Approximately well-balanced Discontinuous Galerkin methods using bases enriched with Physics-Informed Neural Networks

Emmanuel Franck*, Victor Michel-Dansac*, Laurent Navoret*

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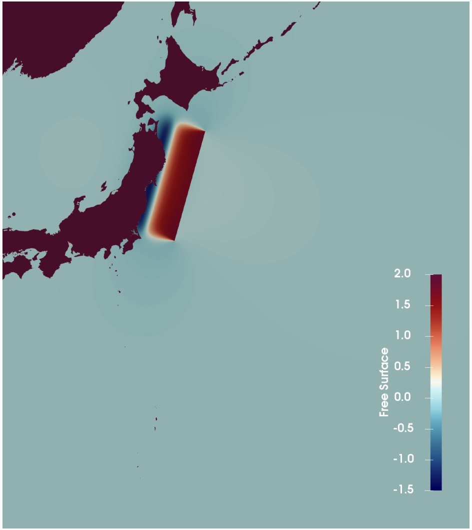
*MACARON project-team, Université de Strasbourg, CNRS, Inria, IRMA, France

Tsunami simulation: naive numerical method

Tsunami initialization



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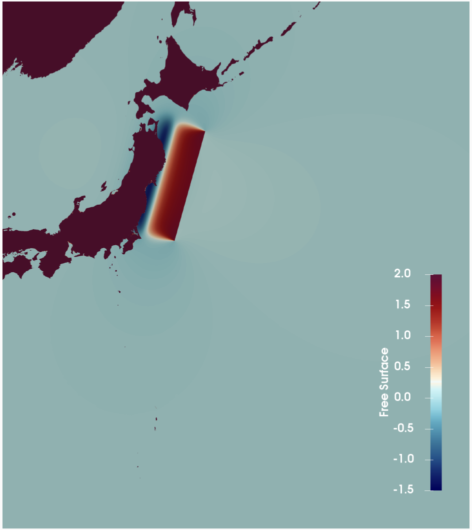
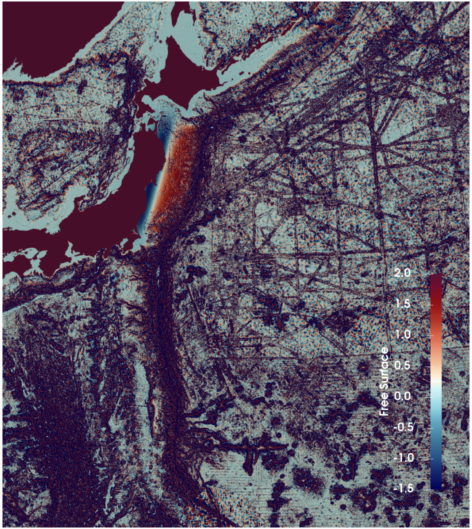


