Artificial neural network for bifurcating phenomena modelled by nonlinear parametrized PDEs

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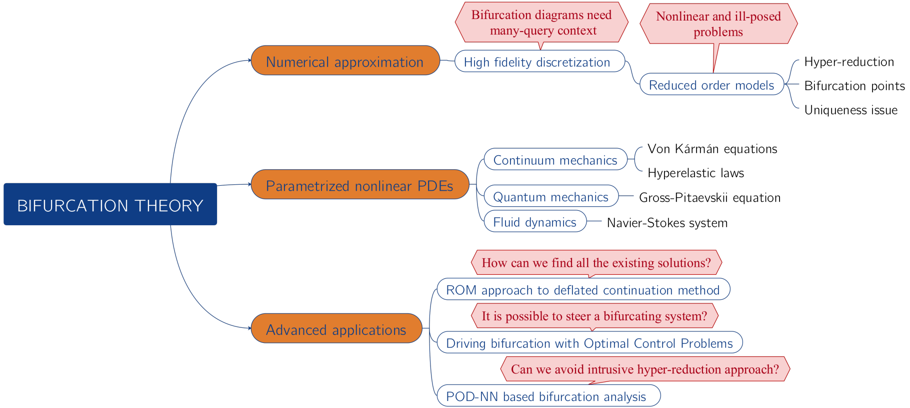
FEniCS 2021
22-26 March

Outline map

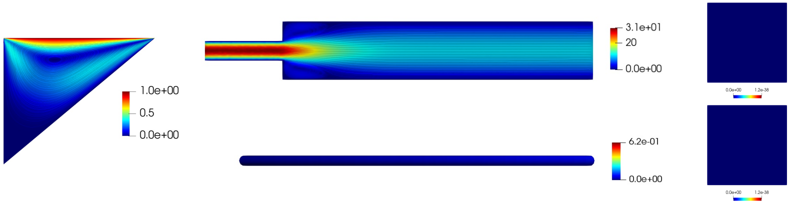


All the simulations were performed within **FEniCS**[1], **RBniCS**[2] and **PyTorch**.

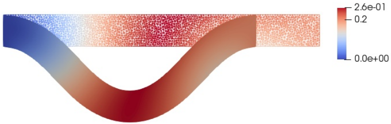
[1] A. Logg et al. *Automated Solution of Differential Equations by the Finite Element Method*. Springer, 2012.
[2] RBniCS - reduced order modelling in FEniCS. https://www.rbnicsproject.org

Preliminary examples

Question:
What have in common complex models coming from different physical contexts?
$\Rightarrow$ Sudden changes linked to qualitatively different behaviour of the solutions.



Example:
The situation for a compressed beam can change abruptly when the load is increased beyond a certain critical level at which the beam buckles.



Bifurcation theory and its numerical approximation

We represent a nonlinear PDE with the parametrized mapping $G : \mathbb{X} \times \mathcal{P} \to \mathbb{X}'$.
Given $\boldsymbol{\mu} \in \mathcal{P} \subset \mathbb{R}^P$, seek $X(\boldsymbol{\mu}) \in \mathbb{X}$ such that:

Strong form

$$G(X(\boldsymbol{\mu}); \boldsymbol{\mu}) = 0, \quad \text{in } \mathbb{X}'. \qquad (1)$$

Weak form

$$g(X(\boldsymbol{\mu}), Y; \boldsymbol{\mu}) = 0, \quad \forall\ Y \in \mathbb{X}. \qquad (2)$$

Consider the finite dimensional space $\mathbb{X}_\mathcal{N} \subset \mathbb{X}$, with dimension $\mathcal{N}$.

