Well-balancing through Scientific Machine Learning

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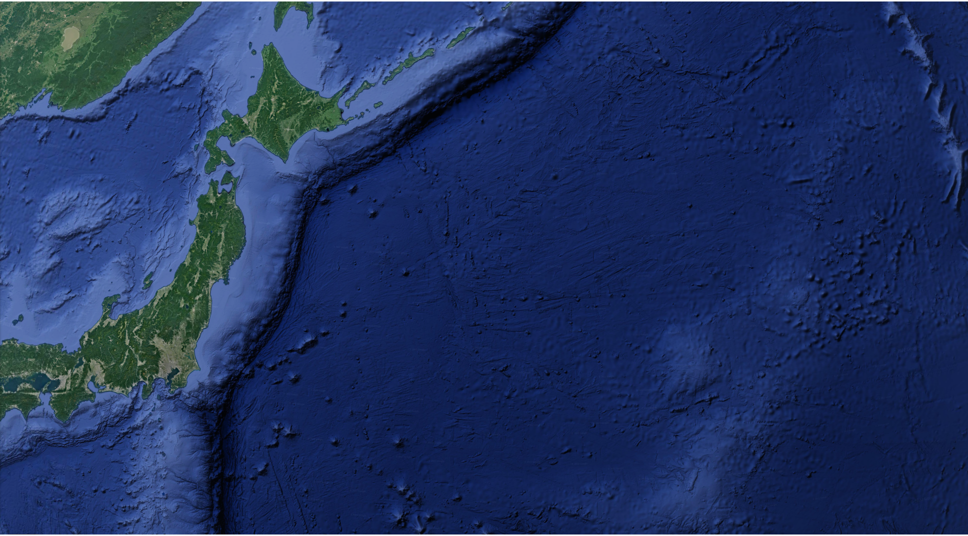
Mathématique Avancée

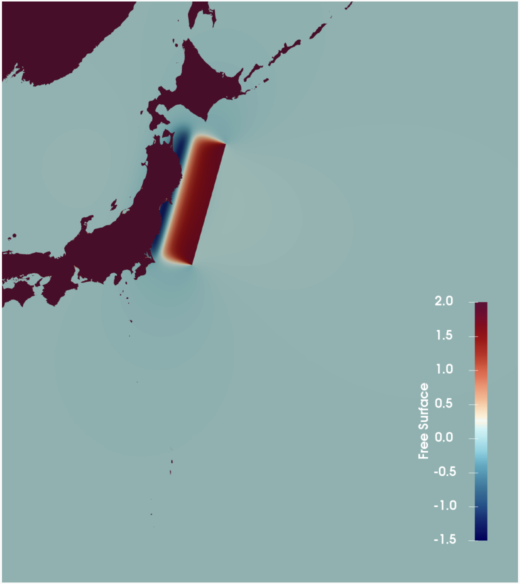
Numerical simulation of a tsunami

Context: 2011 Tōhoku tsunami



Ingredients required for a numerical simulation

Tsunami initialization



Numerical simulation of a tsunami

Starting the simulation with a naive numerical method

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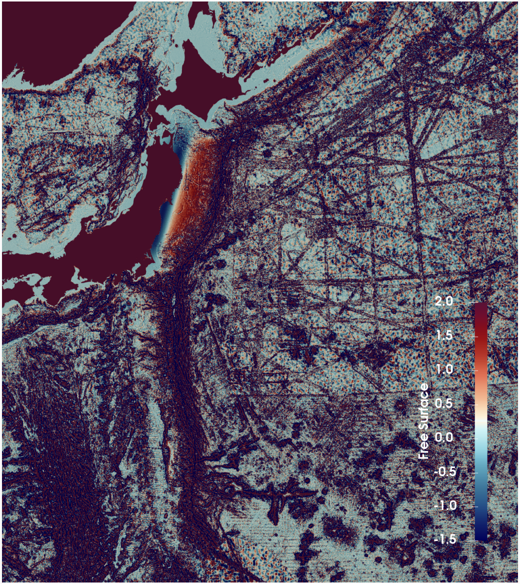

Numerical simulation of a tsunami: failure

... that did not work, the ocean at rest, far from the tsunami, starts spontaneously producing waves.