Simulation with a naive numerical method



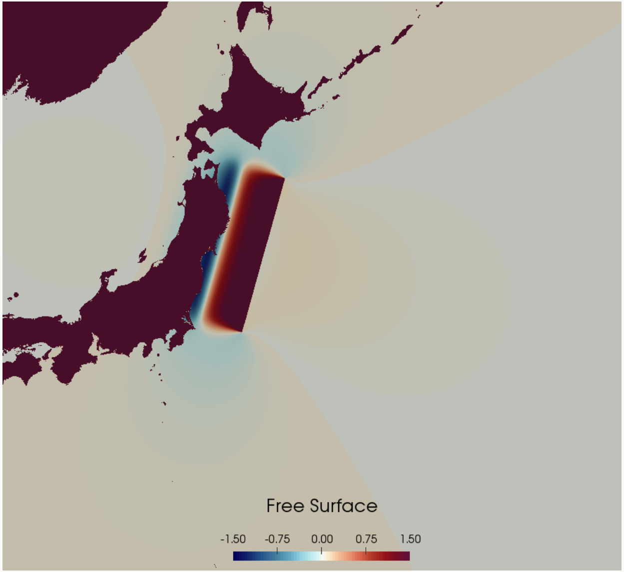
Tsunami simulation: failure

⇝ **The simulation is not usable!**

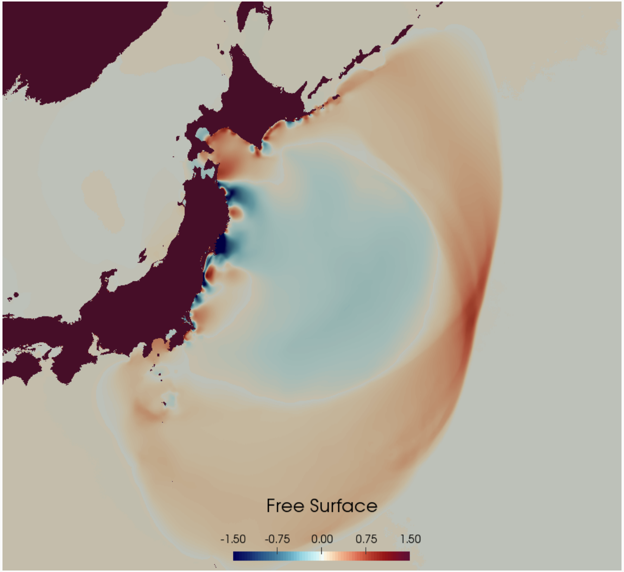
Indeed, the ocean at rest, far from the tsunami, started spontaneously producing waves.

This comes from the non-preservation of stationary solutions, hence the need to develop numerical methods that **preserve stationary solutions**: so-called **well-balanced** methods.

Tsunami simulation: well-balanced method



Tsunami simulation: well-balanced method



Objectives

The goal of this work is to provide a numerical method which:

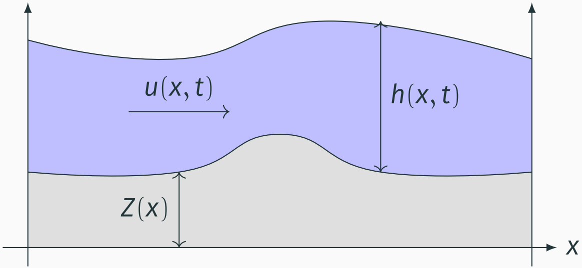
- is able to deal with generic systems,
- can provide a very good approximation of families of steady solutions,
- is as accurate as classical methods on unsteady solutions,
- with provable convergence estimates.

Before outlining the chosen numerical framework, we give an example of a physical model that will be used to validate the method.

The shallow water equations

In one space dimension, the shallow water equations are governed by the following PDE:

$$\begin{cases} \partial_t h + \partial_x q = 0, \\ \partial_t q + \partial_x \left(\dfrac{q^2}{h} + \dfrac{1}{2} g h^2 \right) = -g h \partial_x Z(x). \end{cases}$$

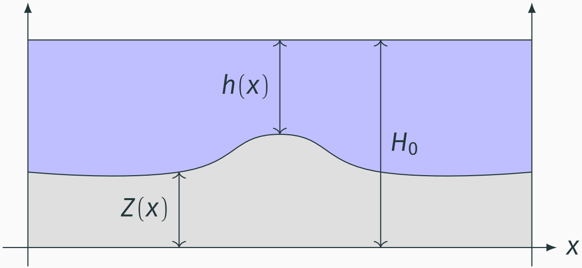


- $h(x,t)$: water depth
- $u(x,t)$: water velocity
- $q = hu$: water discharge
- $Z(x)$: known topography
- g: gravity constant

The shallow water equations: steady solutions

The steady solutions of the shallow water equations are governed by the following ODEs:

$$\begin{cases} \partial_x q = 0, \\ \partial_x \left(\frac{q^2}{h} + \frac{1}{2} g h^2 \right) = -g h \partial_x Z(x), \end{cases} \quad \rightsquigarrow \quad \begin{cases} q = \text{cst} =: q_0, \\ \frac{q_0^2}{2h^2} + g(h + Z) = \text{cst}. \end{cases}$$



If the velocity vanishes, i.e. $q_0 = 0$, we obtain the lake at rest steady solution:

