
<th>order</th>
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<td>3.07</td>
<td>446.71</td>
<td>3.035e-08</td>
<td>2.88</td>
<td>485.69</td>
</tr>
</tbody>
</table>

(c) errors with a three-element basis, $n_G = 3$
Euler-Poisson system in spherical geometry

We consider the Euler-Poisson system in spherical geometry

\[
\begin{aligned}
    \partial_t \rho + \partial_r q &= -\frac{2}{r} q, \\
    \partial_t q + \partial_r \left( \frac{q^2}{\rho} + p \right) &= -\frac{2}{r} \frac{q^2}{\rho} - \rho \partial_r \phi, \\
    \partial_t E + \partial_r \left( \frac{q}{\rho} (E + p) \right) &= -\frac{2}{r} \frac{q}{\rho} (E + p) - q \partial_r \phi, \\
    \frac{1}{r^2} \partial_{rr} (r^2 \phi) &= 4\pi G \rho,
\end{aligned}
\]

The steady solutions at rest are given by

\[
q = 0; \quad \partial_r p + \rho \partial_r \phi = 0; \quad \partial_{rr} (r^2 \phi) = 4\pi r^2 G \rho.
\]

We consider two cases:

- a polytropic pressure law \( p(\rho; \kappa, \gamma) = \kappa \rho^\gamma \) such that the steady solutions satisfy

\[
\frac{d}{dr} \left( r^2 \kappa \gamma \rho^{\gamma-2} \frac{d\rho}{dr} \right) = 4\pi r^2 G \rho,
\]

- a temperature-based pressure law \( p(\rho; \kappa, \alpha) = \kappa \rho T_\alpha \) such that the steady solutions satisfy

\[
\frac{d}{dr} \left( r^2 \kappa \frac{T_\alpha}{\rho} \frac{d\rho}{dr} \right) + \frac{d}{dr} \left( r^2 \kappa \frac{dT_\alpha}{dr} \right) = 4\pi r^2 G \rho;
\]

in practice, we take \( T_\alpha(r) = e^{-\alpha r} \).
Euler-Poisson in spherical geometry: steady solution

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We take a quadrature of degree $n_Q = n_G + 1$.

Results for the polytropic pressure law

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<th>pts</th>
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(a) errors with a one-element basis, $n_G = 1$
Euler-Poisson in spherical geometry: steady solution

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Results for the polytropic pressure law

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<th>pts</th>
<th>$\text{error}^h_\phi$</th>
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(b) errors with a two-element basis, $n_G = 2$
Euler-Poisson in spherical geometry: steady solution

Training takes about 10 minutes on an old GPU, with no data, only the PINN loss. This time, we have two parameters, $\kappa$ and $\gamma$.

We take a quadrature of degree $n_Q = n_G + 1$.

Results for the polytropic pressure law

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(c) errors with a three-element basis, $n_G = 3$
Euler-Poisson in spherical geometry: steady solution

Training takes about 10 minutes on an old GPU, with no data, only the PINN loss. This time, we have two parameters, $\kappa$ and $\gamma$.

We take a quadrature of degree $n_Q = n_G + 1$.

Results for the polytropic pressure law

Statistics: gain with respect to the parameter space (from top to bottom: $n_G = 1, n_G = 2, n_G = 3$)

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Euler-Poisson in spherical geometry: steady solution

Training takes about 10 minutes on an old GPU, with no data, only the PINN loss. This time, we have two parameters, $\kappa$ and $\alpha$.

We take a quadrature of degree $n_Q = n_G + 1$.

Results for the temperature-dependent pressure law

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(a) errors with a oe-element basis, $n_G = 1$
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Results for the temperature-dependent pressure law

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(b) errors with a two-element basis, $n_G = 2$
Euler-Poisson in spherical geometry: steady solution

Training takes about 10 minutes on an old GPU, with no data, only the PINN loss. This time, we have two parameters, $\kappa$ and $\alpha$.