$\rightsquigarrow$ **The simulation is not usable!**

This comes from the non-preservation of stationary solutions:

$$\frac{\partial}{\partial t}u(x,t) + \frac{\partial}{\partial x}f(u(x,t)) = s(u(x,t))$$

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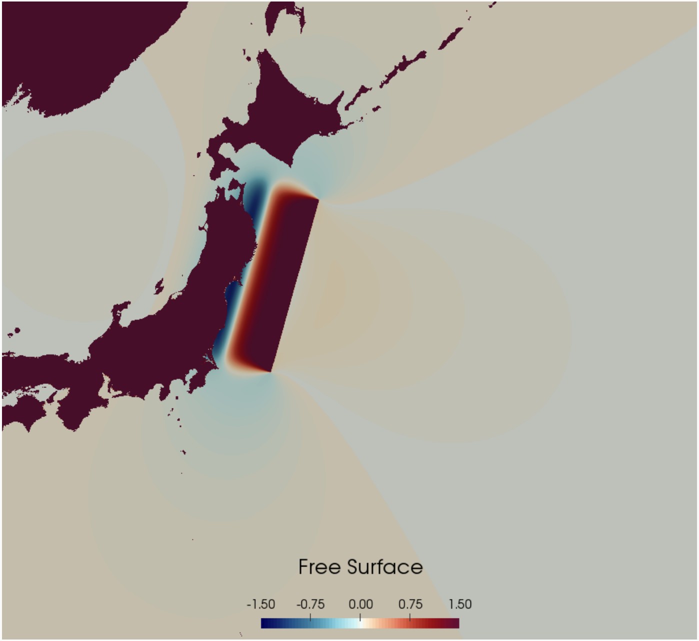
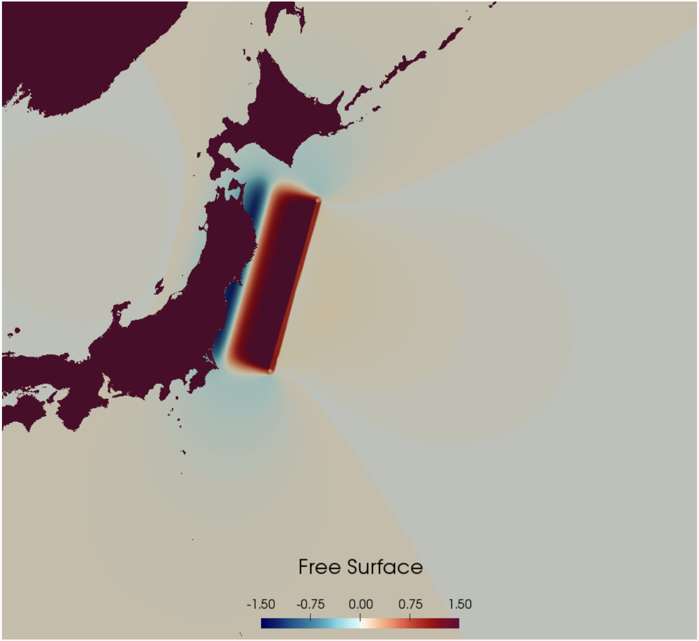
Hence the need to develop numerical methods that **preserve stationary solutions**: so-called **well-balanced** methods.