$$h + Z = \text{cst} =: H_0.$$

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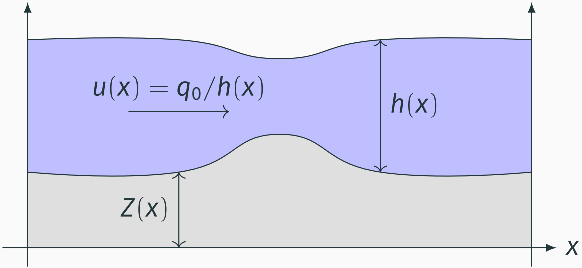
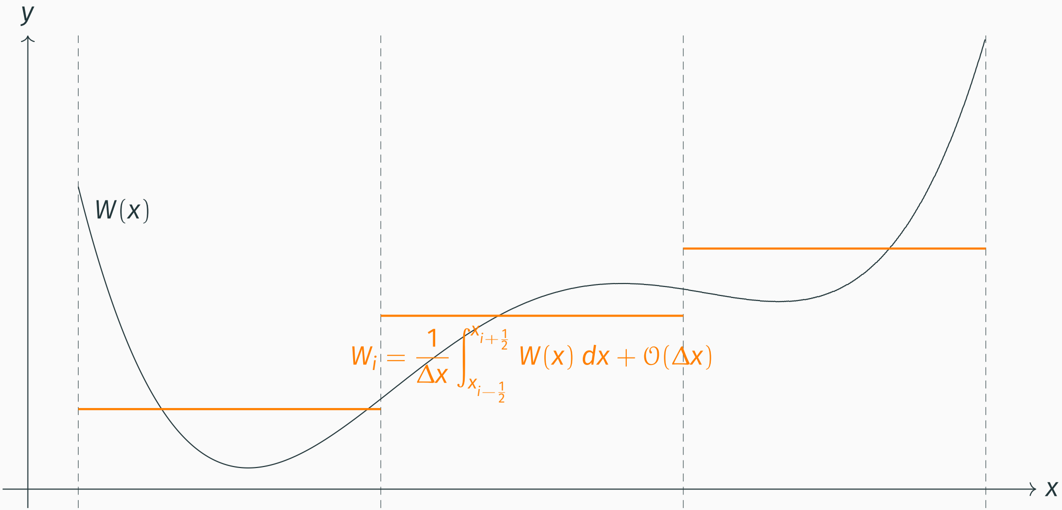


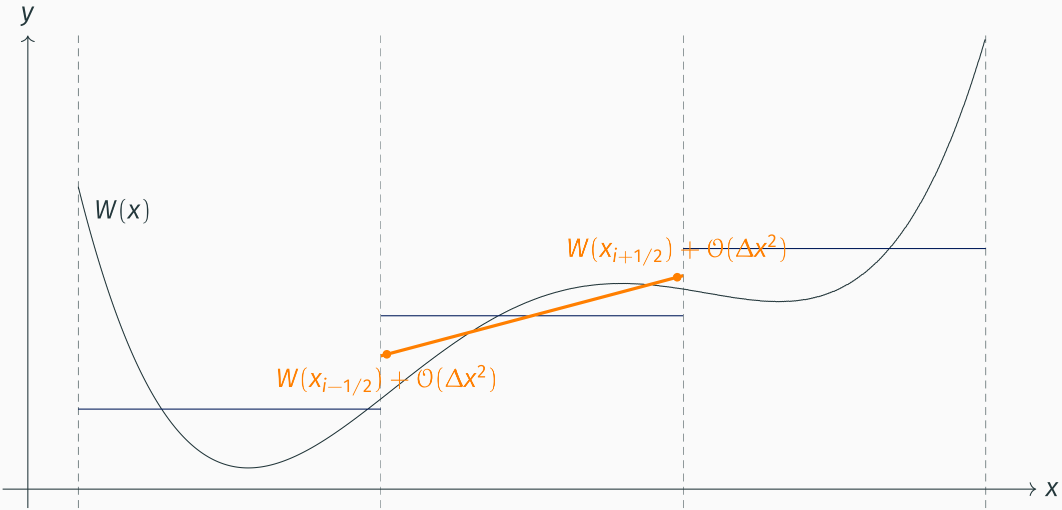
For a nonzero discharge $q_0 \neq 0$, we obtain a moving steady solution: $h(x)$ satisfies a polynomial equation of degree 3 for all x.

The finite volume method, visualized in one space dimension



$$W_i = \frac{1}{\Delta x} \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} W(x)\, dx + \mathcal{O}(\Delta x)$$

The discontinuous Galerkin method, visualized in one space dimension



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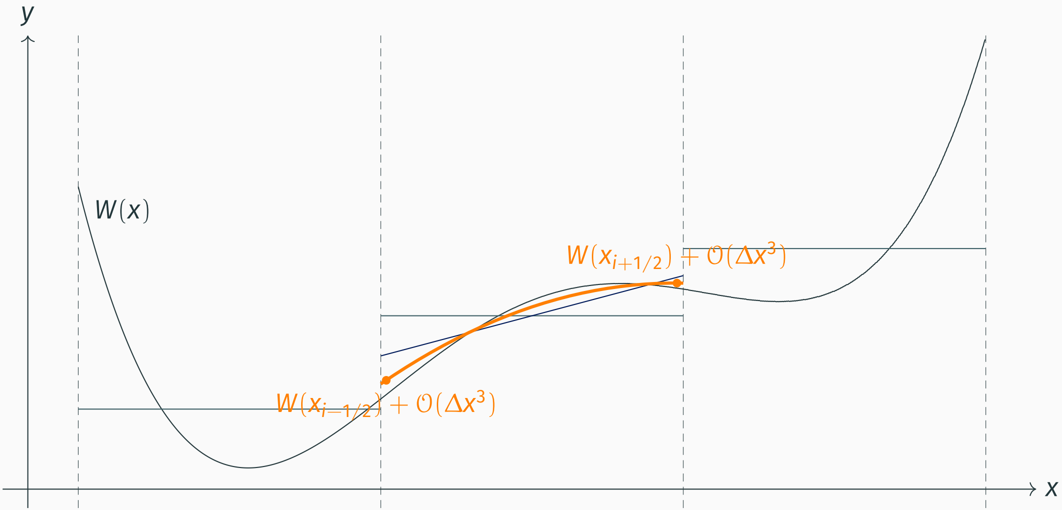