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(c) errors with a three-element basis, $n_G = 3$
2D shallow water system

We consider the 2D shallow water equations

\[
\begin{aligned}
\partial_t h + \nabla \cdot q &= 0 \\
\partial_t q + \nabla \cdot \left( \frac{q \otimes q}{h} + \frac{1}{2} gh^2 \right) &= -gh\nabla Z(x, y; \alpha, r_0)
\end{aligned}
\]

We define the following compactly supported bump function:

\[
\Omega(x, y; \alpha, r_0) = \begin{cases}
\alpha \exp \left( -\frac{1}{\left(1 - \frac{r^2}{r_0^2}\right)^3}\right) & \text{if } r < r_0, \\
0 & \text{otherwise},
\end{cases}
\]

and we take \( Z(x, y; \alpha, r_0) = \Omega(x, y; \alpha, r_0) \).

The steady solution is a \textbf{vortex}, whose amplitude and radius depend on \( \alpha, r_0 \) and an additional parameter \( \Gamma \): this time, we have three parameters, in addition to \( x \) and \( y \).
2D shallow water system: steady solution

Training takes about 20 minutes on an old GPU, with the PINN loss supplemented with data.

We need a high-quadrature, of degree $n_Q = 14$, because of the large derivatives of the compactly supported smooth bump function.

<table>
<thead>
<tr>
<th>pts</th>
<th>$\text{error}_\phi^h$ order</th>
<th>$\text{error}_\phi^{qx}$ order</th>
<th>$\text{error}_\phi^{qy}$ order</th>
<th>$\text{error}_\phi^h$ order</th>
<th>gain</th>
<th>$\text{error}_\phi^{qx}$ order</th>
<th>gain</th>
<th>$\text{error}_\phi^{qy}$ order</th>
<th>gain</th>
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<tr>
<td>20</td>
<td>1.91e-01</td>
<td>1.13e+00</td>
<td>1.13e+00</td>
<td>2.31e-03</td>
<td>82.79</td>
<td>1.02e-03</td>
<td>1116.93</td>
<td>1.01e-03</td>
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<tr>
<td>40</td>
<td>4.72e-02</td>
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<td>2.76e-01</td>
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<td>1222.59</td>
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</table>

(a) errors with a one-element basis, $n_G = 1$
2D shallow water system: steady solution

Training takes about 20 minutes on an old GPU, with the PINN loss supplemented with data.

We need a high-quadrature, of degree \( n_Q = 14 \), because of the large derivatives of the compactly supported smooth bump function.

<table>
<thead>
<tr>
<th>pts</th>
<th>error( \frac{h}{\phi} ) order</th>
<th>error( \frac{q_x}{\phi} ) order</th>
<th>error( \frac{q_y}{\phi} ) order</th>
<th>error( \frac{h}{\phi} ) order</th>
<th>gain</th>
<th>error( \frac{q_x}{\phi} ) order</th>
<th>gain</th>
<th>error( \frac{q_y}{\phi} ) order</th>
<th>gain</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>2.32e-02</td>
<td>2.10e-01</td>
<td>2.10e-01</td>
<td>2.59e-04</td>
<td>89.71</td>
<td>5.49e-04</td>
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<tr>
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<td>7.02e-05</td>
<td>2.91</td>
<td>4.63e-04</td>
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<td>141.49</td>
<td>7.90e-07</td>
<td>586.16</td>
<td>8.02e-07</td>
<td>577.49</td>
</tr>
</tbody>
</table>

(b) errors with a two-element basis, \( n_G = 2 \)
2D shallow water system: steady solution

Training takes about 20 minutes on an old GPU, with the PINN loss supplemented with data.

We need a high-quadrature, of degree \( n_Q = 14 \), because of the large derivatives of the compactly supported smooth bump function.

