Neural implicit representation for PDEs and hybrid numerical methods

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Outline

Numerical Methods and implicit neural representation

Numerical methods

- We begin with a simple example:

$$\begin{cases} L_{t,x}u = \partial_t u - \Delta u = 0 \\ u(t=0,x) = u_0(x) \\ u(x) = g \text{ on } \partial\Omega \end{cases}$$

- Solving a PDE amounts to solving a infinite-dimensional problem.
- **Numerical method**: transform the PDE into a finite-dimensional problem of dimension N with convergence to the PDE solution when $N \to \infty$
- How to summarize most of numerical methods? (drawing from S. Mishra)

$$\begin{tikzcd} X \arrow[r, "\mathcal{G}"] \arrow[d, squiggly, bend right, "\mathcal{E}"'] & Y \arrow[d, bend right, "\mathcal{P}"'] \\ \mathbb{R}^m \arrow[u, bend right, "\mathcal{D}"'] \arrow[r, squiggly, "\mathcal{A}"'] & \mathbb{R}^p \arrow[u, squiggly, bend right, "\mathcal{R}"'] \end{tikzcd}$$

- Definitions:
  - $\mathcal{E}$, the **encoder**, transforms the data (initial conditions, RHS) into a finite dimensional vector. We speak about **degree of freedoms** (DoF).
  - $\mathcal{D}$, the **decoder**, transforms degrees of freedom into a function.
  - $\mathcal{A}$, the **approximator**, transforms the DoF of the inputs into the DoF of the approximate solution.
  - $\mathcal{E} \circ \mathcal{D} \approx I_d$ the **projector** to the final dimension functional space associated to the decoder form.

Why numerical methods require a mesh?

Polynomial Lagrange interpolation

We consider a domain $[a, b]$. There exists a polynomial P of degree k such that, for any $f \in C^0([a, b])$,

$$|f(x) - P(x)| \leq |b - a|^k \max_{x \in [a,b]} |f^{k+1}(x)|.$$

- On small domains ($|b - a| \ll 1$) or for large k, this polynomial gives a very good approximation.
- Very high degrees k can generate oscillations.
- To enfore small domains: we introduce a mesh and a cell-wise polynomial approximation

First step: choose a parametric function

We define a mesh by splitting the geometry in small sub-intervals $[x_i, x_{i+1}]$, and we propose the following candidate to approximate the PDE solution u

$$u_{|[x_i, x_{i+1}]}(t, x) = \sum_{j=1}^{k} \alpha_j(t) \phi_j(x).$$

This is a piecewise polynomial representation.

Finite element, finite volume, discontinuous Galerkin

Finite element method

- **Encoder**: transforms the function f into $\alpha(t)$ the FE DoF (pointwise values, face/edge integral values, . . .)
- **Decoder**: $D(\alpha)(t,x) = \sum_{i=1}^{N} \alpha_i(t)\phi_i(x)$ with $\phi_i(x)$ a compactly supported basis function defined on the whole mesh
- **Approximator**: we plug the decoder in the weak form of the equations to obtain an ODE or an algebraic system on α

Finite volume and discontinuous Galerkin method

- **Encoder**: transforms the function f into $\alpha(t)$ the FE DoF (average values, modal values, nodal values, . . .)
- **Decoder**: $D(\alpha)(t,x)_{|\Omega_j} = \sum_{i=1}^{N} \alpha_i(t)\phi_i(x)$ with $\phi_i(x)$ a local cell-wise basis function.
- **Approximator**: we plug the decoder in the weak form of the equations to obtain an ODE or an algebraic system on α, in each cell

- For this method, the decoder generates a finite-dimensional vector space.
- The method projects a form of the equation on this finite-dimensional space. **Uniqueness** is ensured by the Hilbert projection theorem.
- Convergence is ensured: increasing the number of DoF (mesh, polynomial degree) makes the error decrease.

Spectral methods

Spectral theorem

The spectral theorem in Hilbert spaces proposes an approximation of any function in H by

$$u(x)=\sum_{i=1}^{N}\alpha_i\phi_i(x),$$

with $\phi_i(x)$ the orthonormal global Hilbert basis, and $\alpha_i=\langle f,\phi_i\rangle$.