Discontinuous Galerkin: an example

On the previous slide, the physical unknown W is represented by

- a polynomial of degree 2 in each cell (Galerkin approximation),
- which is Discontinuous at interfaces between cells.

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- a polynomial of degree 2 in each cell (Galerkin approximation),
- which is Discontinuous at interfaces between cells.

Therefore, in each cell Ω_i, W is approximated by

$$W\big|_{\Omega_i} \simeq W_i^{\mathrm{DG}} := \alpha_0 + \alpha_1 x + \alpha_2 x^2 = \sum_{j=0}^{2} \alpha_j x^j,$$

where the polynomial coefficients α_0, α_1 and α_2 are determined to ensure fitness between the unknown at the continuous level, and its polynomial approximation.

Any polynomial of degree two can be exactly represented this way.

Discontinuous Galerkin: polynomial basis

More generally, we define a polynomial basis $\varphi_0, \ldots, \varphi_N$ on each cell Ω_i and approximate the solution in this basis.

A usual example is the following so-called **modal basis**:

$$\forall j \in \{0, \ldots, N\}, \quad \varphi_j(x) = x^j.$$

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Main takeaway: The DG scheme is exact on every function that can be exactly represented in the basis!

Main idea

Recall that the DG scheme will be exact on every function that can be exactly represented in the DG basis, as soon as it is also a solution to the PDE.

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Main idea

Enhance the DG basis by using the steady solution!

$\rightsquigarrow$ If the **steady solution or an approximation thereof is contained in the basis**, then:

- using the exact steady solution in the basis will make the scheme exactly well-balanced;
- using an approximation of the steady solution will make the scheme approximately well-balanced.

Enhanced DG bases

Assume that you know a **prior** W_θ on the steady solution.

It can be the exact steady solution ($W_\theta = W_{\text{eq}}$), or it can be an approximation ($W_\theta \simeq W_{\text{eq}}$).

The goal is now to **enhance the modal basis** V using W_θ:

$$V = \{1, x, x^2, \ldots, x^N\}.$$

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Second possibility: replace the first element with W_θ

$$V_+^\theta = \{W_\theta, x, x^2, \dots, x^N\}.$$

Error estimates

We denote by:

- W_{ex} the exact solution,
- W_{DG} the approximate solution without prior,
- W_{DG}^{θ} the approximate solution with prior W_{θ} and basis V_{*}^{θ}.

For a DG scheme of order $q+1$, we obtain[1] the following error estimates:

$$\left\| W_{\text{ex}} - W_{\text{DG}} \right\| \lesssim \left| W_{\text{ex}} \right|_{H^{q+1}} \Delta x^{q+1},$$

$$\left\| W_{\text{ex}} - W_{\text{DG}}^{\theta} \right\| \lesssim \left| \frac{W_{\text{ex}}}{W_{\theta}} \right|_{H^{q+1}} \Delta x^{q+1} \left\| W_{\theta} \right\|_{L^{\infty}}.$$

Conclusion of the error estimates: the prior W_{θ} needs to provide a **good approximation of the derivatives** of the steady solution.

[1] Rigorous error estimates are written in terms of the error in the projection onto both bases.

Obtaining a prior

For very simple systems, one can use the exact steady solution as a prior.

However, in many cases, even for some simple and well-known systems, one cannot compute the exact steady solution. Therefore, **an approximation is required**.

How to obtain such an approximation?

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However, in many cases, even for some simple and well-known systems, one cannot compute the exact steady solution. Therefore, **an approximation is required**.

How to obtain such an approximation?

1. **First possibility**: use a traditional numerical approximation, obtained by classical ODE solvers (e.g. Runge-Kutta schemes).
2. **Second possibility**: use a Physics-Informed Neural Network (PINN).

Since we need a good approximation of the derivatives, we use a PINN.

