Machine Learning and Reduced Order Modeling for Uncertainty Quantification in Nonlinear PDE Problems

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CASA

TU/e EINDHOVEN UNIVERSITY OF TECHNOLOGY

CWI

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Need for Uncertainty Quantification (UQ)

Need for UQ

NWO Perspective program sling.

- sling. = Sloshing of Liquefied Natural Gas
- Budget: 3.5 M€
- 10 industrial partners, among which:

  Shell, Argos, Total, Damen and *Gaztransport et Technigaz*

NWO Perspective program

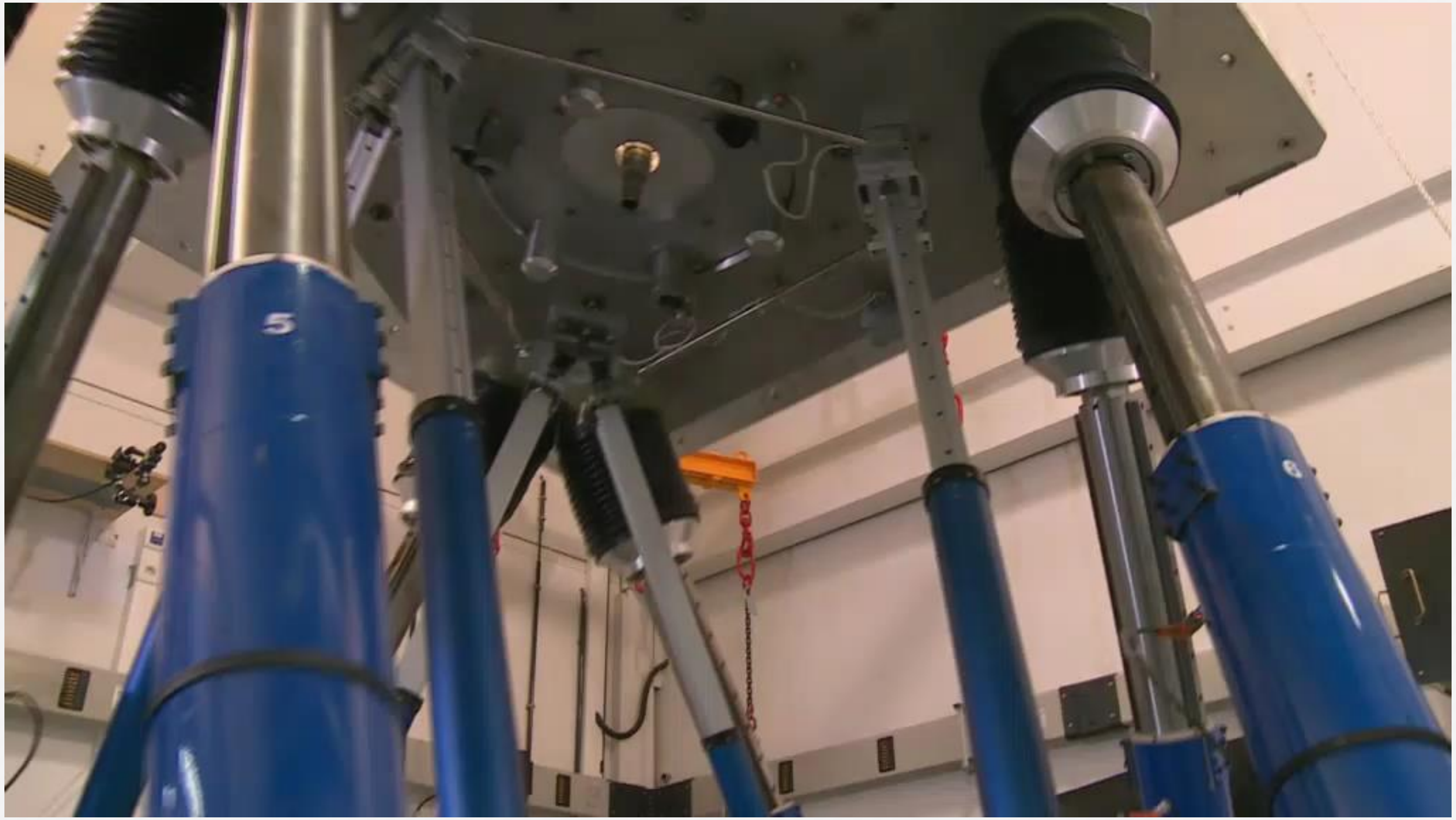
NWO Perspective program

NWO Perspective program sling.

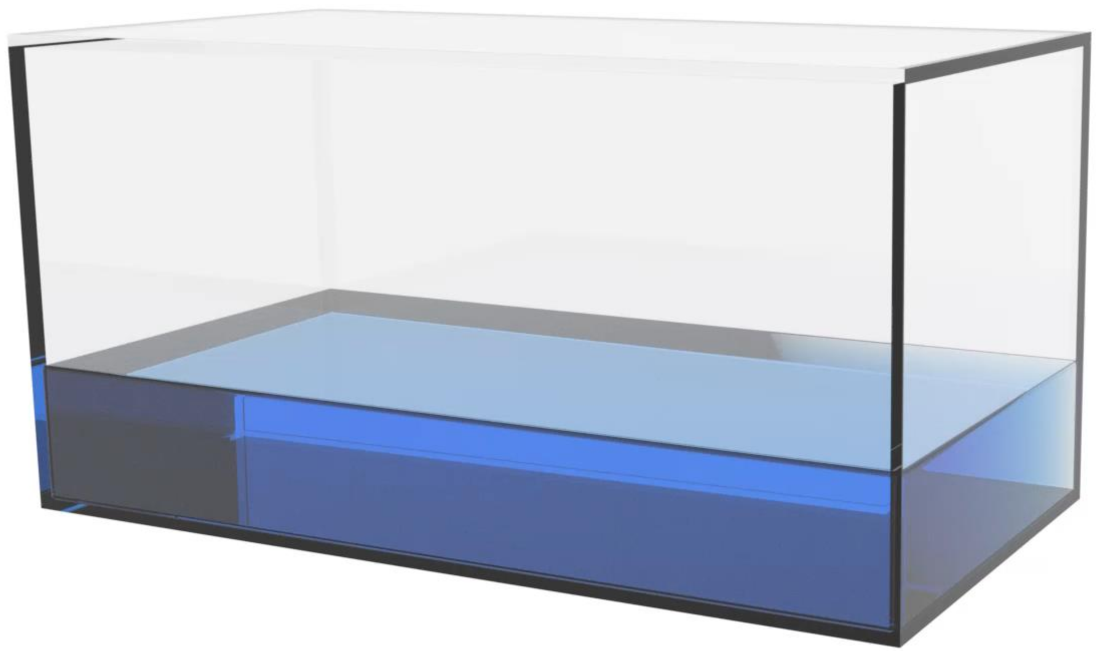
At Gaztransport et Technigaz:

Till recently:
R&D driven by experimental data

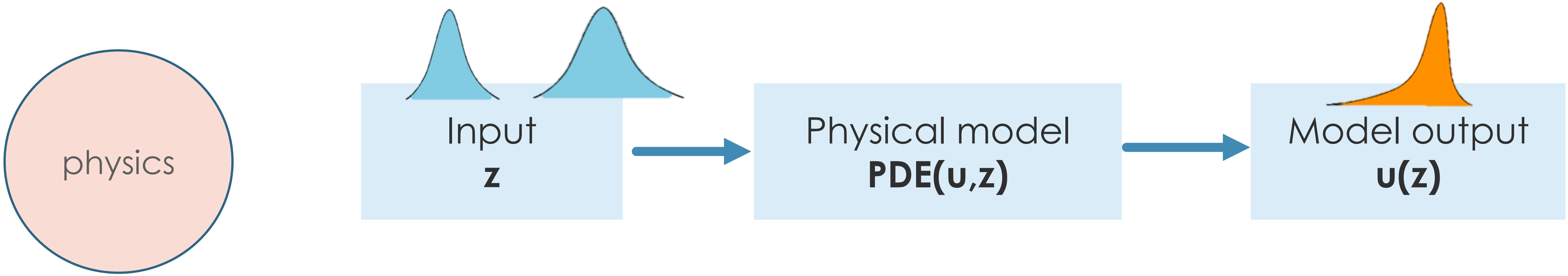
Since recently:
R&D driven by experimental data and computational models