Spectral method

- **Encoder**: Projection of the function f in the spectral basis. DoF: $\alpha_i=\langle f,\phi_i\rangle$
- **Decoder**: $D(\alpha)(t,x)=\sum_{i=1}^{N}\alpha_i(t)\phi_i(x)$ with $\phi_i(x)$ the first modes of the Hilbert basis.
- **Approximator**: we plug the decoder in the weak/strong form of the equations to obtain an ODE or an algebraic system on α.

- For this method, the decoder generates a finite-dimensional vector space.
- The method projects a form of the equation on this finite-dimensional space, using the **Unicity** by Hilbert projection theorem.
- Convergence is ensured: increasing the number of DoF (number of modes) makes the error decrease.

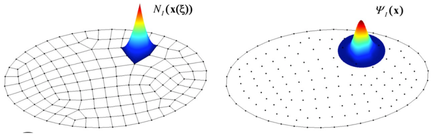
Mesh-free methods

Idea

Represent the solution as a sum of radial basis functions localized at some points:

$$u(x) = \sum_{i=1}^{N} \alpha_i \phi_i(|x - x_j|)$$

with $\phi_i(r)$ a radial basis function such as $\phi(r) = e^{-(\varepsilon r)^2}$ or $\phi(r) = \frac{1}{1+(\varepsilon r)^2}$. Larger values of ε give more localized functions.



Radial basis method

- **Encoder**: Projection of the function f. DoF: weights of the radial functions
- **Decoder**: $D(\alpha)(t,x) = \sum_{i=1}^{N} \alpha_i(t)\phi(|x - x_i|)$ with $\phi(x)$ a radial basis function.
- **Approximator**: just like before, the decoder is plugged in the equation.

- Like before, we have a finite-dimensional function space.
- Convergence: increasing the number of points (DoF) makes the error decrease.

Properties

Space and space-time decoder

- Classical methods (FE/FV/DG/...) involve a decoder where only the space representation is fixed:

$$u(t,x)=\sum_{i=1}^{N}\alpha_i(t)\phi_i(x).$$

- Plugging this decoder in the equation, we obtain an ODE to solve.
- A more recent approach, space-time methods, proposes to fix both space and time representations:

$$u(t,x)=\sum_{i=1}^{N}\alpha_i\phi_i(t,x).$$

- Plugging this decoder in the equation we obtain an algebraic system to solve.

Explicit vs implicit representations

- Representations are called explicit if the degrees of freedom can be explicitly computed and understood from the function.
- FE/FV/DG/spectral methods use explicit representations (average value, ...).
- The radial basis method, however, uses a partially explicit representation. It is difficult to understand the DoF from the function, but they can easily be computed by inverting the mass matrix (projector).

Key idea

Summary

Every previously mentioned space and space-time methods consists in:

1. choosing a linear representation (linear combination of basis functions), either local (on a mesh) or global;
2. plugging this representation into the equation to obtain algebraic relations (linear for linear problems, nonlinear for nonlinear problems) or ODEs.
3. solving this algebraic relation with a linear solver or Newton's method, using a time scheme to solve the ODE.

In all these cases, the decoder is linear with respect to the DoFs, and the representation is either explicit or partially explicit.

Idea

Choose a nonlinear representation given by a neural network. We replace a sum of simple functions with a composition of simple functions.

Important points

Finite-dimensional spaces associated to a nonlinear decoder are not vector spaces but manifolds. So:

- the projector is not unique, and the representations will be implicit.
- Existence and uniqueness? algebraic system replaced with non-convex optimization.

Nonlinear models

- Nonlinear version of classical models: f is represented by the DoF α_i, μ_i, ω_i or Σ_i:

$$f(x;\alpha,\mu,\Sigma)=\sum_{i=1}\alpha_i e^{(x-\mu_i)\Sigma_i^{-1}(x-\mu_i)},\quad f(x;\alpha,\omega)=\sum_{i=1}\alpha_i sin(\omega_i x)$$

- Neural networks (NN).

Layer

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

$$L_l(\mathbf{x}_l)=\sigma(A_l\mathbf{x}_l+\mathbf{b}_l),$$

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

Neural network

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

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

with θ the trainable parameters composed of all the matrices $A_{l,l+1}$ and biases $\mathbf{b}_l$.

- **Go to nonlinear models** allows to use NN which are: accurate global model (mesh free), low frequency (better for generalization) and able to deal with large dimension.
- **Go to nonlinear models**: would allows to use less degrees of freedom.