Parameterized families of steady solutions

We consider a parametric system of p balance laws, with unknown $W : R^{1+d+m} \to \mathbb{R}^p$,

$$\partial_t W(t, x; \mu) + \nabla \cdot F(W(t, x; \mu)) = S(W(t, x; \mu)),$$

where $t > 0$ and $x \in \Omega \subset \mathbb{R}^d$, and with $\mu \in \mathbb{P} \subset \mathbb{R}^m$ some parameters.

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Steady solutions satisfy

$$\nabla \cdot F(W(x; \mu)) = S(W(x; \mu)),$$

which is nothing but a parametric, time-independent PDE.

Therefore, the above PDE defines a parameterized family of steady solutions.

Parametric PINNs

Ommitting the boundary conditions, a parametric PDE is the following problem:

$$\text{find } W \text{ such that } \mathcal{D}(W, x; \boldsymbol{\mu}) = 0 \text{ for all } x \in \Omega \text{ and } \boldsymbol{\mu} \in \mathbb{P} \subset \mathbb{R}^m.$$

The parametric PINN

$$W_\theta : \Omega \times \mathbb{P} \subset \mathbb{R}^{m+d} \to \mathbb{R}^p$$
$$(x, \boldsymbol{\mu}) \mapsto W_\theta(x; \boldsymbol{\mu})$$

should approximately satisfy the above PDE, and the problem becomes:

$$\text{find } \theta_{\text{opt}} \text{ such that } \mathcal{D}(W_{\theta_{\text{opt}}}, x; \boldsymbol{\mu}) \simeq 0 \text{ for all } x \in \Omega \text{ and } \boldsymbol{\mu} \in \mathbb{P} \subset \mathbb{R}^m.$$

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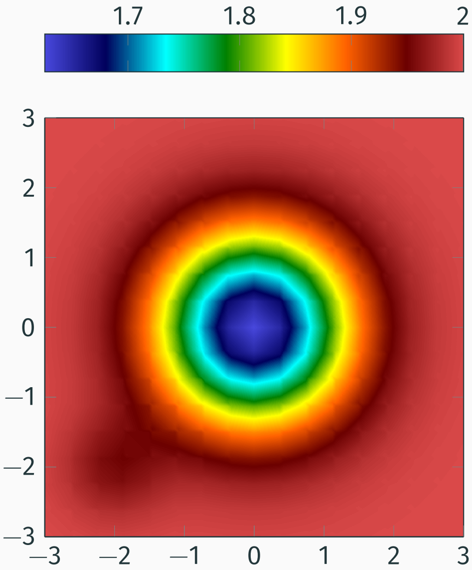
To find θ_{opt}, the minimization problem simply reads:

$$\theta_{\text{opt}} = \underset{\theta}{\operatorname{argmin}} \int_{\mathbb{P}} \int_{\Omega} \|\mathcal{D}(W_\theta, x; \boldsymbol{\mu})\|_2^2 \, dx d\boldsymbol{\mu}.$$

Perturbation of a shallow water steady solution



PINN trained on a parametric steady solution, driven by the topography

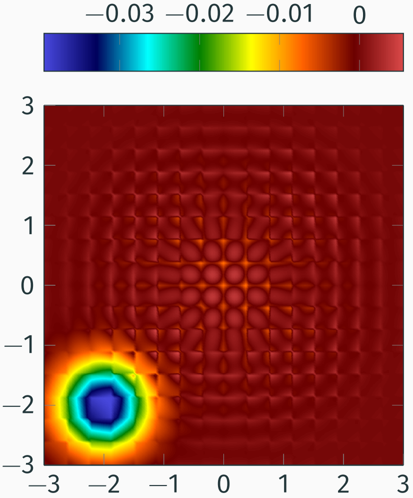
$$Z(x;\mu) = \Gamma \exp\left(\alpha(r_0^2 - \|x\|^2)\right),$$

with physical parameters

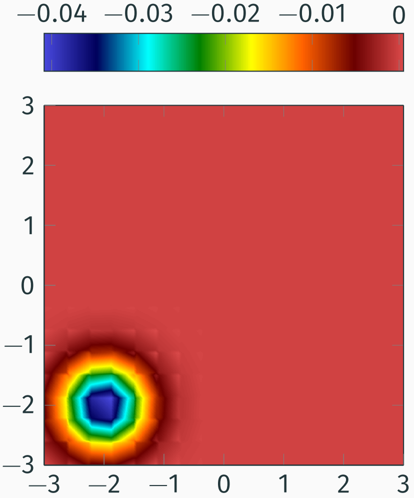
$$\mu \in \mathbb{P} \iff \begin{cases} \alpha \in [0.25, 0.75], \\ \Gamma \in [0.1, 0.4], \\ r_0 \in [0.5, 1.25]. \end{cases}$$

Left plot: initial condition, made of a perturbed steady solution.