Algorithm 1 A pseudo-code for the reconstruction of a branch

1: $\mathrm{X}_0 = \mathrm{X}_{guess}$ ▷ Initial guess
2: **for** $\boldsymbol{\mu}_j \in \mathcal{P}_K$ **do** ▷ **Continuation loop**
3: $\quad \mathrm{X}_j^{(0)} = \mathrm{X}_{j-1}$ ▷ Continuation guess
4: $\quad$ **while** $||\mathrm{G}_\mathcal{N}(\mathrm{X}_j^{(k)}; \boldsymbol{\mu}_j)||_{\mathbb{X}_\mathcal{N}} > \epsilon$ **do** ▷ **Newton method**
5: $\quad\quad \mathrm{J}_\mathcal{N}(\mathrm{X}_j^{(k)}; \boldsymbol{\mu}_j)\delta\mathrm{X} = \mathrm{G}_\mathcal{N}(\mathrm{X}_j^{(k)}; \boldsymbol{\mu}_j)$ ▷ **Galerkin-FE method**
6: $\quad\quad \mathrm{X}_j^{(k+1)} = \mathrm{X}_j^{(k)} - \delta\mathrm{X}$
7: $\quad$ **end while**
8: $\quad \mathrm{J}_\mathcal{N}(\mathrm{X}_j; \boldsymbol{\mu}_j)\mathrm{X}_e = \sigma_{\boldsymbol{\mu}_j}\mathrm{M}_\mathcal{N}\mathrm{X}_e$ ▷ Eigenproblem for stability
9: **end for**

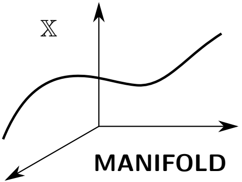
Reduced Order Models (ROMs)[3,4]

We focus on **Reduced Basis** (RB) method based on **POD** strategy, defining

$$\mathbb{X}_N = span\{\Sigma^m,\ m = 1, \cdots, N\} \subset \mathbb{X}_{\mathcal{N}}, \quad \text{where} \quad N \ll \mathcal{N},$$

where $\{\Sigma^m\}_{m=1}^{N}$ are the basis functions obtained from the **snapshots** $\{X_{\mathcal{N}}(\boldsymbol{\mu}^n)\}_{n=1}^{N_{train}}$.

$$\underbrace{G(X(\boldsymbol{\mu}); \boldsymbol{\mu}) = 0}_{\text{Partial differential equation}}$$



[3] J. S. Hesthaven, G. Rozza, and B. Stamm. *Certified Reduced Basis Methods for Parametrized Partial Differential Equations*. Springer International Publishing, 2015.

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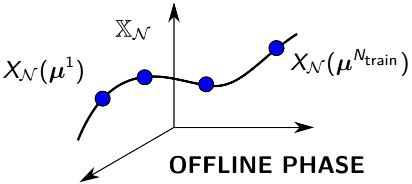

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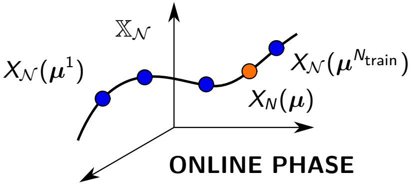

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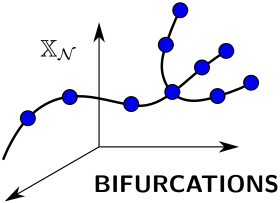
- **Global approach**:
  Pros: single space encoding all branches
  Cons: larger N and higher errors.



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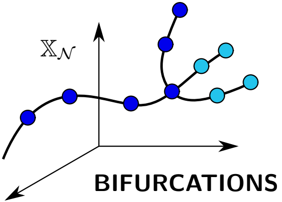
- **Global approach**:
  Pros: single space encoding all branches
  Cons: larger N and higher errors.
- **Branch-wise approach**:
  Pros: low dimensional space
  Cons: hidden unsampled branch.



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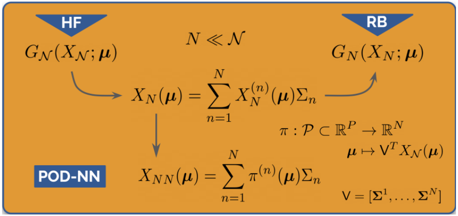
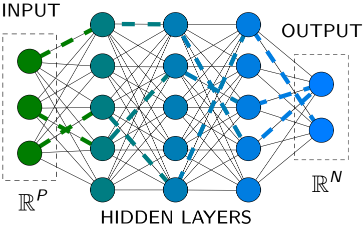
Motivations for non-intrusive approach

[5]**Goal**: Investigate efficiently complex **bifurcating** behaviour in a **real-time** context.