Space-time approach: PINNs I

Idea of PINNs

- For u in some function space $\mathcal{H}$, we wish to solve the following PDE:

$$\partial_t u = \mathcal{F}(u, \nabla u, \Delta u) = F(u).$$

- Classical representation for space-time approach: $u(t,x) = \sum_{i=1}^N \theta_i \phi_i(x,t)$
- Deep representation: $u(t,x) = u_{nn}(x,t;\theta)$ with u_{nn} a NN with trainable parameters θ.

- Since ANNs are C^p functions, we can compute $\partial_t u_{nn}(x,t;\theta)$, $\partial_{x^p} u_{nn}(x,t;\theta)$ and

$$r(x,t) = \partial_t u_{nn}(x,t;\theta) - \mathcal{F}(u_{nn}(x,t;\theta), \nabla u_{nn}(x,t;\theta), \Delta u_{nn}(x,t;\theta))$$

- Since the subspace of NN functions is not a vector space, we cannot "project" this residue.

Conclusion

We move away from solving algebraic equations on the parameters, and go towards non-convex optimization.

Space-time approach: PINNs II

- We define the residual of the PDE:

$$R(t,x) = \partial_t u_{nn}(t,x;\theta) - \mathcal{F}(u_{nn}(t,x;\theta), \partial_x u_{nn}(t,x;\theta), \partial_{xx} u_{nn}(t,x;\theta))$$

- To learn the parameters θ in $u_{nn}(t,x;\theta)$, we minimize:

$$\theta = \arg\min_{\theta} \left(J_r(\theta) + J_b(\theta) + J_i(\theta) \right),$$

with

$$J_r(\theta) = \int_0^T \int_{\Omega} |R(t,x)|^2 dxdt$$

and

$$J_b(\theta) = \int_0^T \int_{\partial\Omega} \| u_{nn}(t,x;\theta) - g(x) \|_2^2 dxdt, \quad J_i(\theta) = \int_{\Omega} \| u_{nn}(0,x;\theta) - u_0(x) \|_2^2 dx.$$

- If these residuals are all equal to zero, then $u_{nn}(t,x;\theta)$ is a solution of the PDE.
- To complete the determination of the method, we need a way to compute the integrals. In practice we use Monte Carlo.
- **Important point**: the derivatives are computed exactly using automatic differentiation tools and back propagation. Valid for any decoder proposed.

Space-time approach: PINNs II

- We define the residual of the PDE:

$$R(t,x) = \partial_t u_{nn}(t,x;\theta) - \mathcal{F}(u_{nn}(t,x;\theta), \partial_x u_{nn}(t,x;\theta), \partial_{xx} u_{nn}(t,x;\theta))$$

- To learn the parameters θ in $u_{nn}(t,x;\theta)$, we minimize:

$$\theta = \arg\min_{\theta} \Big(J_r(\theta) + J_b(\theta) + J_i(\theta) \Big),$$

with

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

with (t_n, x_i) sampled uniformly or through importance sampling, and

$$J_b(\theta) = \sum_{n=1}^{N_b} \sum_{i=1}^{N_b} |u_{nn}(t_n, x_i; \boldsymbol{\theta}) - g(x_i)|^2, \quad J_i(\theta) = \sum_{i=1}^{N_i} |u_{nn}(0, x_i; \boldsymbol{\theta}) - u_0(x_i)|^2.$$

- If these residuals are all equal to zero, then $u_{nn}(t,x;\theta)$ is a solution of the PDE.
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PINNs for parametric PDEs

- **Advantages of PINNs**: mesh-less approach, not too sensitive to the dimension.
- **Drawbacks of PINNs**: they are often not competitive with classical methods.
- Interesting possibility: use the strengths of PINNs to solve PDEs parameterized by some $\boldsymbol{\mu}$.
- The neural network becomes $u_{nn}(t, x, \boldsymbol{\mu}; \theta)$.

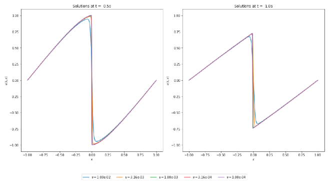
New Optimization problem for PINNs

$$\min_{\theta} J_r(\theta) + \ldots,, \quad \text{with}$$

$$J_r(\theta) = \int_{V_\mu} \int_0^T \int_\Omega \left\| \partial_t u_{nn} - \mathcal{L}\left(u_{nn}(t,x,\boldsymbol{\mu}), \partial_x u_{nn}(t,x,\boldsymbol{\mu}), \partial_{xx} u_{nn}(t,x,\boldsymbol{\mu})\right) \right\|_2^2 dxdt$$

with V_μ a subspace of the parameters $\boldsymbol{\mu}$.