Perturbation of a shallow water steady solution

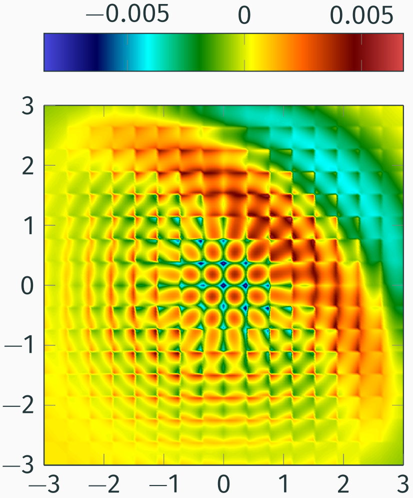


(a) classical basis



(b) enhanced basis

Perturbation of a shallow water steady solution



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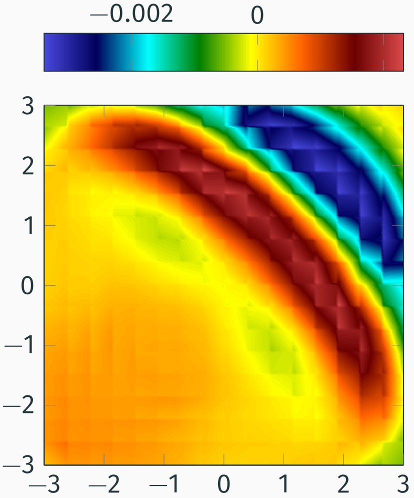


(b) enhanced basis

Why do we need well-balanced methods?

Example of a physical model: the shallow water equations

Numerical method overview: Discontinuous Galerkin

Enhancing DG with Scientific Machine Learning

PINNs for parameterized families of steady solutions

Validation

Conclusion and related work

Conclusion and related work

We have obtained:

- an approximately well-balanced DG scheme,
- for parameterized families of steady solutions,
- which works for arbitrary hyperbolic balance laws.

Related work include using ML tools for

- enriching finite element approximation spaces
  (Frédérique Lecourtier's talk in MS025A, on Thursday afternoon),
- predicting an initial guess for Newton's method,
- performing shape optimization with a volume constraint.

Article presenting this work: E. Franck, V. Michel-Dansac and L. Navoret.
"Approximately WB DG methods using bases enriched with PINNs.", *J. Comput. Phys.*, 2024
git repository: https://github.com/Victor-MichelDansac/DG-PINNs

Thank you for your attention!

Exact imposition of the boundary conditions

For the moment, the **boundary conditions are viewed as constraints**, and the solution will not exactly satisfy them.

This can be remedied by introducing a **suitable ansatz**[2]. To that end, we define

$$\widetilde{W}_\theta = \mathcal{B}(W_\theta, x, t; \mu), \quad \text{such that} \quad \widetilde{W}_\theta(x, t; \mu) = g(x, t; \mu) \quad \text{for } x \in \partial\Omega.$$

Clearly, the new approximate solution $\widetilde{W}_\theta$ exactly satifies the boundary conditions.

Moreover, the boundary loss function can be eliminated, thus **reducing competition** between the loss functions.

$\rightsquigarrow$ How to get such an ansatz? We check on an example.

[2] I. E. Lagaris et al., *IEEE Trans. Neural Netw.* (1998)

Exact imposition of the boundary conditions: example

Let us go back to the parameterized Laplace equation, where $\mu = (\alpha, \beta)$:

$$\begin{cases} \Delta W(x;\mu) + \beta W(x;\mu) = f(x;\mu) & \text{for } (x,\mu) \in \Omega \times \mathbb{P}, \\ W(x;\mu) = 0 & \text{for } (x,\mu) \in \partial\Omega \times \mathbb{P}. \end{cases}$$

Homogeneous Dirichlet BC are imposed on $\Omega = (0,1)^2$, and so we define the ansatz

$$\widetilde{W_\theta} = \mathcal{B}(W_\theta, x; \mu) = x_1(1-x_1)\, x_2(1-x_2)\, W_\theta.$$

This obviously satisfies the boundary conditions, since $\forall x \in \partial\Omega, \widetilde{W_\theta}(x;\mu) = 0$.