NWO Perspective program

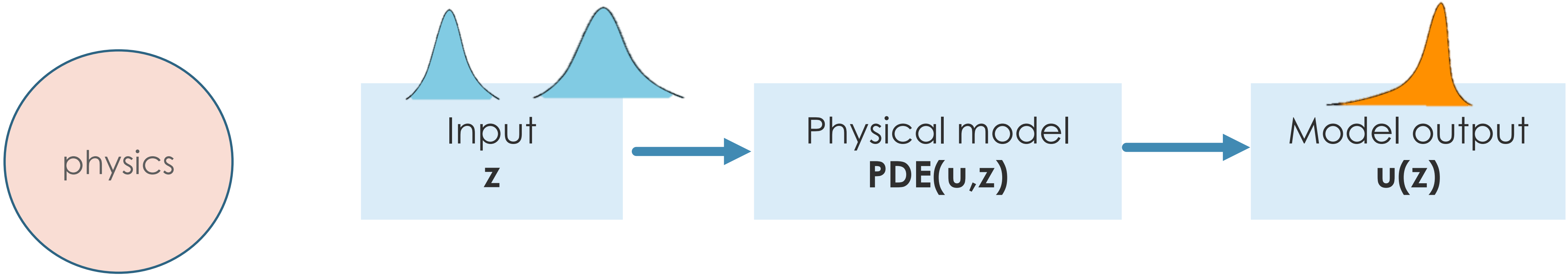


Old UQ (Monte Carlo)



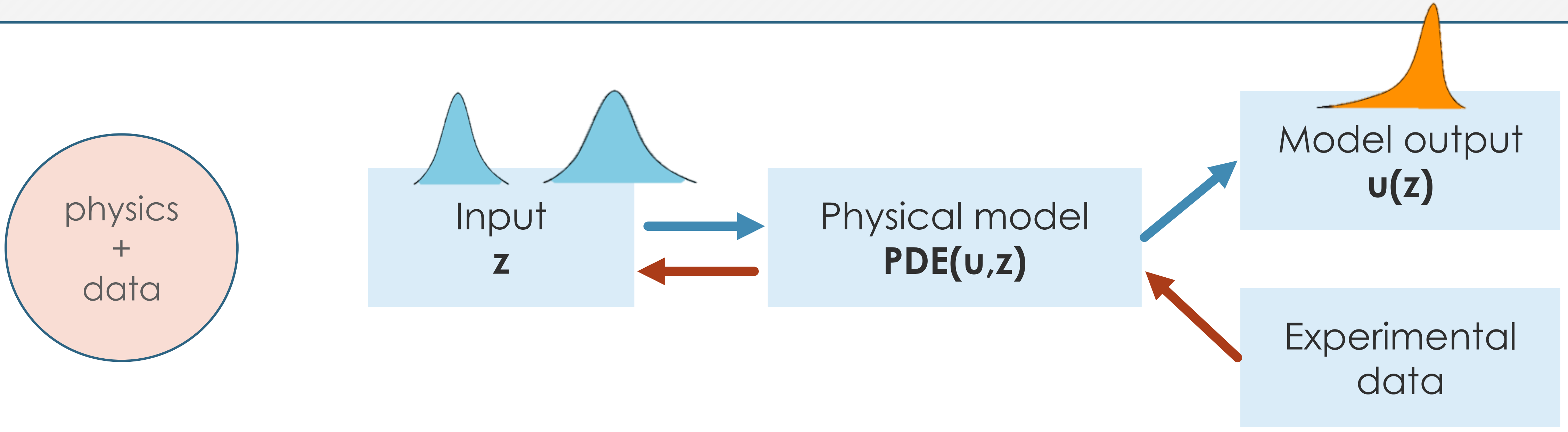
Computationally very, very expensive !

Existing UQ (Polynomial chaos)



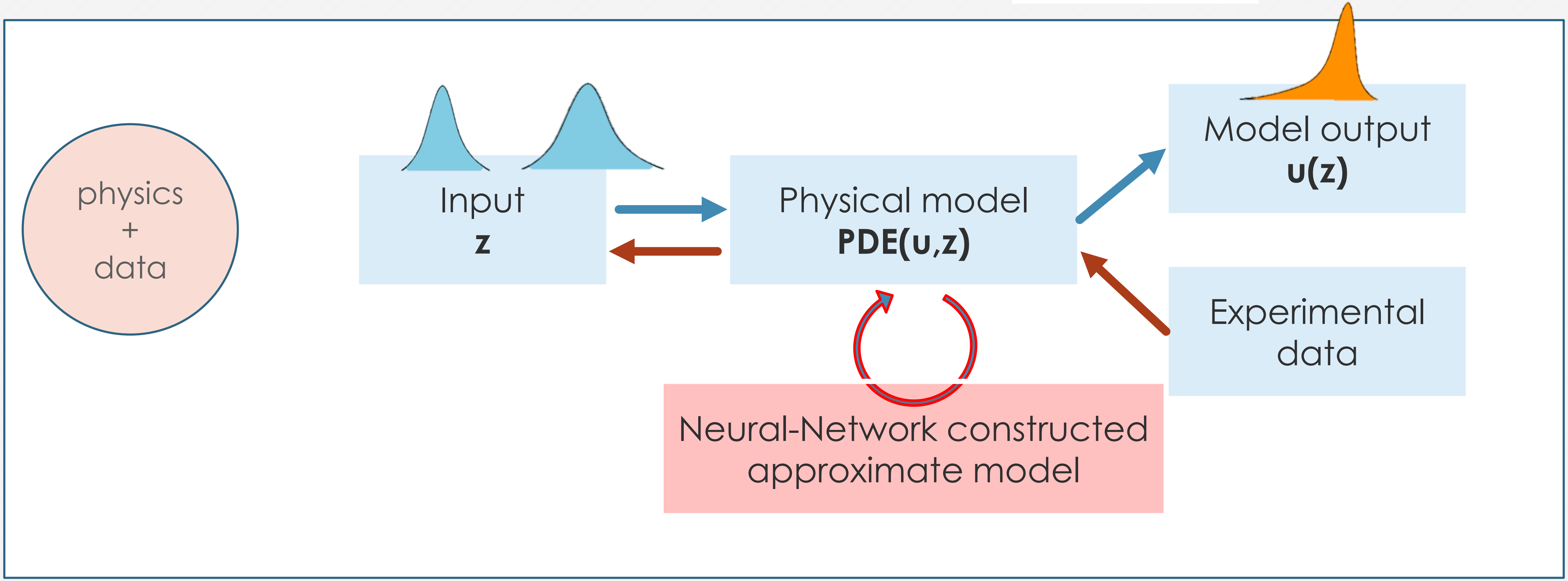
Still computationally expensive, but less

Existing UQ (Polynomial Chaos)



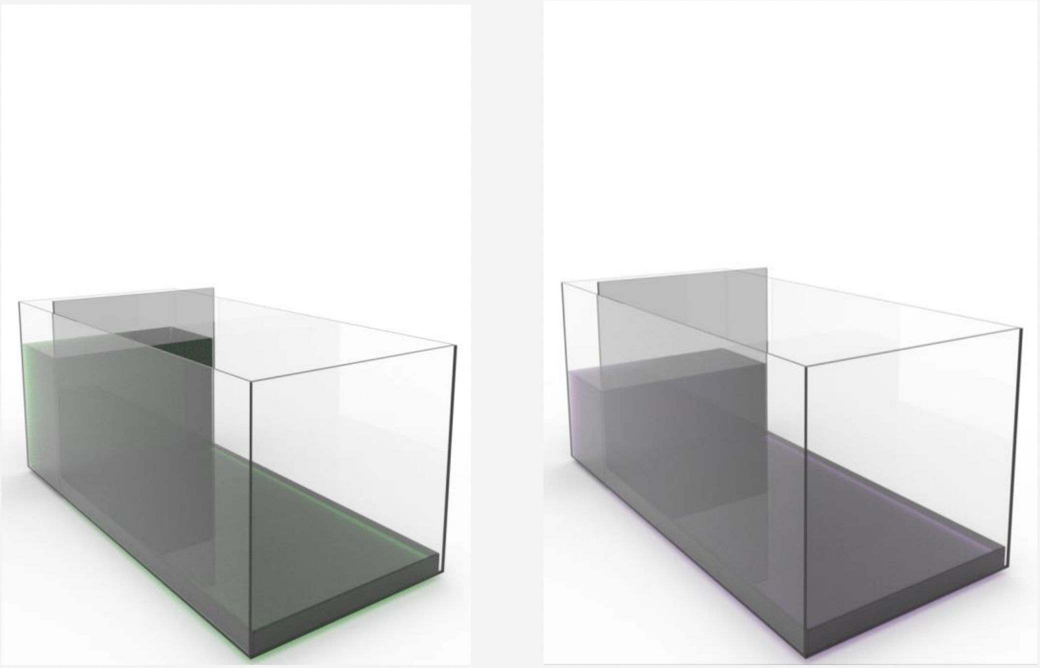
Computationally very expensive !