- Application to the Burgers equations with many viscosities $[10^{-2}, 10^{-4}]$:



- Training for $\mu = 10^{-4}$: 2h. Training for the full viscosity subset: 2h.

Spatial approach: Neural Galerkin I

- We solve the following PDE:

$$\partial_t u = \mathcal{F}(u, \nabla u, \Delta u) = F(u).$$

- Classical representation: $u(t,x) = \sum_{i=1}^N \theta_i(t)\phi_i(x)$
- Deep representation: $u(t,x) = u_{nn}(x;\theta(t))$ with u_{nn} a neural network, with parameters $\theta(t)$, taking x as input.
- We want that:

$$F(u_{nn}(x;\theta(t))) = \partial_t u_{nn}(x;\boldsymbol{\theta(t)}) = \left\langle \nabla_\theta u_{nn}(x;\boldsymbol{\theta}), \frac{d\theta(t)}{dt} \right\rangle$$

- How to find an equation for $\frac{d\theta(t)}{dt}$?
- We solve the minimization problem:

$$\frac{d\theta(t)}{dt} = \arg\min_{\boldsymbol{\eta}} J(\boldsymbol{\eta}) = \arg\min_{\boldsymbol{\eta}} \int_\Omega |\langle \nabla_\theta u_{nn}(x;\theta), \boldsymbol{\eta}\rangle - F(u_{nn}(x;\theta(t)))|^2 dx.$$

- The solution is given by

$$\boxed{M(\theta(t))\frac{d\theta(t)}{dt} = F(x, \theta(t))}$$

with

$$M(\theta(t)) = \int_\Omega \nabla_\theta u_{nn}(x;\theta) \otimes \nabla_\theta u_{nn}(x;\theta) dx, \quad F(x,\theta(t)) = \int_\Omega \nabla_\theta u_{nn}(x;\theta) F(u_{nn}(x;\theta)) dx.$$

Spatial approach: Neural Galerkin II

- How to estimate $M(\theta(t))$ and $F(x,\theta(t))$?
- **Firstly**: we need to differentiate the network with respect to θ and to x (in the function F). This can easily be done with automatic differentiation.
- **Secondly**: How to compute the integrals? Monte Carlo approach.
- So, we use:

$$M(\theta(t)) \approx \sum_{i=1}^{N} \nabla_\theta u_{nn}(x_i;\theta) \otimes \nabla_\theta u_{nn}(x_i;\theta)$$

  and the same for $F(x,\theta(t))$.
- **Summary**: we obtain an ODE in time (as usual) and a mesh-less method in space.
- Like in the case of PINNs, we can apply this framework to parametric PDEs and larger dimensions.
- We solve the following PDE:

$$\partial_t u = \mathcal{F}(u,\nabla u,\Delta u,\alpha) = F(u;\mu).$$

- Deep representation: $u(t,x,\mu) = u_{nn}(x,\mu;\theta(t))$
- The solution is given by

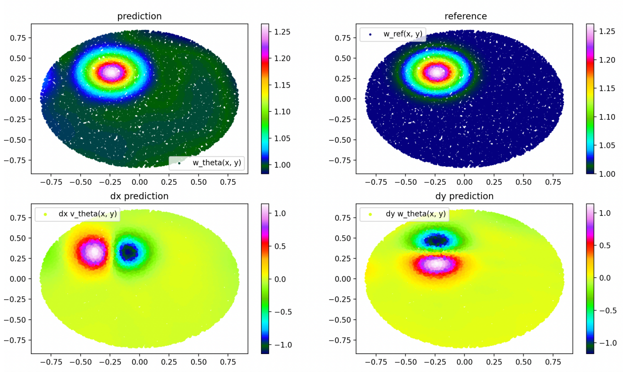
$$\boxed{M(\theta(t))\frac{d\theta(t)}{dt} = F(x,\theta(t),\mu)}$$

  with

$$M(\theta(t)) = \int_{V_\mu}\int_\Omega \nabla_\theta u_{nn}(x,\mu;\theta) \otimes \nabla_\theta u_{nn}(x,\mu;\theta) dx d\mu.$$

