Non-linear reduction for data-driven non-intrusive reduced-order models with parallel autoencoders

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Introduction

The completely **data-driven non-intrusive ROM** using **linear reduction** methods such as the **POD** fails for problems characterised by a slow decay of the Kolmogorov N-width. In this ongoing research, we are exploring the usage of a **non-linear reduction** approach such as the **autoencoder** neural network instead of the linear POD, to tackle various types of problems within the **HPC** framework, taking the advantage of **data parallelism** techniques.

1 - The traditional data-driven non-intrusive ROM

Using Proper Orthogonal Decomposition with Interpolation (PODI):

Starting from a **parametric** geometrical model; if we have a database of **parameter** values $\mathbf{\Xi} = [\boldsymbol{\mu}_1 \dots \boldsymbol{\mu}_N]$ and a database of **snapshots** $\mathbf{\Theta} = [u(\boldsymbol{\mu}_1) \dots u(\boldsymbol{\mu}_N)]$ as in [1], we can apply the **Singular Value Decomposition (SVD)** to the **snapshots matrix** $\mathbf{\Theta}$:

$$\mathbf{\Theta} = \mathbf{\Psi}\mathbf{\Sigma}\mathbf{\Phi}^T$$

where $\mathbf{\Psi}$ and $\mathbf{\Phi}$ are the left and right singular vectors matrices of $\mathbf{\Theta}$, and $\mathbf{\Sigma}$ is the diagonal matrix containing the singular values in decreasing order. The columns of Ψ are called the **POD modes** ψ and the **modal coefficients** α can be obtained through $\alpha = \mathbf{\Psi}^T\mathbf{\Theta}$ as mentioned in [2].

Then the **reduced solution** of the problem can be viewed as a **linear combination** of the POD modes ψ multiplied by the modal coefficients α as follows:

$$u^N = \sum_{i=0}^{N} \alpha_i \psi_i$$

Q: How to get value of the modal coefficients α for each new parameter?

In the offline phase: We **compute the full-order solution** using the high-fidelity solver for some parameter points $\boldsymbol{\mu}_k \in \mathbf{\Xi}$. Since the high fidelity solution $u(\boldsymbol{\mu}_k)$ and the reduced solution $u^N(\boldsymbol{\mu}_k)$ are assumed to be equal by construction, we have the following:

$$\forall \boldsymbol{\mu}_k \in \mathbf{\Xi} : u(\boldsymbol{\mu}_k) = u^N(\boldsymbol{\mu}_k) = \sum_{i=0}^{N} \alpha_i(\boldsymbol{\mu}_k)\psi_i$$

Now for the set of parameters $\boldsymbol{\mu}_k$, we can compute the corresponding coefficients $\alpha(\boldsymbol{\mu}_k)$.

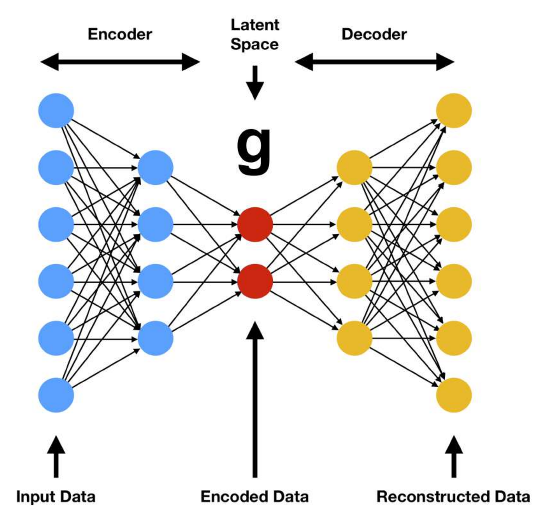
In the online phase: Since we obtained pairs of $(\boldsymbol{\mu}_k, \alpha(\boldsymbol{\mu}_k))$, for each new parameter $\boldsymbol{\mu}_{\text{new}}$, we **interpolate the previously computed coefficients** $\alpha(\boldsymbol{\mu}_k)$ to find the new coefficients $\alpha(\boldsymbol{\mu}_{\text{new}})$. The new reduced solution can be obtained by:

$$u^N_{new} = \sum_{i=0}^{N} \alpha_i(\boldsymbol{\mu}_{new})\psi_i$$

2 - From Linear to non-linear reduction

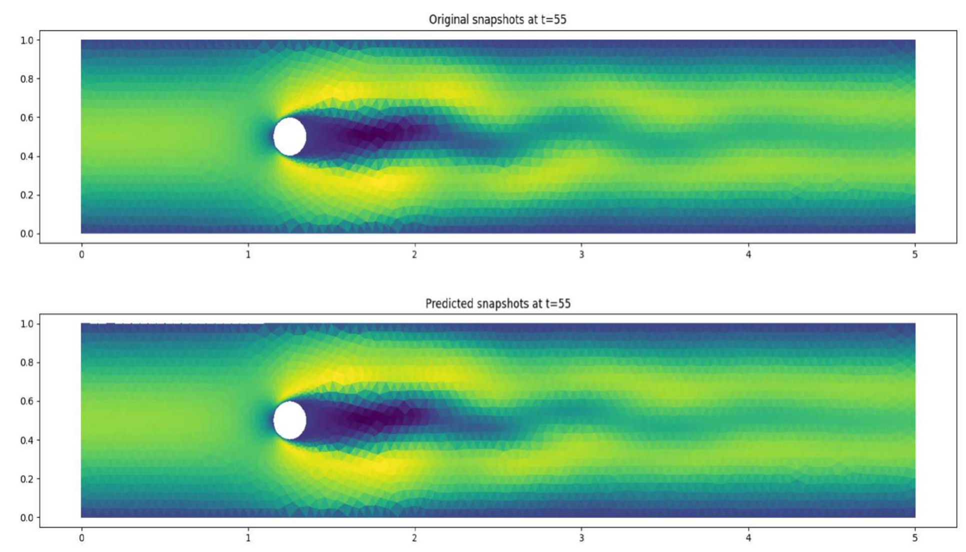
Linear reduction: SVD $\rightsquigarrow$ $u(\boldsymbol{\mu}) \approx \sum_{i=0}^{N} \alpha_i(\boldsymbol{\mu})\psi_i$

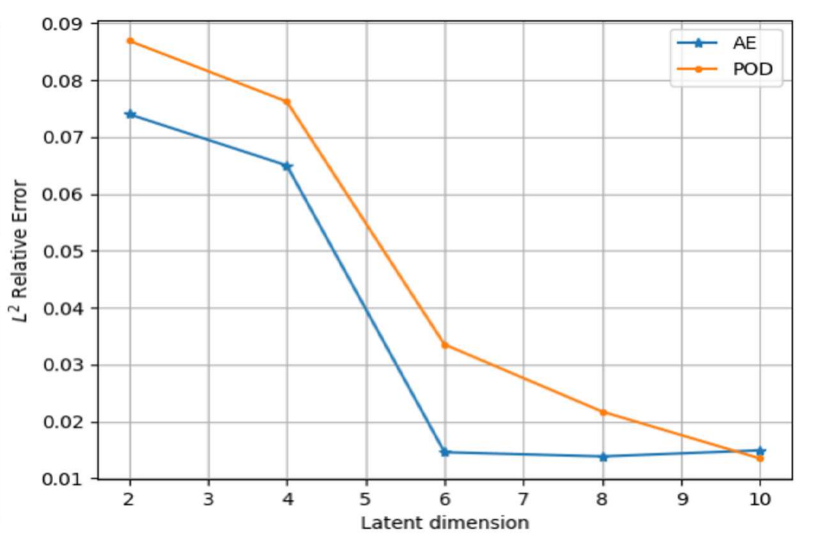
Non-linear activation $\left(\sum_{i=1}^{N}(x_i w_i) + \text{bias}\right)$



Non-linear reduction: AE $\rightsquigarrow$ $u(\boldsymbol{\mu}) \approx f(\boldsymbol{g})$