New UQ – with Machine Learning – in



Multigrid neural networks

- **Goal:** computationally very efficient approximate model
- **Approach:** grid coarsening (multigrid)
- **Idea**: neural networks learn relative solution errors between grid levels
- **Assumption:** less samples needed on finer grids (because of less variance)

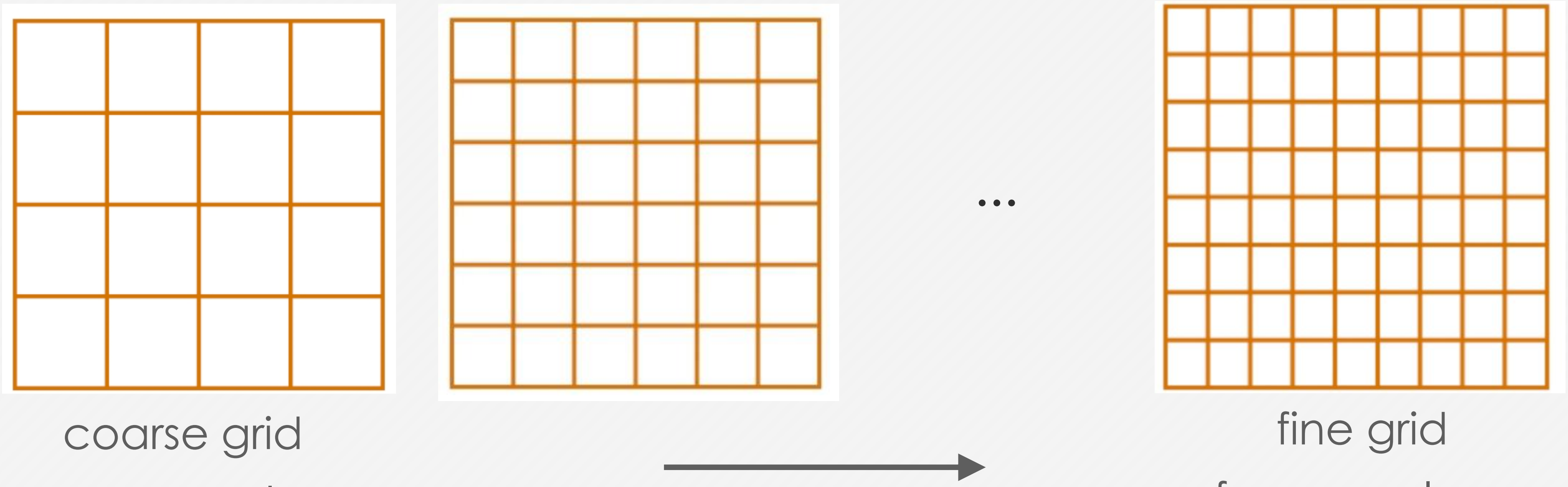


Sloshing is very sensitive to uncertainty in parameters

Y. van Halder, B. Sanderse, B. Koren, Multi-level neural networks for PDEs with uncertain parameters, ArXiv 2004.131128, 2020

Multigrid expansion

PDE(u,z) | $u^1(z)$ | $u^2(z)$ | … | $u^N(z)$



coarse grid

many samples **z**

fine grid

few samples **z**

Multigrid expansion: $$u(z) \approx u^3(z) = u^1(z) + (u^2(z) - u^1(z)) + (u^3(z) - u^2(z)) = u^1(z) + e^2(z) + e^3(z)$$

Neural network design

- **Idea 1**:
  Relative solution error is related to local truncation error:

$$u(z) \to \tau(z) \to e(z)$$

Neural network design

- **Idea 1**:
  Relative solution error is related to local truncation error:

$$u(z) \to \tau(z) \to e(z)$$

- Construct neural network *P* to relate *u* to e:

$$e(z) \approx P(u(z))$$

$$\begin{aligned} u^3(z) &= u^1(z) + e^2(z) + e^3(z) \\ &= u^1(z) + P^2(u^1(z)) + P^3(u^2(z)) \end{aligned}$$

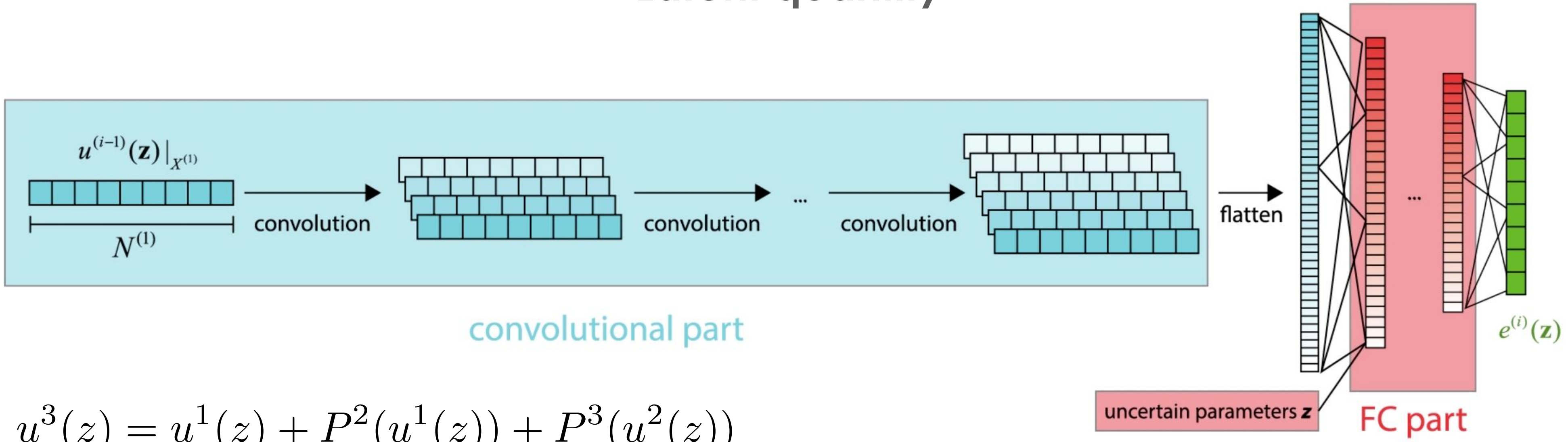
Neural network design

$$u(z) \rightarrow \tau(z) \rightarrow e(z)$$

Convolutional neural network

Fully connected neural network

Latent quantity

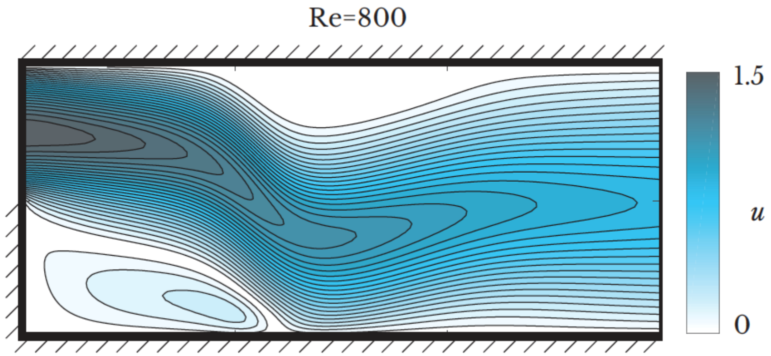


$$u^3(z) = u^1(z) + P^2(u^1(z)) + P^3(u^2(z))$$

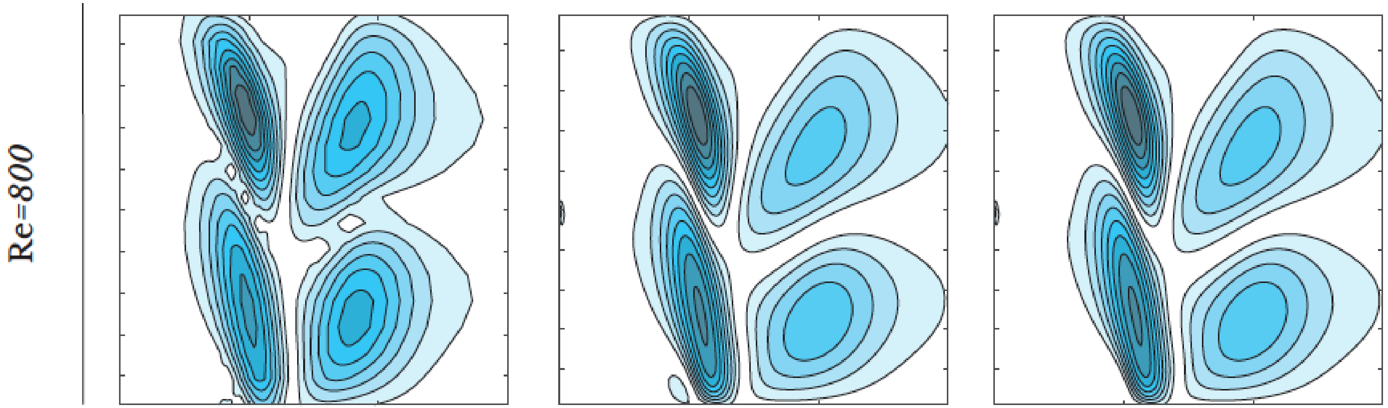
Neural network design

- **Idea 2:**

Relative errors e(z) have similar spatial structure: $e^2(z) \sim e^3(z) \sim \dots$