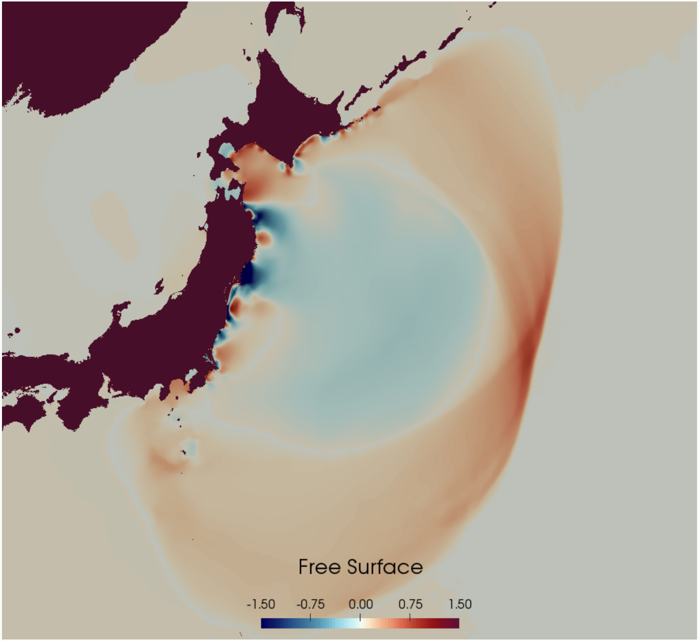
Numerical simulation of a tsunami: well-balanced method



Numerical simulation of a tsunami: well-balanced method



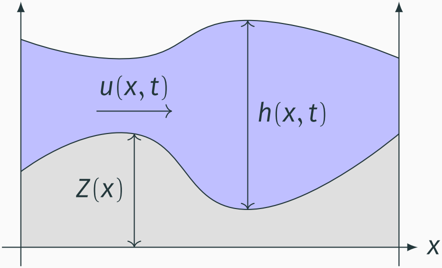
Numerical simulation of a tsunami: well-balanced method



The shallow water equations

The shallow water equations are governed by the following PDE:

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

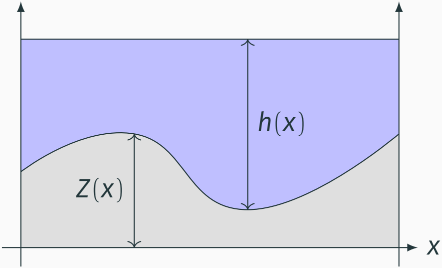


- $h(x, t)$: water height
- $u(x, t)$: water velocity
- $q = hu$: water discharge
- $Z(x)$: known topography
- g: gravity constant

The shallow water equations: steady solutions

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

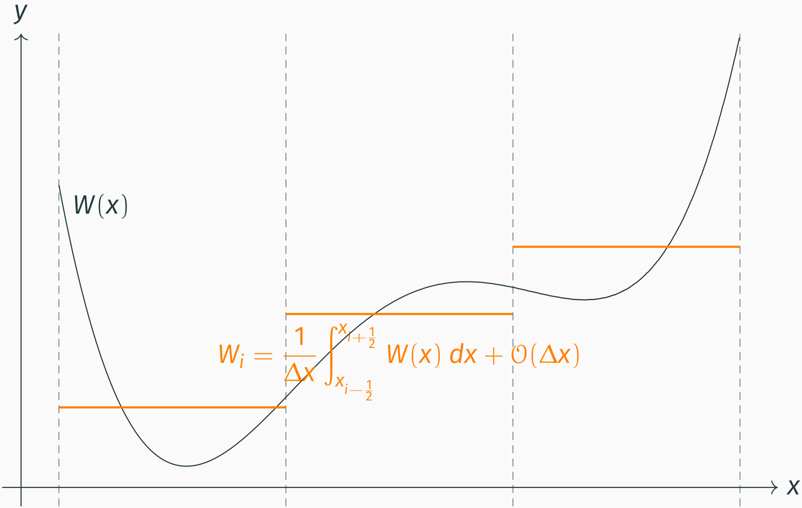
$$\begin{cases} \partial_x q = 0, \\ \partial_x \left(\dfrac{q^2}{h} + \dfrac{1}{2} g h^2 \right) = -g h \partial_x Z(x). \end{cases}$$