3 - Preliminary results



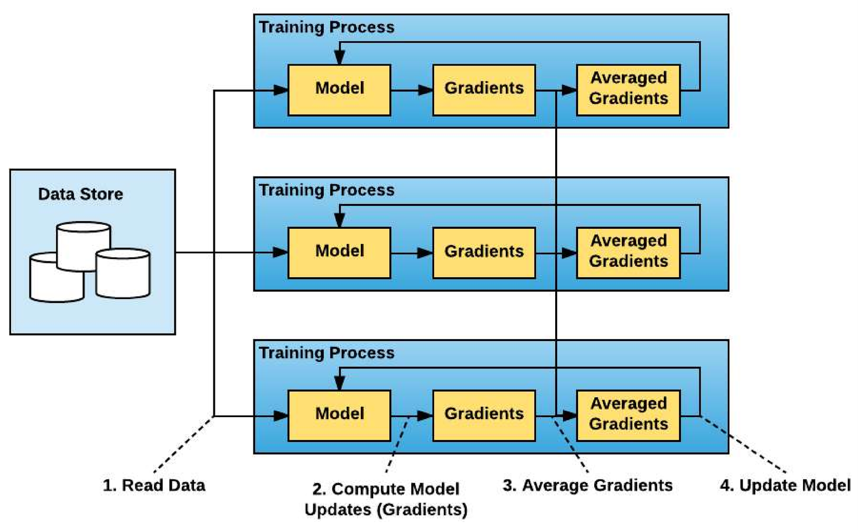


Note:
The non-linear reduction can achieve **smaller** solution manifolds with **better** accuracy.

4 - Data parallelism

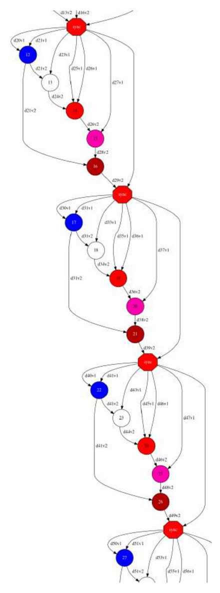
Input of large-sized batches from FOM:

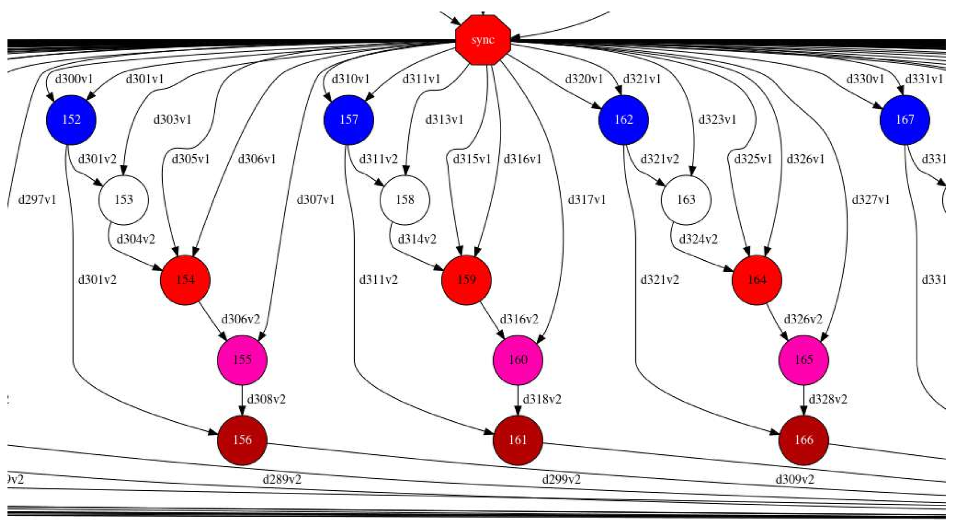
1. **Divide** into **mini-batches** and **distribute** them across processing units.
2. **Replicate the full model** on each processing units to treat a mini-batch.
3. Perform **training locally** and **synchronise local gradients**.
4. The **average** of the local gradients is used to **update** the local models.



5 - Parallel execution

Simultaneous execution of the same functions for multiple predictions or error calculations:





6 - Computational science and engineering softwares: `mathlab.sissa.it/cse-software`

EZyRB
`github.com/mathLab/EZyRB`
`mathlab.github.io/EZyRB`

EZyRB is a python library for data-driven (non-intrusive) model order reduction with linear and non-linear reduction and different approximation methods.

COMPSs
`github.com/bsc-wdc/compss`
`compss-doc.readthedocs.io/en/stable/index.html`

COMPSs is a programming model to ease the development of applications for distributed infrastructures, such as Clusters, Clouds and Containerised Platforms.

EDDL
`github.com/deephealthproject/eddl`
`deephealthproject.github.io/eddl/index.html`

EDDL is an optimised tensor library for distributed deep learning with hardware transparency support for CPUs, GPUs and FPGAs.

References and Acknowledgements

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[3] M. Tezzele, N. Demo, A. Mola, and G. Rozza, "An integrated data-driven computational pipeline with model order reduction for industrial and applied mathematics," in *Novel Mathematics Inspired by Industrial Challenges*, pp. 179–200, Springer, 2022.

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