$e^2(z)$ **$e^3(z)$** **$e^4(z)$**



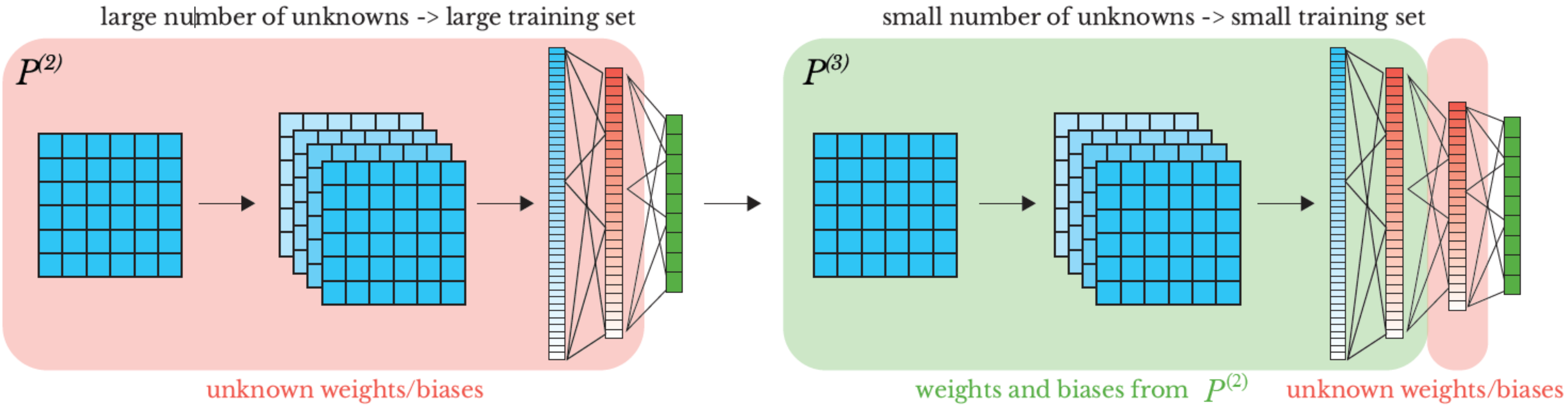
coarse grid → fine grid

Neural network design

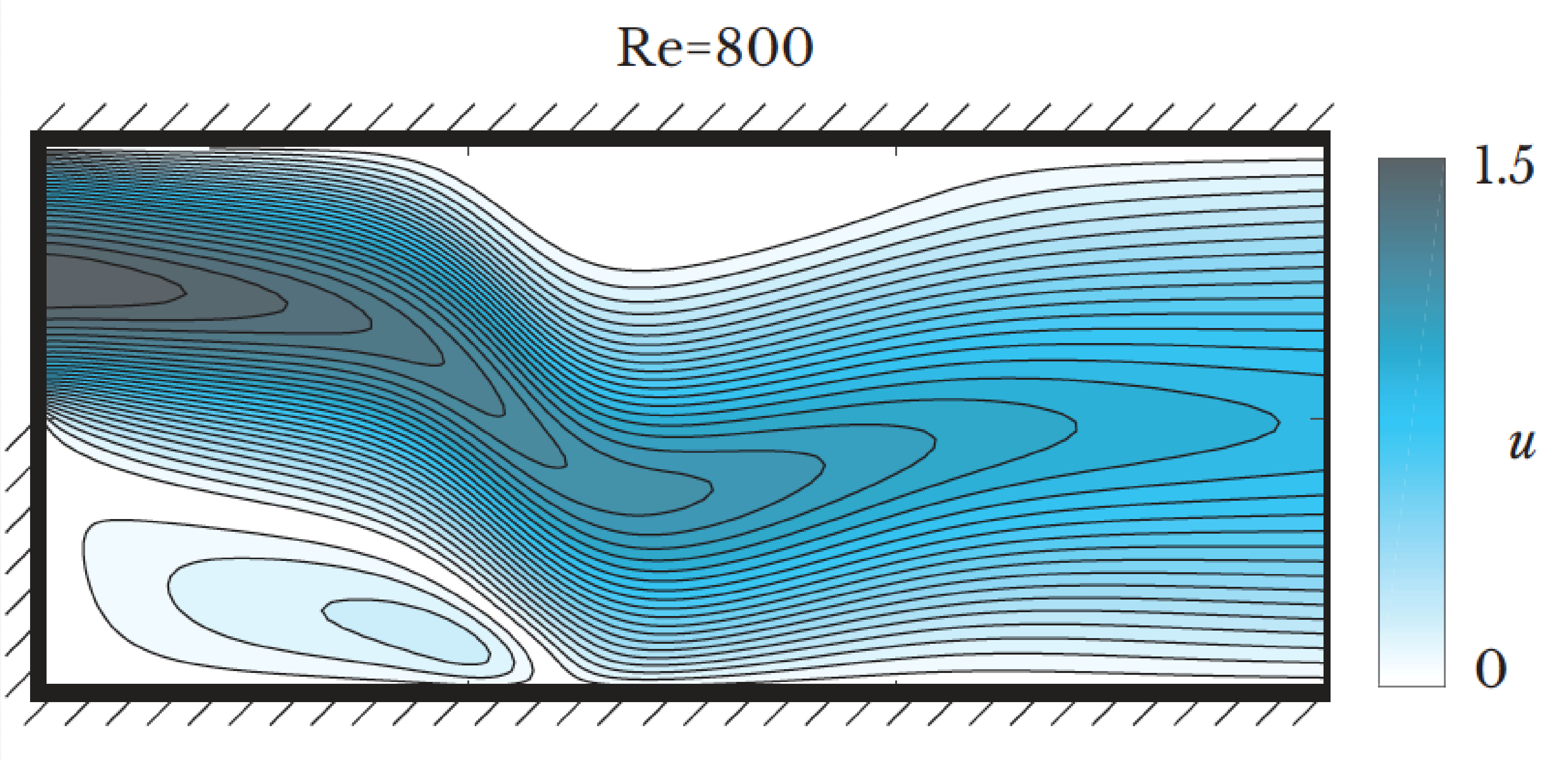
- **Idea 2:**

  Relative errors e(z) have similar spatial structure: $e^2(z) \sim e^3(z) \sim \ldots$