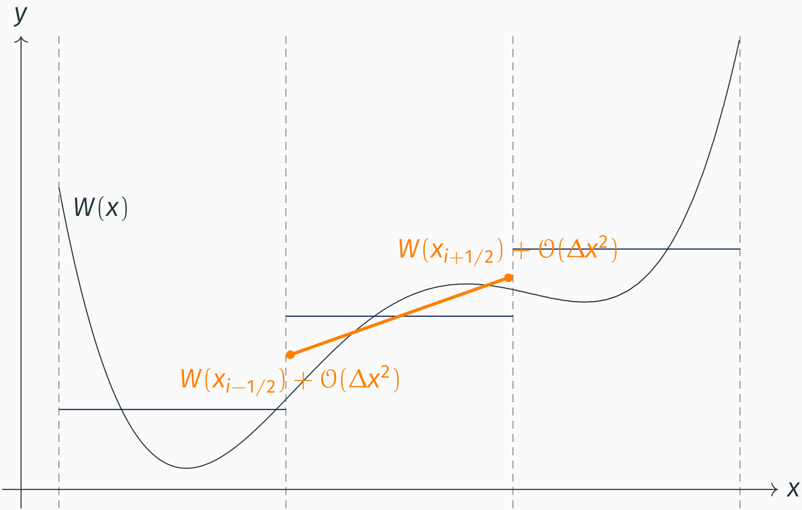
For the shallow water equations, if the velocity vanishes, we obtain the lake at rest steady solution:

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

Finite volume method, visualized



Discontinuous Galerkin, visualized



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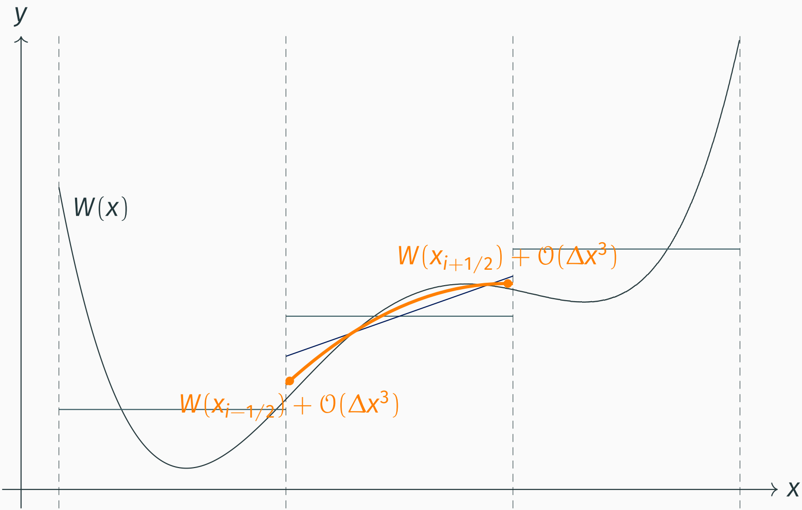

Discontinuous Galerkin: an example

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

- a polynomial of degree 2 in each cell (Galerkin approximation),
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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 continuous data 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 $\varphi_0, \dots, \varphi_N$ on each cell Ω_i and approximate the solution in this basis.

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

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

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

Main idea

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Enhance the DG basis by using the steady solution!

$\rightsquigarrow$ If **the basis is enhanced with an approximation of the steady solution**, then the enhanced DG scheme will provide a better approximation of the steady solution than the classical version.

Enhanced DG bases

Assume that you know a **prior** $\overline{W}$ on the steady solution.

The goal is now to **enhance the modal basis** V using $\overline{W}$:

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

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A possibility is to replace the first element with $\overline{W}$

$$\bar{V} = \{\overline{W}, x, x^2, \ldots, x^N\}.$$

We can prove that the prior $\overline{W}$ needs to provide a **good approximation of the derivatives** of the steady solution (in addition to the steady solution itself).