Spatial approach: Neural Galerkin III

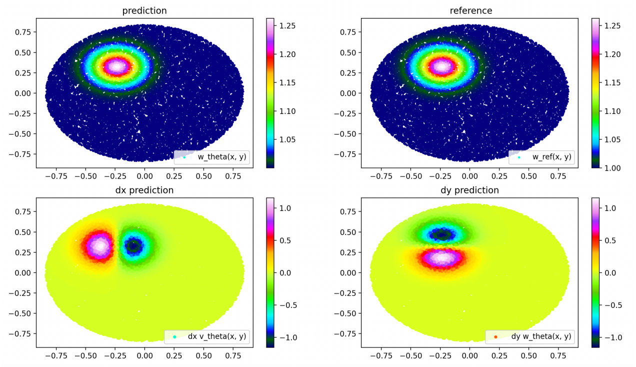
- We solve the advection-diffusion equation $\partial_t \rho + \boldsymbol{a} \cdot \nabla \rho = D \Delta \rho$ with a Gaussian function as initial condition.
- Case 1: with a neural network (2200 DOF)



- 5 minutes on CPU, MSE error around 0.0045.

Spatial approach: Neural Galerkin III

- We solve the advection-diffusion equation $\partial_t \rho + \boldsymbol{a} \cdot \nabla \rho = D \Delta \rho$ with a Gaussian function as initial condition.
- Case 2: with a Gaussian mixture (one Gaussian):



- 5 sec on CPU. MSE around 1.0^{-6}. Decoder perfect to represent this test case.

Summary

New numerical methods

New numerical methods are derived using nonlinear models like neural networks. Same spirit as classical methods: plug an Ansatz into the equation to obtain equations on DoFs.

- **Classical numerics**: they use Ansatz $f(t,x;\theta)$ plugged into the equations.
  - Space time Ansatz
    $$f(t,x;\theta)=\sum_{i=1}\theta_i\phi_i(t,x)$$
    gives a algebraic system on θ (linear for linear PDE, nonlinear else).
  - Space Ansatz
    $$f(t,x;\theta)=\sum_{i=1}\theta_i(t)\phi_i(x)$$
    gives a linear/non-linear ODE on θ + algebraic system on θ for initial projection.

Drawbacks

- less accurate than classical approaches especially in low dimension
- convergence and theoretical study difficult,

Advantages

- mesh free
- more efficient in large dimension and for parametric PDEs, perfect for GPUs
- more freedom on the chosen structure (the decoder)

Summary

New numerical methods

New numerical methods are derived using nonlinear models like neural networks. Same spirit as classical methods: plug an Ansatz into the equation to obtain equations on DoFs.

- **Neural method**: idem.
  - PINNs (Space time Ansatz)

    $$f(t,x;\theta) = u_{nn}(t,x;\theta)$$

    replace algebraic system on θ by non-convex optimization.
  - Neural Galerkin (Space Ansatz)

    $$f(t,x;\theta) = u_{nn}(x;\theta(t))$$

    gives a nonlinear on $\theta(t)$ + non-convex optimization for initial projection.

Drawbacks

- less accurate than classical approaches especially in low dimension
- convergence and theoretical study difficult,

Advantages

- mesh free
- more efficient in large dimension and for parametric PDEs, perfect for GPUs
- more freedom on the chosen structure (the decoder)

Application to numerical methods

Hybrid predictor-corrector methods

Hybrid methods

In this context, hybrid methods combine classical numerical methods and numerical methods based on Implicit Neural representation (IRM).

Objectives

Taking the best of both worlds: the accuracy of classical numerical methods, and the mesh-free large-dimensional capabilities of IRM-based numerical methods.

General Idea

- **Offline process**: train a Neural Network (PINNs, NGs, NOs or CROM) to obtain a large family of approximate solutions.
- **Online process**: predict the solution associated to our test case using the NN.
- **Online process**: correct the solution with a numerical method.

Predictor-Corrector: using PINNs in a FE method

- We consider the following elliptic problem:

$$\begin{cases} Lu = -\partial_{xx} u + v\partial_x u + ru = f, & \forall x \in \Omega \\ u = g, & \forall x \in \partial\Omega \end{cases}$$

- We assume that we have a continuous prior of the solution given by a parametric PINN $u_\theta(x)$
- We propose the following corrections of the finite element basis functions:

$$u(x) = u_\theta(x) + p_h(x), \quad u(x) = u_\theta(x) p_h(x),$$

with $p_h(x)$ a perturbation discretized using P_k Lagrange finite element.