- Use **transfer learning** to train subsequent neural networks

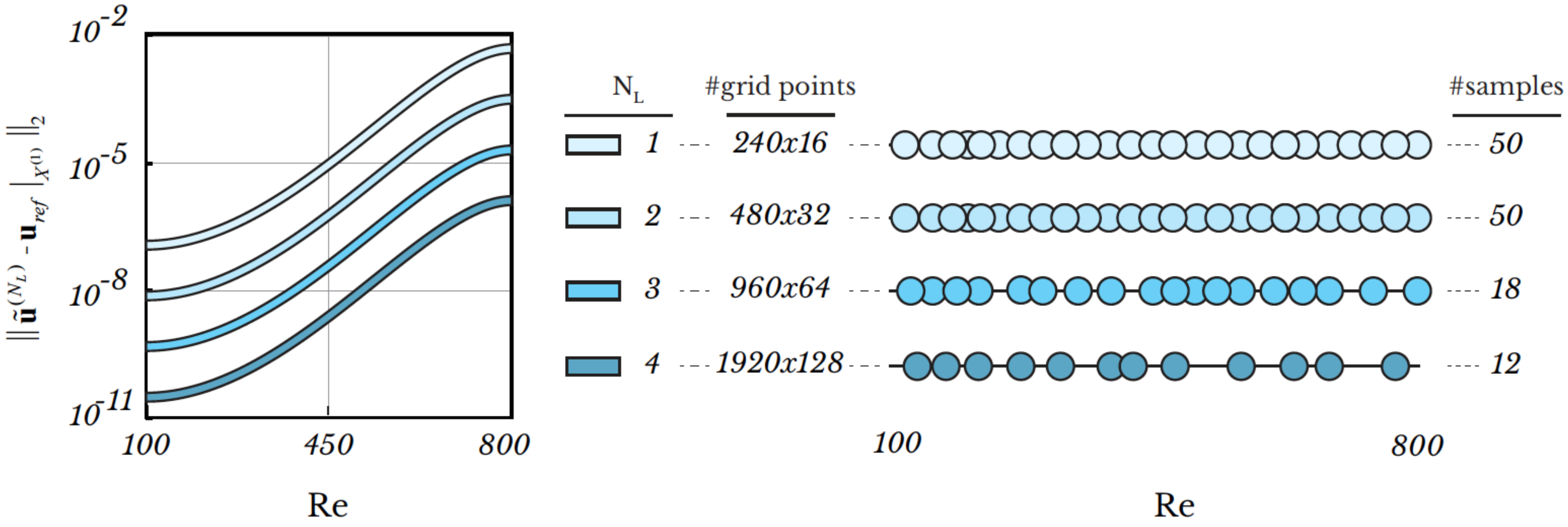


Backward-facing step flow



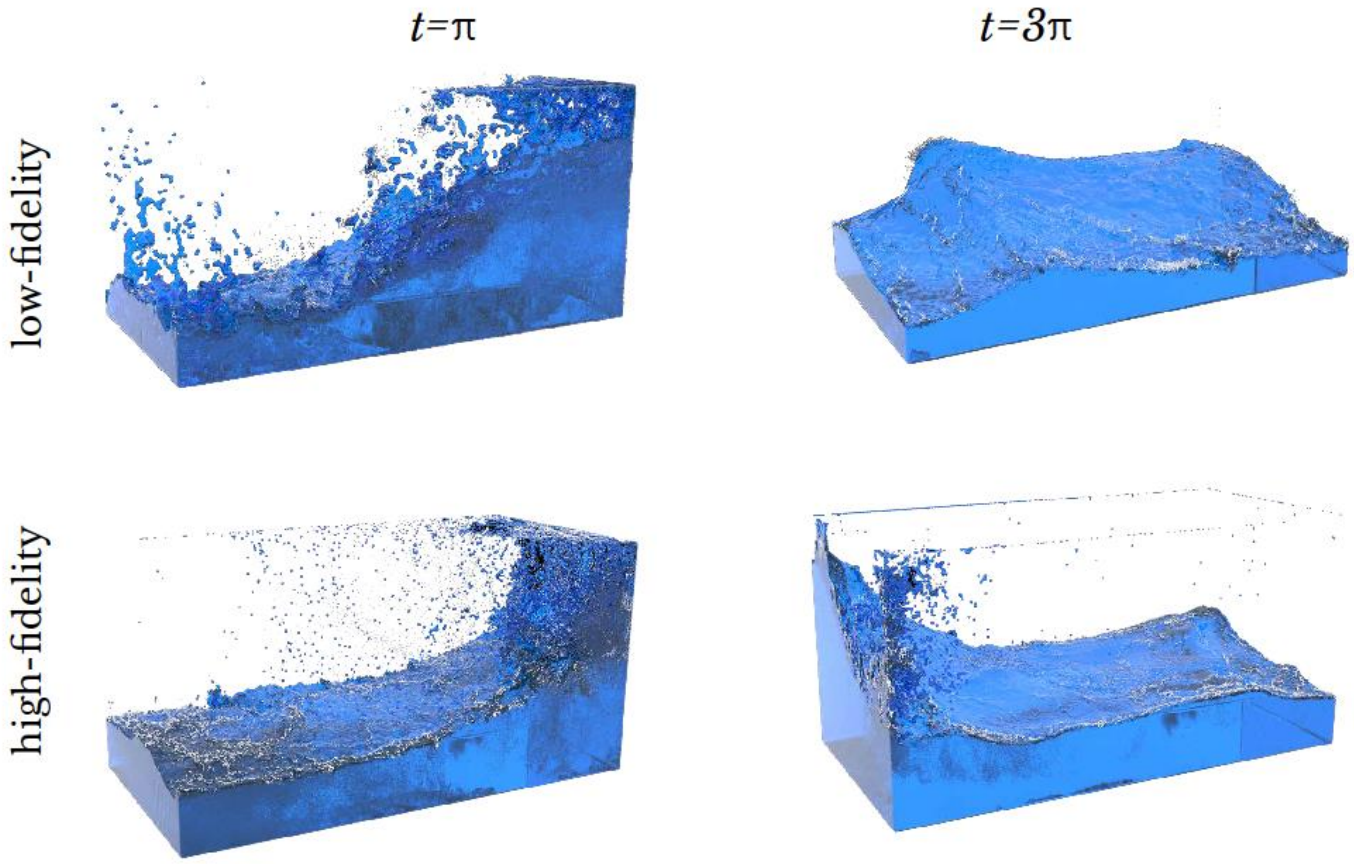
Backward-facing step flow

- Uncertainty in Reynolds number

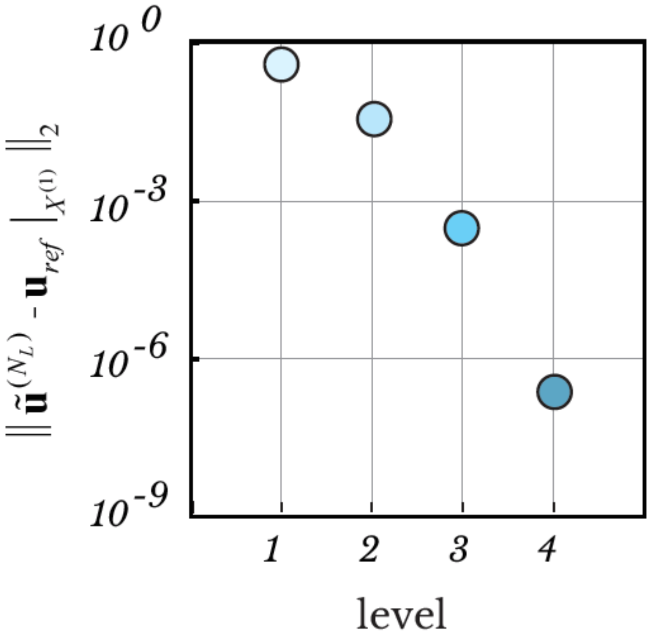


Sloshing

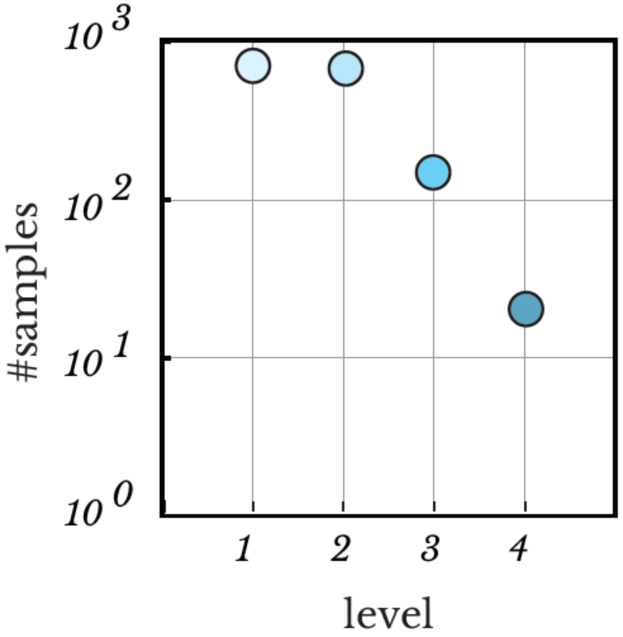
- Two uncertainties in prescribed rotational gravitational field (rotation around two axes)
- Particle-in-cell method