$\rightsquigarrow$ A Physics-Informed Neural Network (**PINN**) is the ideal candidate!

Steady solutions as boundary value problems

As seen in the previous section, we seek an approximation of a steady solution using a PINN.

A **steady solution** is nothing but the **solution to a boundary value problem (BVP)**:

$$\begin{cases} \mathcal{D}(W, x) = 0 & \text{for } x \in \Omega, \\ W(x) = g(x) & \text{for } x \in \partial\Omega, \end{cases}$$

where $\mathcal{D}$ is a differential operator containing derivatives of W.

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Since their derivatives are easily computable by automatic differentiation, they are therefore **natural objects to approximate solutions to PDEs or ODEs**.

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Definition: PINN

A PINN is a neural network with input x and trainable weights θ, approximating the solution to a PDE or ODE, and denoted by $W_\theta(x)$.

PINNs: using the ODE residual

Recall that the PINN W_θ approximates the solution to the BVP

$$\begin{cases} \mathcal{D}(W, x) = 0 & \text{for } x \in \Omega, \\ W(x) = g(x) & \text{for } x \in \partial\Omega. \end{cases}$$

Based on this observation, we know that the PINN W_θ should approximately satisfy the above BVP:

$$\begin{cases} \mathcal{D}(W_\theta, x) \simeq 0 & \text{for } x \in \Omega, \\ W_\theta(x) \simeq g(x) & \text{for } x \in \partial\Omega. \end{cases}$$

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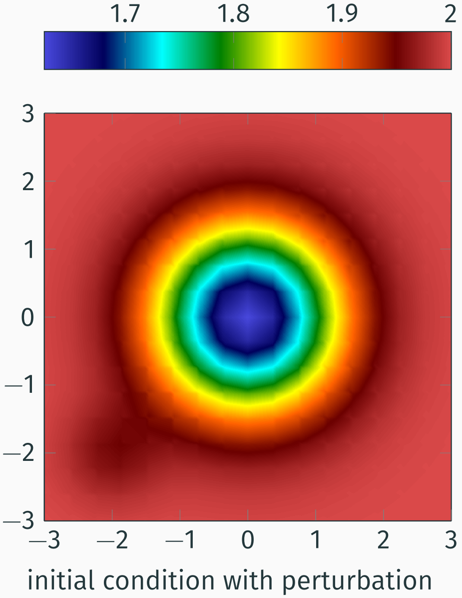
The idea behind PINNs training is to find the optimal weights θ_{opt} by **minimizing a loss function built from the ODE residual**:

$$\theta_{\text{opt}} = \underset{\theta}{\operatorname{argmin}} \left(\int_\Omega \|\mathcal{D}(W_\theta, x)\|_2^2 \, dx + \int_{\partial\Omega} \|W_\theta(x) - g(x)\|_2^2 \, dx. \right)$$

The Monte-Carlo method is used for the integrals, which makes the whole approach **mesh-less** and able to deal with **parametric BVPs**.

Perturbation of a shallow water steady solution



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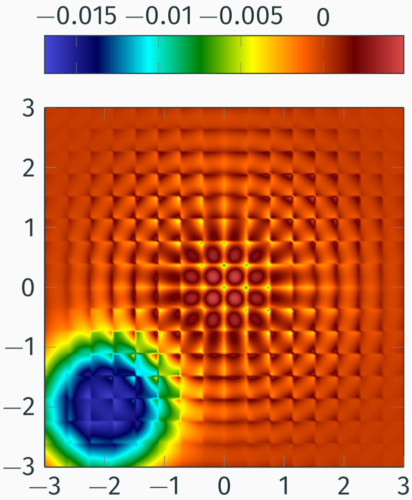
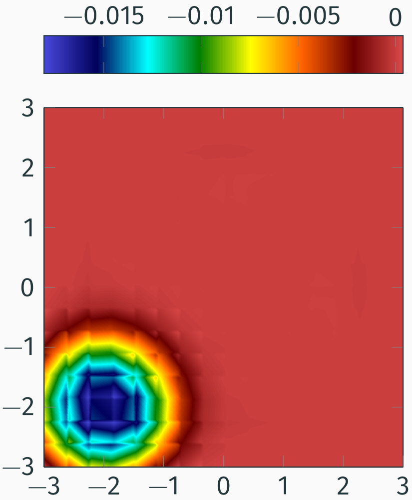