- For the **first approach (additive prior)**, we solve in practice:

$$\begin{cases} Lp_h(x) = f - Lu_\theta(x), & \forall x \in \Omega \\ p_h(x) = g - u_\theta(x), & \forall x \in \partial\Omega \end{cases}$$

- For the **second approach (multiplicative prior)**, we need $u_\theta(x) \neq 0$, so we take $M > 0$ and we solve:

$$\begin{cases} L(u_\theta(x) p_h(x)) = f, & \forall x \in \Omega \\ p_h(x) = \frac{g}{u_\theta(x)} + M, & \forall x \in \partial\Omega \end{cases}$$

Theory for hybrid EF

- Approach one: we rewrite the Cea lemma for $u_h(x) = u_\theta(x) + p_h(x)$. We obtain

$$\| u - u_h \| \leq \frac{M}{\alpha} \| u - u_\theta - I_h(u - u_\theta) \|$$

  with I_h the interpolator. Using the classical result of P_k Lagrange interpolator we obtain

$$\| u - u_h \|_{H^m} \leq \frac{M}{\alpha} C h^{k+1-m} \underbrace{\left(\frac{| u - u_\theta |_{H^m}}{| u |_{H^m}} \right)}_{gain} | u |_{H^m}$$

- Approach two: $u_h(x) = u_\theta(x) p_h(x)$. We use a modified interpolator:

$$I_{mod,h}(f) = \sum_{i=1}^{N} \frac{f(x_i)}{u_\theta(x_i)} \phi_i(x) u_\theta(x)$$

  using $I_{mod,f}(f) = I_h(\frac{f}{u_\theta}) u_\theta(x)$, the Cea lemma and interpolation estimate we have:

$$\| u - u_h \|_{H^m} \leq \frac{M}{\alpha} C h^{k+1-m} \underbrace{\left(\frac{| \frac{u}{u_\theta} |_{H^m} \| u_\theta(x) \|_{L^\infty}}{| u |_{H^m}} \right)}_{gain} | u |_{H^m}$$

- The prior must give a good approximation of the m^{th} derivative.

EF for elliptic problems

- First test:

$$-\partial_{xx} u = \alpha \sin(2\pi x) + \beta \sin(4\pi x) + \gamma \sin(8\pi x)$$

We train with $(a, b, c) \in [0, 1]^3$ and test with $(a, b, c) \in [0, 1.2]^3$.

method:	average gain	variance gain
additive prior with PINNs	273	13000
Multiplicative prior $M = 3$ with PINNs	92	4000
Multiplicative prior $M = 100$ with PINNs	272	13000
additive prior with NN	15	18
Multiplicative prior $M = 3$ with NN	11	17.5
Multiplicative prior $M = 100$ with NN	15	18

- The PINN is trained with the physical loss, the NN with only data, no physics.
- The NN is able to better learn the solution itself, but the approximation of derivatives is less accurate than with the PINN.

EF for elliptic problems

- Second test:

$$v\partial_x u - \frac{1}{P_e}\partial_{xx} u = r$$

We train with $r \in [1,2]$, $Pe \in [10,100]$. We test with $(r, Pe) = (1.2, 40)$ and $(r, Pe) = (1.5, 90)$

Case 1	Classical FE		Additive prior			Multiplicative prior		
	error	order	error	order	gain	error	order	gain
10	$1.07e^{-1}$	–	$2.70e^{-3}$	–	40	$2.29e^{-4}$	–	467
20	$3.36e^{-2}$	1.97	$8.00e^{-4}$	1.76	42	$9.06e^{-5}$	1.93	371
40	$9.09e^{-3}$	1.89	$2.01e^{-4}$	2.00	45	$2.63e^{-5}$	1.97	345
80	$2.32e^{-3}$	1.97	$5.01e^{-5}$	1.99	46	$6.37e^{-6}$	1.99	365
160	$5.82e^{-4}$	1.99	$1.30e^{-6}$	1.97	45	$1.77e^{-6}$	2.0	289