Sloshing

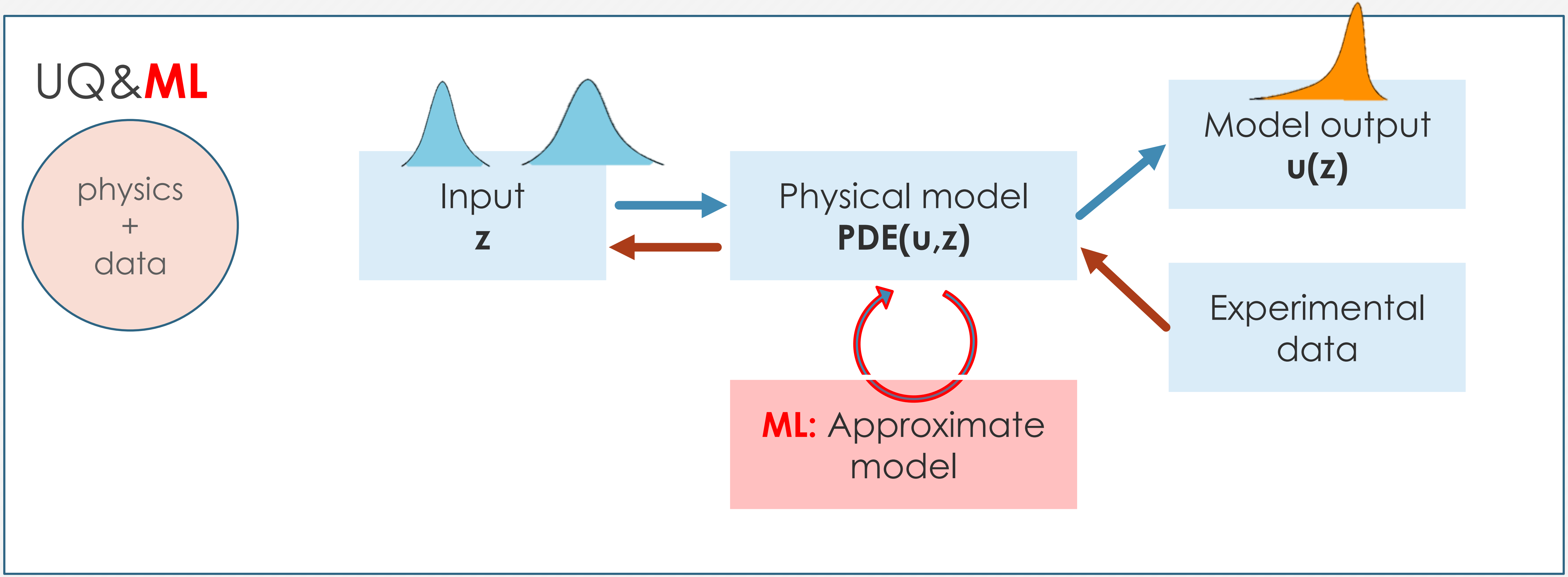


error decreases
rapidly

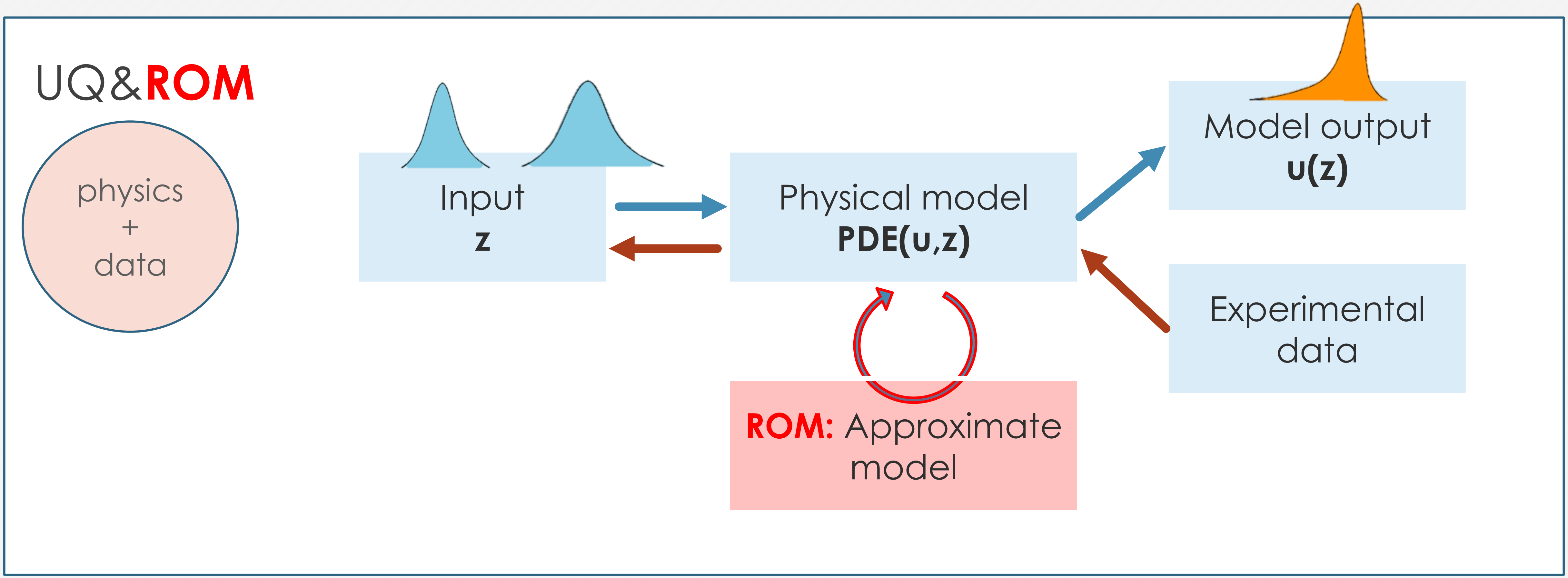


#samples decreases
rapidly

UQ with ML-constructed approximate model

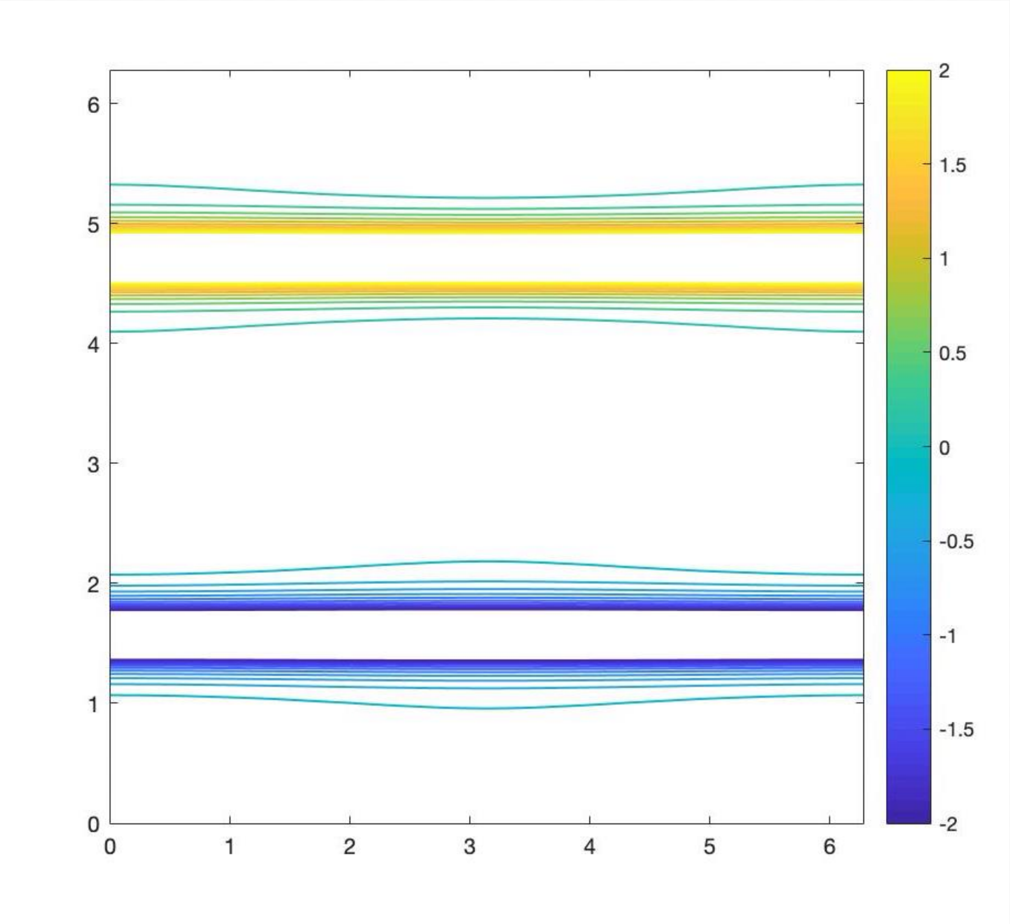


UQ with ROM-constructed approximate model

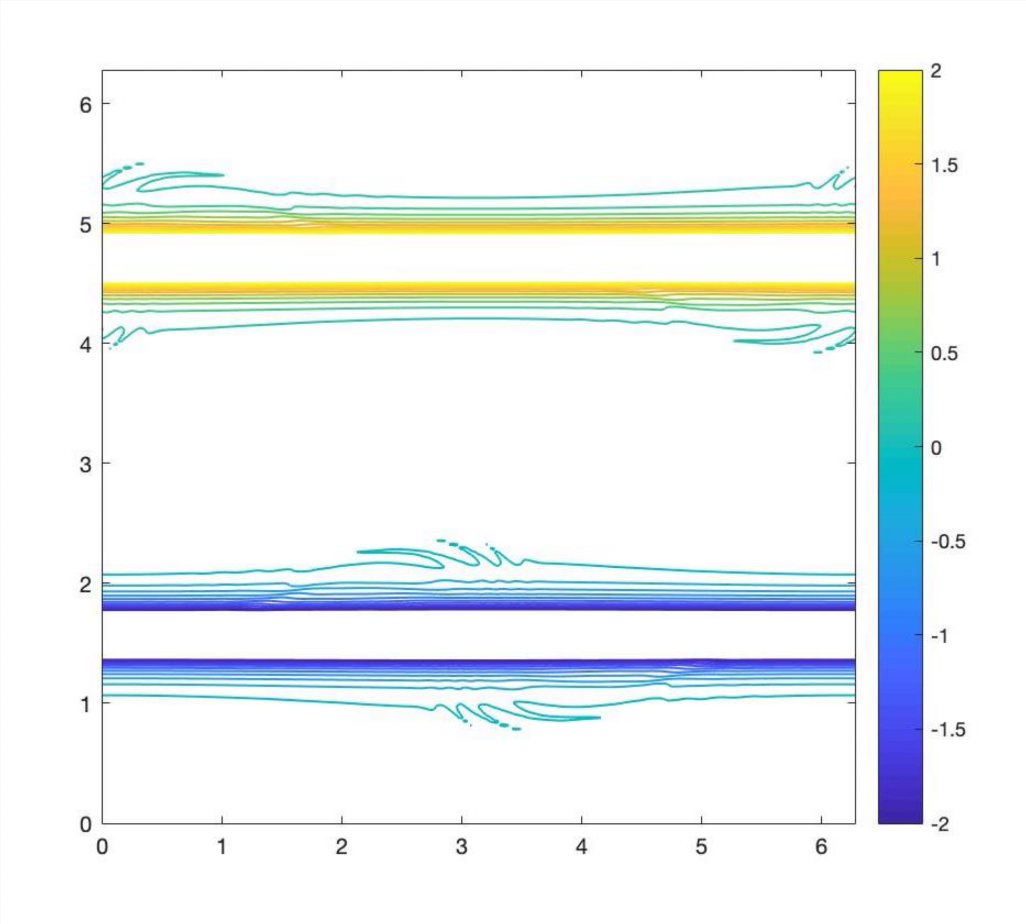


B. Sanderse, Non-linearly stable reduced-order models for incompressible flow with energy-conserving finite volume methods, *Journal of Computational Physics*, 2020