Therefore, the loss function only has to ensure that $\widetilde{W_\theta}$ approximates the solution to the PDE in the interior of Ω, through minimizing the loss function

$$\mathcal{J}_{\text{PDE}}(\theta) = \int_{\mathbb{P}} \int_{\Omega} \left\| \Delta \widetilde{W_\theta}(x;\mu) + \beta \widetilde{W_\theta}(x;\mu) - f(x;\mu) \right\|_2^2 dx\, d\mu.$$

PINNs as a DG prior: perturbed steady solution

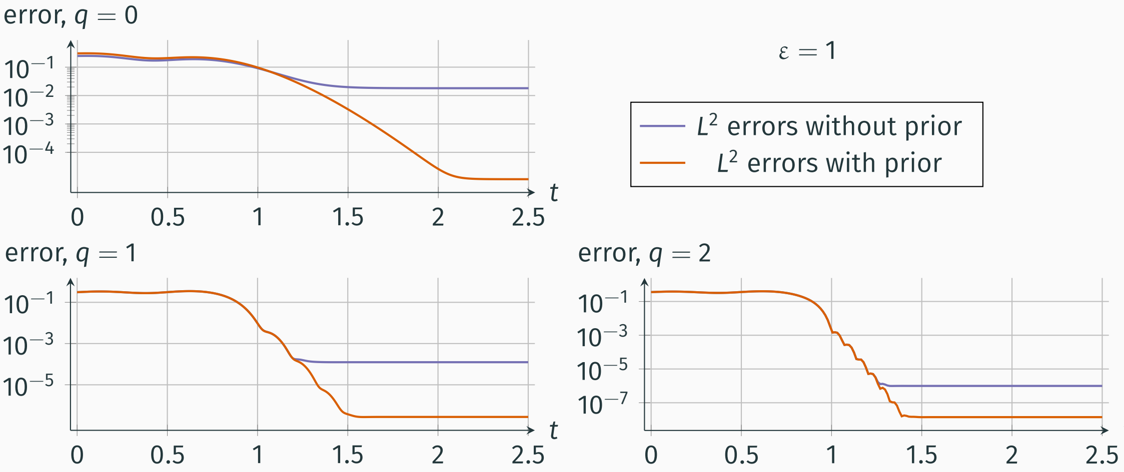
We use the DG scheme to solve the advection equation with a **perturbation of the steady solution as initial condition**:

$$\begin{cases} \partial_t W + \partial_x W = aW + bW^2 & \text{for } x \in (0,1),\ t \in (0,T), \\ W(0,x) = (1 + \varepsilon \sin(2\pi x))\, W_{\text{eq}}(x) & \text{for } x \in (0,1), \\ W(t,0) = u_0 & \text{for } t \in (0,T). \end{cases}$$

We expect:

- both schemes to **converge (in time)** towards the original, unperturbed steady solution;
- the DG scheme with prior to provide a **better approximation of the unperturbed steady solution** than the classical DG scheme.

PINNs as a DG prior: perturbed steady solution



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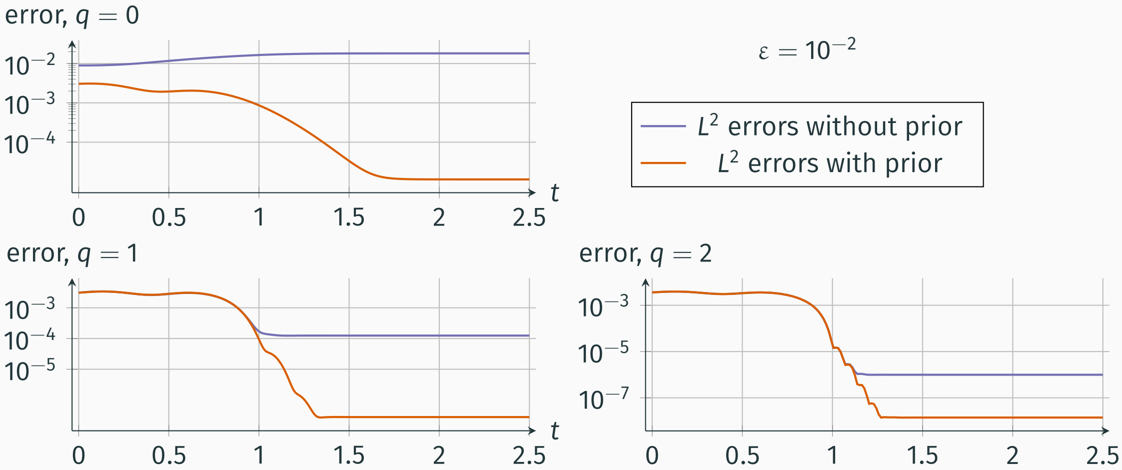