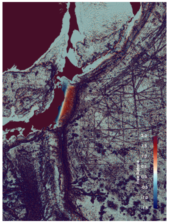
Case 2	Classic		additive prior			Multiplicative prior		
	error	order	error	order	gain	error	order	gain
10	$2.65e^{-1}$	–	$1.51e^{-1}$	–	1.7	$9.33e^{-4}$	–	284
20	$1.06e^{-1}$	1.32	$6.04e^{-2}$	1.33	1.7	$3.84e^{-4}$	1.28	276
40	$3.46e^{-2}$	1.62	$1.96e^{-2}$	1.62	1.8	$1.13e^{-4}$	1.76	305
80	$9.50e^{-3}$	1.86	$5.32e^{-3}$	1.87	1.8	$3.26e^{-5}$	1.80	291
160	$2.43e^{-3}$	1.86	$2.43e^{-3}$	1.86	1.8	$8.67e^{-6}$	1.91	280

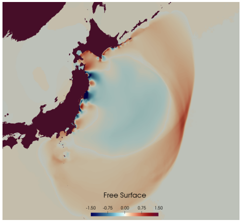
Hyperbolic systems with source terms

- In the team, most of us are interested in hyperbolic systems:

$$\partial_t \boldsymbol{U} + \nabla \cdot \boldsymbol{F}(\boldsymbol{U}) = \boldsymbol{S}(\boldsymbol{U})$$

- It is important to have a good preservation of the steady state $\nabla \cdot \boldsymbol{F}(\boldsymbol{U}) = \boldsymbol{S}(\boldsymbol{U})$.
- **Example**: Lake at rest for shallow water:
- **Exactly Well-Balanced schemes**: exact preservation of the steady state. **Approximately Well-Balanced schemes**: preserve with a high-accuracy than the scheme the steady state.
- Building exact WB schemes is difficult for some equilibria, or for 2D flows.





Idea

Compute offline a family of equilibria with parametric PINNs (or NOs) and plug the equilibrium in the DG basis to obtain a more accurate scheme around steady states.

Theory for hybrid DG

- Theory for the scalar case.
- The classical modal DG scheme uses the local representation:

$$u_{|\Omega_k}(x) = \sum_{l=0}^{q} \alpha_l \phi_l(x)^k, \text{ with } \quad [\phi_1^k, \dots \phi_q^k] = [1, (x - x_k), \dots (x - x_k)^q]$$

- If $u_\theta(x)$ is an approximation of the equilibrium, we propose to take as basis:

$$V_1 = [u_\theta(x), (x - x_k), \dots (x - x_k)^q], \text{ or } V_2 = u_\theta(x)[1, (x - x_k), \dots (x - x_k)^q]$$

Estimate on the projector for V2

Assume that the prior u_θ satisfies

$$u_\theta(x;\mu)^2 > m^2 > 0, \quad \forall x \in \Omega, \quad \forall \mu \in \mathbb{P}.$$

and still consider the vector space V_2. For any function $u \in H^{q+1}(\Omega)$,

$$\| u - P_h(u) \|_{L^2(\Omega)} \lesssim \left| \frac{u}{u_\theta} \right|_{H^{q+1}(\Omega)} (\Delta x_k)^{q+1} \| u_\theta \|_{L^\infty(\Omega)}.$$

- Adding a stability estimate, we can also prove the convergence.

Euler-Poisson system in spherical geometry

- We consider the Euler-Poisson system in spherical geometry

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

- **First application**: we consider the barotropic pressure law $p(\rho;\kappa,\gamma) = \kappa\rho^\gamma$ such that the steady solutions satisfy

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

- The PINN yields an approximation of $\rho_\theta(x,\kappa,\gamma)$
- **Second application**: we consider the ideal gas pressure law $p(\rho;\kappa,\gamma) = \kappa\rho T(r)$, with $T(r) = e^{-\alpha r}$, such that the steady solutions satisfy

$$\frac{d}{dr}\left(r^2 \kappa \frac{T}{\rho}\frac{d\rho}{dr} \right) + \frac{d}{dr}\left(r^2 \kappa \frac{dT}{dr} \right) = 4\pi r^2 G \rho,$$

- The PINN yields an approximation of $\rho_\theta(x,\kappa,\alpha)$

- To simulate a flow around a steady solution, we need a scheme that is very accurate on the steady solution.