Roll-up of shear flow

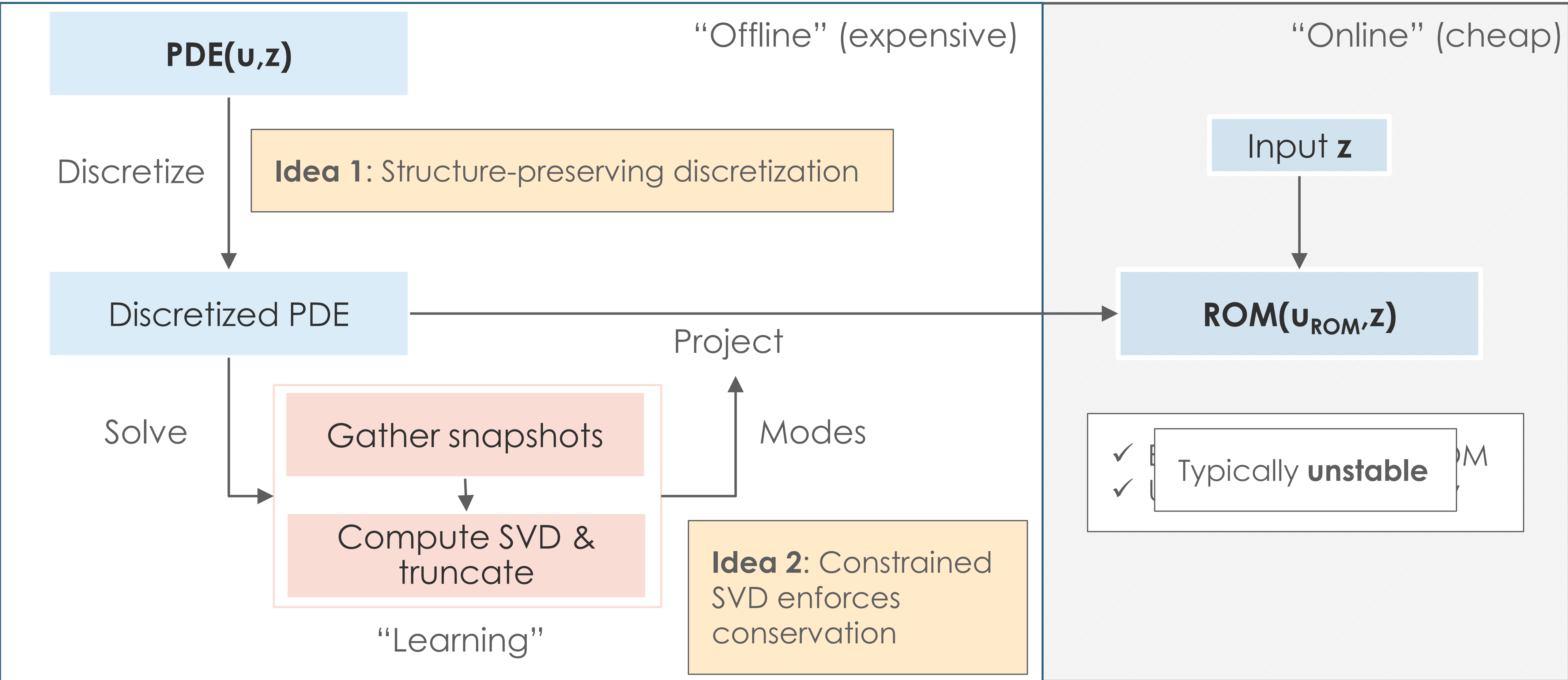


Full-order model (FOM),
Initial condition
40,000 degrees of freedom

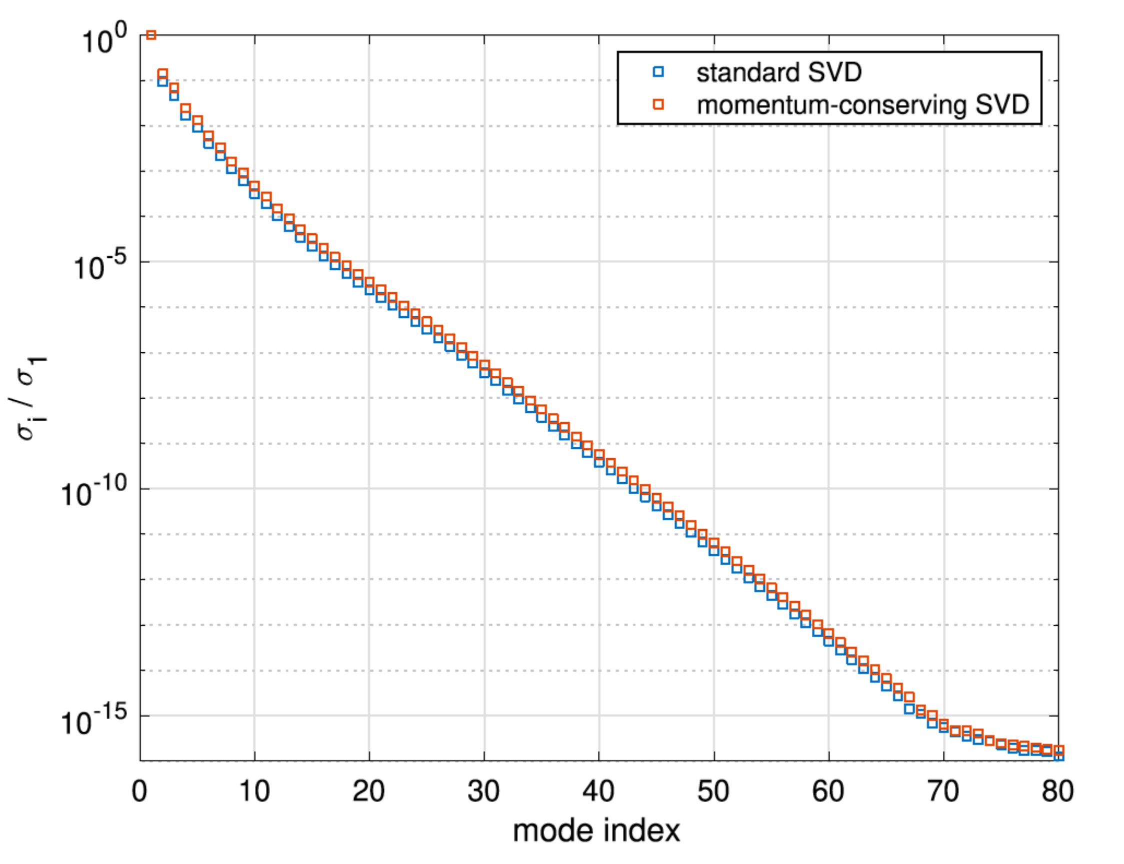


Reduced-order model (ROM),
16 degrees of freedom

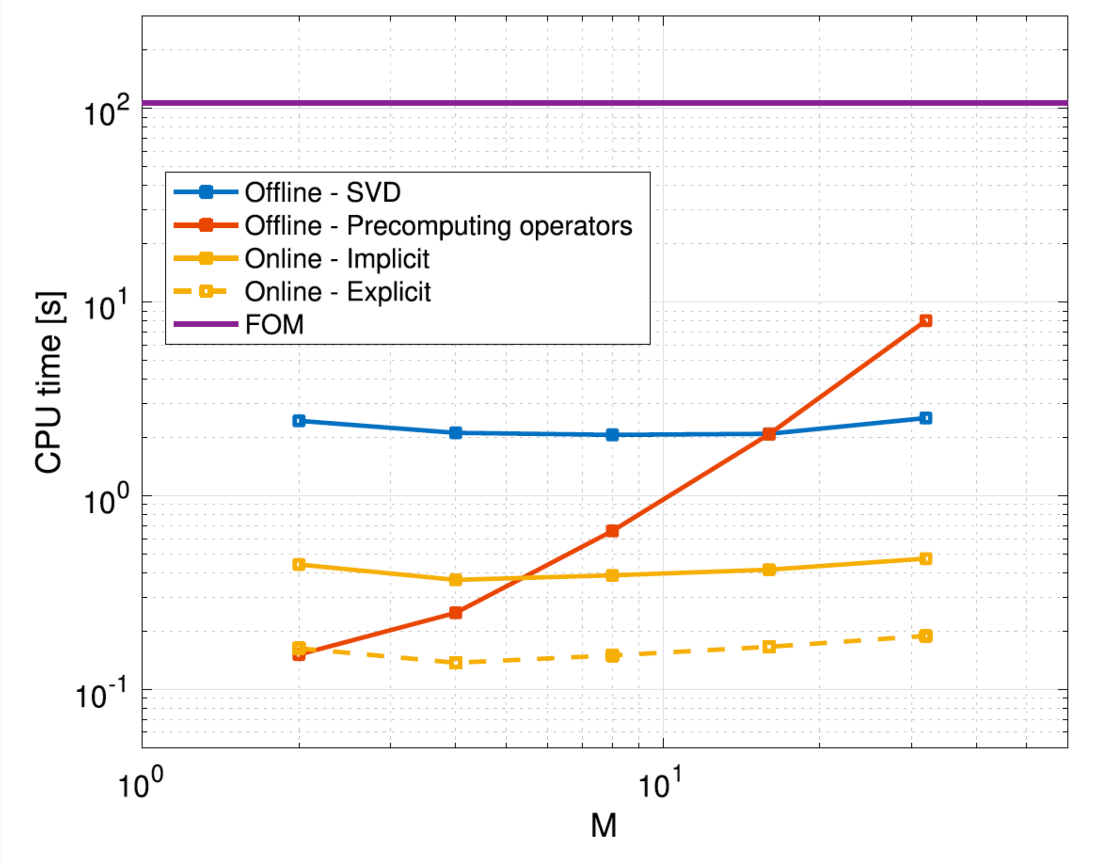
Structure-preserving ROM



Speed-up: O(10^2-10^3)

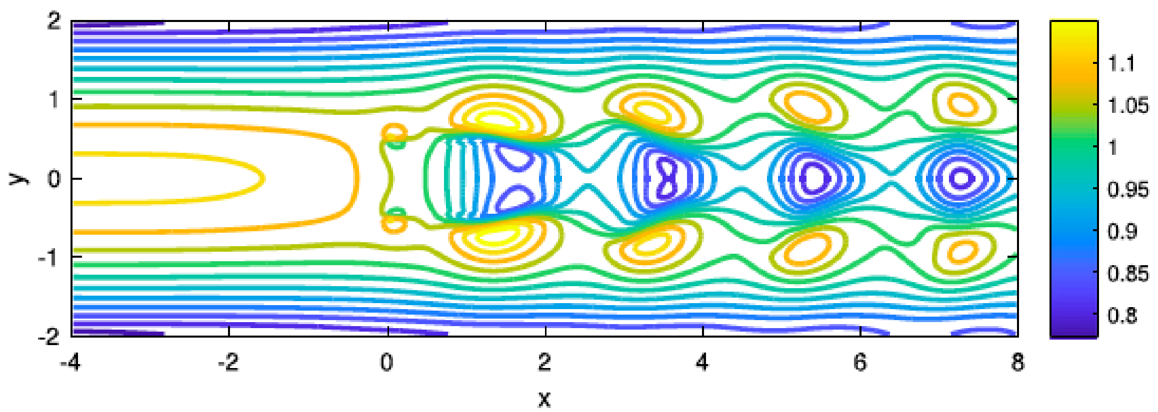


Singular value decay = "potential for reduction"

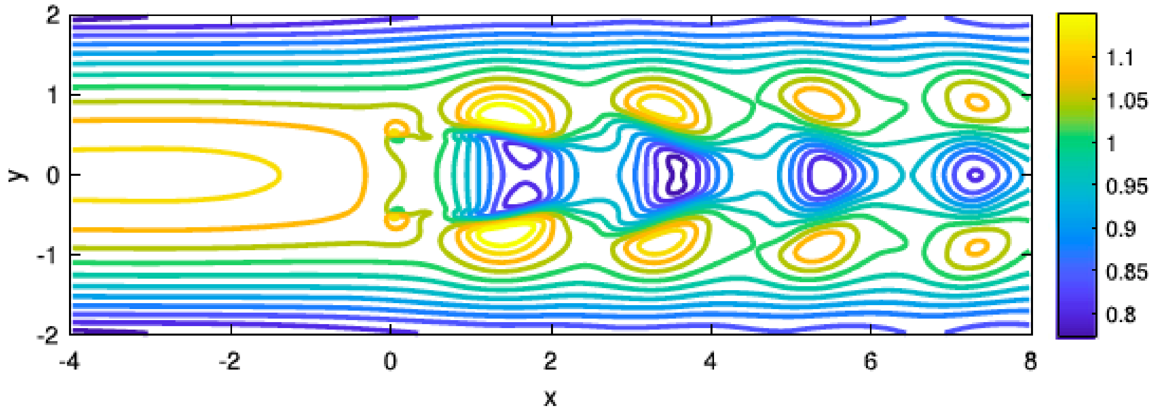


Speed-up

ROM for wind-farm aerodynamics



FOM
57,840 degrees of freedom



ROM
10 degrees of freedom

Advantages

Multigrid neural networks:

- ✓ Uncertainties computable on coarse grids
- ✓ Non-intrusive, not PDE-specific
- ✓ Based on error structure between grid levels

Structure-preserving ROMs:

- ✓ Time-dependent approximation to entire solution
- ✓ Very large speed-ups
- ✓ Structure-preservation of continuous equations: stability guaranteed

Challenges

Multigrid neural networks:

- Time-dependent QoIs
- High-dimensional spaces of uncertain parameters

Structure-preserving ROMs:

- Intrusive (code access required)
- Requires identification of "structure" and associated discretization

Thank you for your interest