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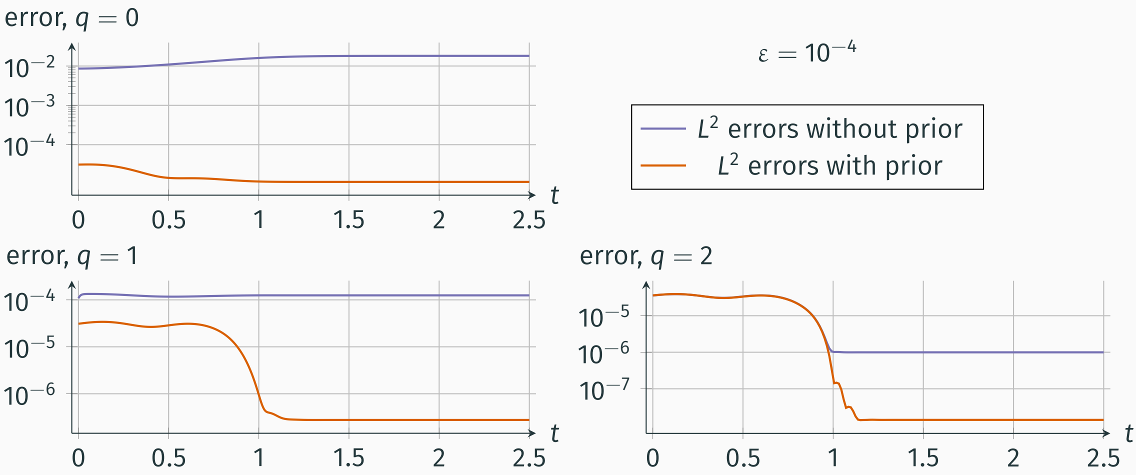

PINNs as a DG prior: unsteady solution

We use the DG scheme to solve the advection of a Gaussian bump:

$$
\begin{cases}
\partial_t W + \partial_x W = aW + bW^2 & \text{for } x \in (0,1),\ t \in (0,T), \\
W(0,x) = 0.1(1 + e^{-100(x-0.5)^2}) & \text{for } x \in (0,1), \\
W(t,0) = 0.1(1 + e^{-25}) & \text{for } t \in (0,T).
\end{cases}
$$

We expect the prior not to alter the convergence:

- both schemes to converge with the **same error rate**;
- the DG scheme with prior to provide a **similar approximation** to the classical DG scheme.

PINNs as a DG prior: unsteady solution

We compute the errors in x between the exact and approximate solutions:

- for several numbers of basis elements and discretization cells,
- using $a = 0.75$; $b = 0.75$; $u_0 = 0.15$.

	without prior		with prior		
cells	error	order	error	order	gain
10	4.04e-02	—	5.04e-02	—	0.80
20	3.46e-02	0.22	4.28e-02	0.24	0.81
40	2.84e-02	0.28	3.50e-02	0.29	0.81
80	2.15e-02	0.40	2.64e-02	0.40	0.81
160	1.47e-02	0.55	1.81e-02	0.55	0.81

(a) Errors with a basis composed of one element.

PINNs as a DG prior: unsteady solution

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	without prior		with prior		
cells	error	order	error	order	gain
10	1.92e-02	—	1.93e-02	—	1.00
20	6.26e-03	1.62	6.27e-03	1.62	1.00
40	1.19e-03	2.39	1.20e-03	2.39	1.00
80	1.99e-04	2.59	1.99e-04	2.59	1.00
160	4.19e-05	2.24	4.20e-05	2.24	1.00

(b) Errors with a basis composed of two elements.

PINNs as a DG prior: unsteady solution

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	without prior		with prior		
cells	error	order	error	order	gain
10	5.15e-03	—	5.15e-03	—	1.00
20	4.56e-04	3.50	4.56e-04	3.50	1.00
40	4.55e-05	3.32	4.55e-05	3.32	1.00
80	5.42e-06	3.07	5.42e-06	3.07	1.00
160	6.75e-07	3.01	6.75e-07	3.01	1.00

(c) Errors with a basis composed of three elements.

PINNs as a DG prior: unsteady solution

We compute the errors in x between the exact and approximate solutions:

- for several numbers of basis elements and discretization cells,
- using $a = 0.75$; $b = 0.75$; $u_0 = 0.15$.

	without prior		with prior		
cells	error	order	error	order	gain
10	4.72e-04	—	4.72e-04	—	1.00
20	2.87e-05	4.04	2.87e-05	4.04	1.00
40	1.81e-06	3.99	1.81e-06	3.99	1.00
80	1.14e-07	3.98	1.14e-07	3.98	1.00
160	7.20e-09	3.99	7.20e-09	3.99	1.00

(d) Errors with a basis composed of four elements.