Results

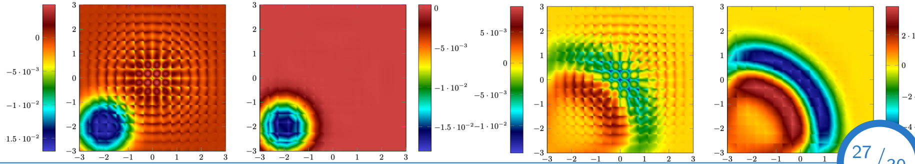
- Training takes about 10 minutes on an old GPU,with **no data**, only the PINN loss.
- We take a quadrature of degree $n_Q = n_G + 1$ (sometimes, more accurate quadrature formulas are needed).
- Barotropic case:

	minimum gain			average gain			maximum gain		
q	ρ	Q	E	ρ	Q	E	ρ	Q	E
0	19.14	2.33	17.04	233.48	3.73	197.28	510.42	4.48	371.87
1	7.61	8.28	6.98	158.25	188.92	130.57	1095.68	1291.90	1024.59
2	0.14	0.22	2.99	12.11	16.55	23.73	89.47	109.93	169.28

- ideal gas case:

	minimum gain			average gain			maximum gain		
q	ρ	Q	E	ρ	Q	E	ρ	Q	E
0	13.30	1.05	16.24	151.96	1.88	150.63	600.13	2.91	473.83
1	6.30	7.53	5.40	72.63	77.20	51.09	321.20	302.58	257.19
2	3.35	3.45	2.20	18.96	22.58	13.56	55.47	63.45	47.83

- 2D shallow water equations: equilibrium with $\boldsymbol{u} \neq 0$ + small perturbation. Plot the deviation to equilibrium:



Conclusion

Conclusion and Adverts!

Short conclusion

Using nonlinear implicit representations, we proposed new numerical/reduced modeling methods whose advantages/drawbacks are very different to those of classical approaches. We will continue to investigate hybrid approaches.

Scimba

- For the PEPR Numpex, we are currently writing the Scimba code. It contains for PINNs, Neural Galerkin, Neural operator methods, . . . ; the goal is for this code to be shared by different teams.
- If you are interested to try these methods, play with Scimba, or participate contact us!

Macaron

- Our Inria team TONUS/MACARON will specialize in the hybridation between ML and numerical methods for PDEs.
- We regularly have PhD, post-doc and even permanent positions open on these subjects. If you are interested, contact us :)

Main references

- PINNs:
  - *Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations*, M. Raissi, P. Perdikaris, G.E. Karniadakis
  - *An Expert's Guide to Training Physics-informed Neural Networks*, S. Wang, S. Sankaran, H. Wang, P. Perdikaris
  - *Estimates on the generalization error of Physics Informed Neural Networks (PINNs) for approximating PDEs*, S. Mishra, R. Molinaro
- Neural Galerkin:
  - *Neural Galerkin Scheme with Active Learning for High-Dimensional Evolution Equations*, J. Bruna, B. Peherstorfer, E. Vanden-Eijnden
  - *A Stable and Scalable Method for Solving Initial Value PDEs with Neural Networks*, M. Finzi, A. Potapczynski, M. Choptuik, A. Gordon Wilson
- Neural Operator:
  - *Fourier Neural Operator for Parametric Partial Differential Equations*, Z.i Li, N. Kovachki, K. Azizzadenesheli, B. Liu, K. Bhattacharya, A. Stuart, A. Anandkumar
  - *Neural Operator: Learning Maps Between Function Spaces*, N. Kovachki, Z. Li, B. Liu, K. Azizzadenesheli, K. Bhattacharya, A. Stuart, A. Anandkumar
  - *MOD-Net: A Machine Learning Approach via Model-Operator-Data Network for Solving PDE*, L. Zhang, T. Luo, Y. Zhang, Weinan E, Z. Xu, Z. Ma
- Deep Predictor for Newton:
  - *Accelerating hypersonic reentry simulations using deep learning-based hybridization (with guarantees)*, P. Novello, G. Poëtte, D. Lugato, S. Peluchon, P. Marco Congedo
  - *DeepPhysics: a physics aware deep learning framework for real-time simulation*, A. Odot , R. Haferssas, S. Cotin
  - *Accelerating Newton convergence for nonlinear elliptic PDE using neural operator approach*, E. Franck, R. Hild, V. Vigon, V. Michel-Dansac, J. Aghili. En cours de rédaction.
- Hybrid methods:
  - *Enhanced Finite element by neural networks for elliptic problems*, H. Barucq, E Franck, F. Faucher, N. Victorion. En cours de rédaction
  - *Approximately well-balanced Discontinuous Galerkin methods using bases enriched with Physics-Informed Neural Networks*, E. Franck, V. Michel-Dansac, L. Navoret. Arxiv preprint.