(a) $T = 0.1$, classical basis



(b) $T = 0.1$, enhanced basis

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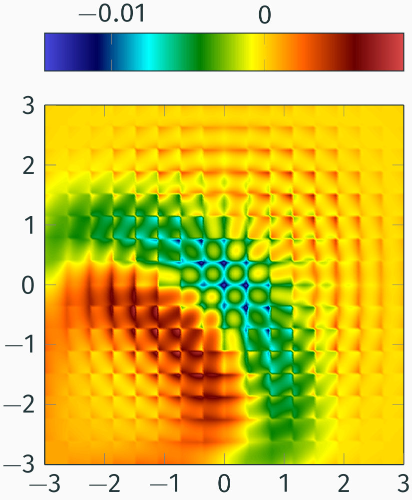
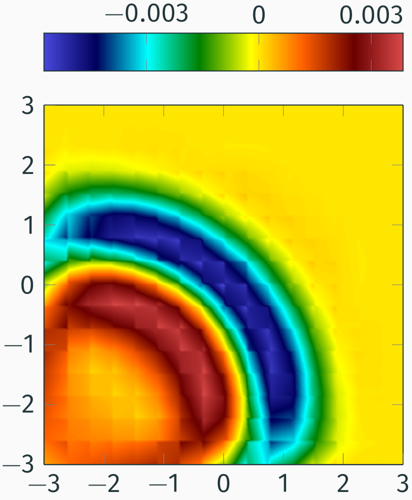
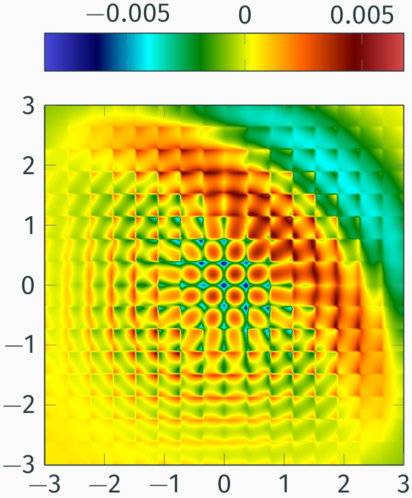