[6]**How**: **POD-NN** approach combining ROMs and learning of reduced coefficients.





POD-NN approach:
approximate $\pi : \mathcal{P} \subset \mathbb{R}^P \to \mathbb{R}^N$ such that $\boldsymbol{\mu} \mapsto \mathsf{V}^T X_{\mathcal{N}}(\boldsymbol{\mu})$ from a training set given by the pairs $\{(\boldsymbol{\mu}^i, \mathsf{V}^T X_{\mathcal{N}}(\boldsymbol{\mu}^i))\}_{i=1}^{N_{train}}$ obtained from the offline POD procedure.

[5] F. Pichi, F. Ballarin, G. Rozza, and J. S. Hesthaven. *Artificial neural network for bifurcating phenomena modelled by nonlinear parametrized PDEs.* Preprint, 2020.

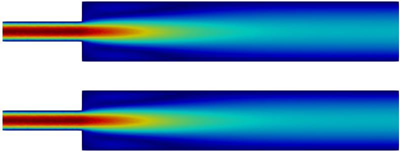
[6] J. S. Hesthaven and S. Ubbiali. *Non-intrusive reduced order modeling of nonlinear problems using neural networks.* Journal of Computational Physics, 363:55–78, 2018.

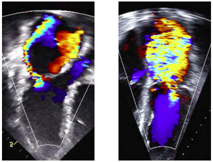
Navier-Stokes application: the Coanda effect in a channel

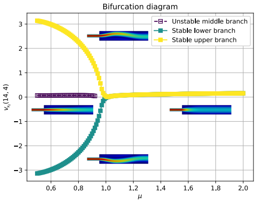
NS system for viscous, steady and incompressible flow

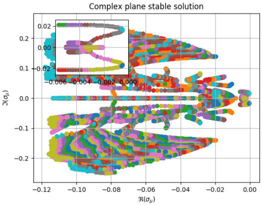
$$\begin{cases} -\mu\Delta v + v\cdot\nabla v + \nabla p = 0 & \text{in } \Omega,\\ \nabla\cdot v = 0 & \text{in } \Omega,\end{cases} \quad \text{with} \quad \begin{cases} v = v_{\text{in}} & \text{on } \Gamma_{\text{in}},\\ v = 0 & \text{on } \Gamma_0,\\ -pn + (\mu\nabla v)n = 0 & \text{on } \Gamma_{\text{out}},\end{cases}$$

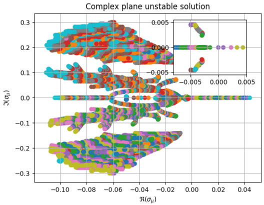
ISSUE: For viscosities $\mu \leq \mu^* \approx 0.96$ **wall-hugging** (stable) phenomena occur.









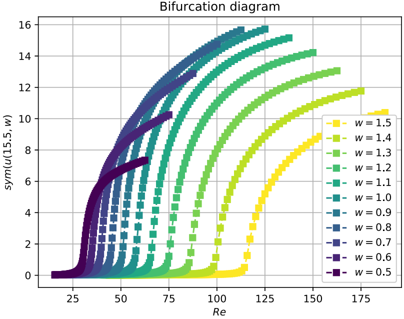


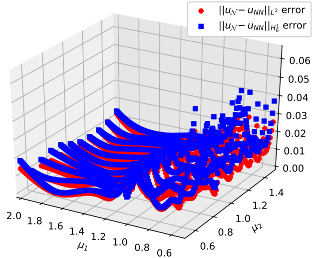
Navier-Stokes application: the Coanda effect in a channel

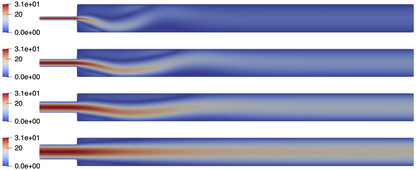
SETTING

Parameter space $P = 2$, $(\mu, w) \in \mathcal{P} = [0.5, 2] \times [0.5, 1.5]$, viscosity and ch. width.
RB dimension $N_u = 50$, $N_p = 24$. **Network** 2 layers, 15 neurons, $N_{train} = 200 \cdot 6$.