<table>
<thead>
<tr>
<th>pts</th>
<th>( \text{error}^h_{\phi} ) order</th>
<th>( \text{error}^{q_x}_{\phi} ) order</th>
<th>( \text{error}^{q_y}_{\phi} ) order</th>
<th>( \text{error}^h_{\bar{\phi}} ) order gain</th>
<th>( \text{error}^{q_x}_{\bar{\phi}} ) order gain</th>
<th>( \text{error}^{q_y}_{\bar{\phi}} ) order gain</th>
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</thead>
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<tr>
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<td>6.05e-02 —</td>
<td>6.05e-02 —</td>
<td>3.05e-04 —</td>
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<td>1.60e-03 —</td>
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<tr>
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<td>4.35e-03 3.80</td>
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<td>4.35e-06 8.55</td>
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<td>2.73e-04 3.99</td>
<td>2.73e-04 3.99</td>
<td>1.30e-07 3.99</td>
<td>2.84e-07 3.94</td>
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<td>160</td>
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<td>1.81e-05 3.91</td>
<td>8.17e-09 3.99</td>
<td>1.59e-08 4.15</td>
<td>1.62e-08 4.16</td>
</tr>
</tbody>
</table>

(c) errors with a three-element basis, \( n_G = 3 \)
Future work and extension
Operator learning

- Parametric PINNs make it possible to approximate a family of PDE solutions, but we need a parametrisation (e.g. of the topography).
- **More general**: Operator learning
- Principle: we consider
  \[ -\partial_x (\alpha(x) \partial_x u(x)) = f(x) \]
- Formally there exist a operator \( G^+ : \mathcal{H}^2 \rightarrow \mathcal{H} \), with \( \mathcal{H} \) an Hilbert space, defined by
  \[ G^+(\alpha(x), f(x)) \rightarrow u(x) \]

Neural operator

Construct a neural network \( G^+_\theta \), approximation of \( G^+ \), where the result and, if possible, the input, do not depend on the mesh resolution.

Next

- this week: construct Neural operator which takes the topography a input, and gives the equilibrium for the 2D Shallow Water equations.
- 2-year post-doc position in Strasbourg to improve neural operators for time-dependent hyperbolic systems.
MHD equilibrium

- For Tokamaks and stellarators, we solve flows around equilibrium.
- General equilibrium:
  \[ \nabla P = J \times B \]
  with \( \mu_0 \mathcal{J} = \nabla \times \mathcal{B} \).

- Tokamak equilibrium
  \[ -\Delta^* \psi(R, Z) = -\mu_0 R^2 \frac{dP(\psi, \mu_1)}{d\psi} - \frac{1}{2} \frac{dF(\psi, \mu_2)}{d\psi} \]
  with \( \mu_1, \mu_2 \) some parameters.

Aim

Solve the equilibrium family with PINNs/Neural operator, and couple with a DG scheme, or another efficient scheme.
Coming back to time-dependant problems:

$$\partial_t u + a\partial_x u = u^2$$

If the prior is perfect in time and space and the quadrature also the spatial part is exact but it change nothing for the time part.

The modification only acts on the spatial error.

Using DG in time or other approaches, we wish to obtain a very accurate approximation in time around a family of space-time solution.

Example: a compressible scheme which would be more accurate around a family of incompressible flows.

Direct optimization of the basis functions to minimize the error on some solutions
## Conclusion

### PINNs

Physics-Informed neural networks and neural operators are a good way to compute and store large families of solutions.

### Enhanced DG

Using this prior in the basis, we significantly increase the accuracy around these families of steady states (including steady solution with no analytical expression).

### Questions

Can we obtain entropy stability?

### General

Neural networks are interesting for PDEs but we do not have the same guarantees of classical numerical methods. Using the NN as a "predictor/preconditioner" for the numerical method, we hope to gain in CPU time, accuracy, and retain good convergence properties.
Thank you for your attention!

Finite Volumes for Complex Applications 10 (FVCA10), in Strasbourg, 30/10/2023 – 03/11/2023