(c) $T = 0.6$, classical basis

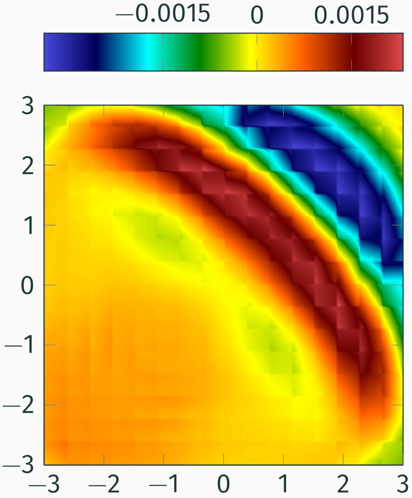


(d) $T = 0.6$, enhanced basis

Perturbation of a shallow water steady solution



(e) $T = 1.2$, classical basis

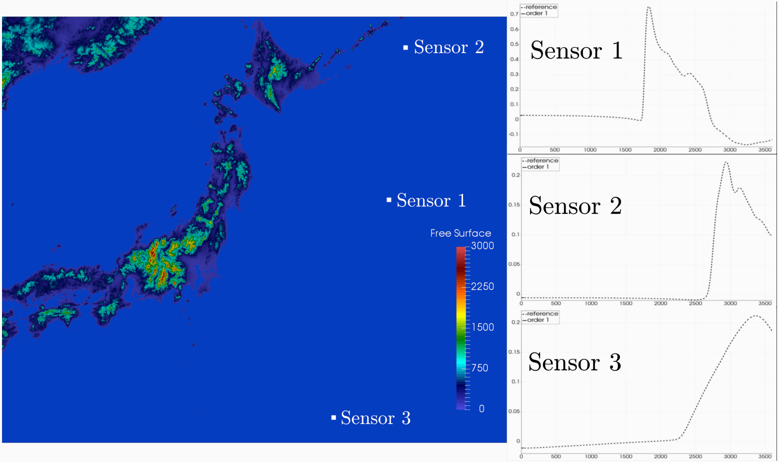


(f) $T = 1.2$, enhanced basis

Thank you for your attention!

Ingredients required for a numerical simulation

Fourth step: Verification of the numerical results

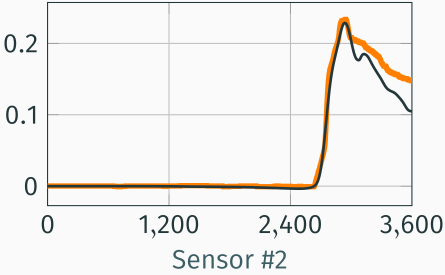


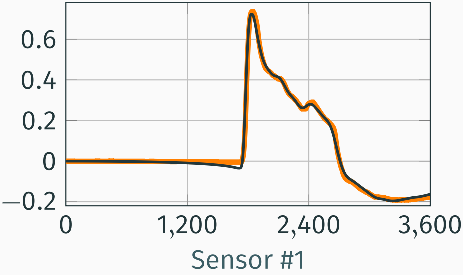
Simulation of the 2011 Japan tsunami

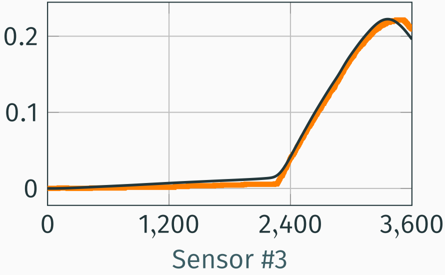
Water depth at sensors:

- #1: 5700 m;
- #2: 6100 m;
- #3: 4400 m.

Plots of the time variation
of the water height (in meters).
data in black, simulation in orange







PINNs: advantages and drawbacks

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The most interesting use of PINNs, in our case, is to deal with **parametric ODEs and PDEs**, where dimension-insensitivity is paramount.

Parametric PINNs: approximation using the ODE residual

The parametric PINN $W_\theta(x;\boldsymbol{\mu})$, with parameters $\boldsymbol{\mu} \in \mathbb{P} \subset \mathbb{R}^m$ approximates the solution to the parametric BVP

$$\begin{cases} \mathcal{D}(W, x; \boldsymbol{\mu}) = 0 & \text{for } x \in \Omega, \boldsymbol{\mu} \in \mathbb{P}, \\ W(x) = g(x; \boldsymbol{\mu}) & \text{for } x \in \partial\Omega, \boldsymbol{\mu} \in \mathbb{P}. \end{cases}$$

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The loss function then becomes

$$\mathcal{J}_{\text{ODE}}(\theta) = \underbrace{\int_{\mathbb{P}} \int_{\Omega} \|\mathcal{D}(W_\theta, x; \mu)\|_2^2 \, dx d\mu}_{\mathcal{J}_\Omega(\theta)} + \underbrace{\int_{\mathbb{P}} \int_{\partial\Omega} \|W_\theta(x; \mu) - g(x; \mu)\|_2^2 \, dx d\mu}_{\mathcal{J}_{\text{boundary}}(\theta)}.$$