POD-NN speed-up $= 10^6$
$\epsilon_{NN}^{max} = 0.0625$, $\overline{\epsilon}_{NN} = 0.0118$.
RB speed-up $= 1.5$
$\epsilon_{RB}^{max} = 0.7553$, $\overline{\epsilon}_{RB} = 0.0129$.

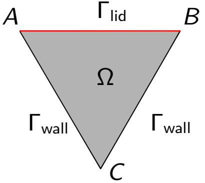






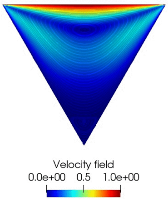
Navier-Stokes application: triangular cavity flow

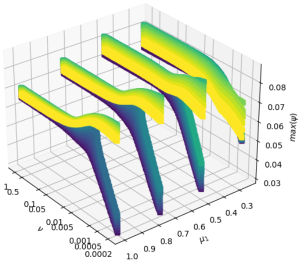
Towards multiple bifurcating regimes:
existence of a critical angle for the parametrized geometry causing a vortex attaching to vertex B increasing the Reynolds number.

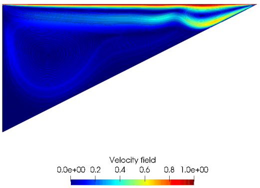


SETTING

Parameter space P = 3, $(\nu, \mu_1, \mu_2) \in \mathcal{P} = [2 \cdot 10^{-4}, 1] \times [-0.5, 0.5] \times [-.25, -1]$, viscosity and bottom vertex position. **RB dimension** $N_u = 100$, $N_p = 44$.
Network 3 layers, 20 neurons, log-equispaced sampling, tanh, epochs, Adam opt.





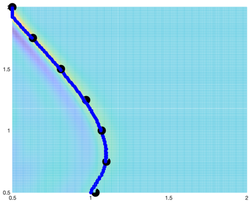


A reduced manifold based bifurcation diagram

Aim: efficiently reconstruct a bifurcation diagram, where the output is entirely based on the **reduced coefficients** appearing in the RB expansion.

Idea: take advantage of the **non-smoothness** of the manifold, constructing a **detection tool** that is able to track the critical points employing its **curvature**.

Result: L^2 relative error for the vector of the **critical points** is of the order 10^{-2}.



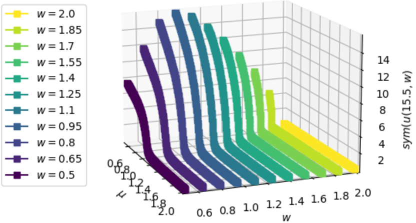


Figure: Multi-parameter Coanda test case: (Left) Reduced manifold based bifurcation diagram reconstruction. (Right) RB/POD-NN based 3D bifurcation diagram.

Conclusions and Perspectives

- △ We described the general framework for the approximation of bifurcating nonlinear parametrized PDEs.
- △ We investigated the intrusive Reduced Basis method to obtain an efficient evaluation of the bifurcation diagrams.
- △ We applied the non-intrusive POD-NN technique to recover the decoupling between offline and online phases.
- △ We presented an application of the methodology to the multi-parameter test cases: the Coanda effect in a channel and the triangular cavity flow.
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- ▽ Reduce the number of training points needed incorporating physics with Physics Informed Neural Networks (PINNs).
- ▽ Embed Automatic Machine Learning (AutoML) to select best configuration for the hyper-parameters of the neural network.
- ▽ Improve the decay of the POD-NN technique w.r.t. the number of RB modes by developing new algorithmic procedure.

List of publications

[1] F. Pichi and G. Rozza. Reduced basis approaches for parametrized bifurcation problems held by non-linear Von Kármán equations. *Journal of Scientific Computing*, 81(1):112–135, 2019.

[2] D. B. P. Huynh, F. Pichi, and G. Rozza. *Reduced Basis Approximation and A Posteriori Error Estimation: Applications to Elasticity Problems in Several Parametric Settings*, pages 203–247. Springer International Publishing, Cham, 2018.

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[8] F. Pichi. Reduced order models for parametric bifurcation problems in nonlinear PDEs. Ph.D. Thesis, 2020.

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