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pyforce: Python Framework for data-driven model Order Reduction of multi-physiCs problEms

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Summary

pyforce (Python Framework for data-driven model Order Reduction of multi-physiCs problEms) is a Python library implementing Data-Driven Reduced Order Modelling (DDROM) techniques (Riva et al., 2024) for applications to multi-physics problems, mainly in the nuclear engineering world. These techniques have been implemented upon the dolfinx package (Baratta et al., 2023) (currently v0.6.0), part of the FEniCSx project, to handle mesh generation, integral calculation and functions storage. The package is part of the ROSE (Reduced Order modelling with data-driven techniques for multi-phySics problEms) framework, which is one of the main research topics investigated at the ERMETE-Lab: in particular, the focus of the research activities is on mathematical algorithms aimed at reducing the complexity of multi-physics models with a focus on nuclear reactor applications, searching for optimal sensor positions and integrating experimental data to improve the knowledge on the physical systems.

Statement of need

Innovative reactor technologies in the framework of Generation IV are usually characterised by harsher and more hostile environments than standard nuclear systems, for instance, due to the liquid nature of the fuel or the adoption of liquid salt and molten as coolant. This framework poses more challenges in the monitoring of the system itself; since placing sensors inside the reactor itself is a nearly impossible task, it is crucial to study innovative methods able to combine different sources of information, namely mathematical models and measurements data (i.e., local evaluations of quantities of interest) in a quick, reliable and efficient way. These methods fall into the Data-Driven Reduced Order Modelling framework, they can be very useful to learn the missing physics or the dynamics of the problem, in particular, they can be adapted to generate surrogate models able to map the out-core measurements of a simple field (e.g., neutron flux and temperature) to the dynamics of non-observable complex fields (precursors concentration and velocity).

The techniques implemented here follow the same underlying idea expressed in Figure 1. They all share the typical offline/online paradigm of ROM techniques: the former is computationally expensive and it is performed only once, whereas the latter is cheap from the computational point of view and allows to have quick and reliable evaluations of the state of the system by merging background model knowledge and real evaluations of quantities of interest (Yvon Maday et al., 2014). During the offline (also called training) phase, a *high-fidelity* or Full Order Model (FOM), usually parameterised partial differential equations, is solved several times to obtain a collections of snapshots $\mathbf{u}_{FOM} \in \mathbb{R}^{\mathcal{N}_h}$, given $\mathcal{N}_h$ the dimension of the spatial mesh, which are dependent on some parameters μ_n; then, these snapshots are used to generate a reduced representation through a set of basis functions $\{\psi_n(\mathbf{x})\}$, in this way the degrees of freedom are decresed from $\mathcal{N}_h$ to N, provided that $\mathcal{N}_h >> N$. This allows to approximate any solution of the FOM as follows

$$u(\mathbf{x};\mu) \simeq \sum_{n=1}^{N} \alpha_n(\mu)\cdot\psi_n(\mathbf{x}) \qquad (1)$$

with $\alpha_n(\mu)$ as the reduced coefficients, embedding the parametric dependence. Moreover, a reduced representation allows for the search of the optimal positions of sensors in the physical domain in a more efficient manner.

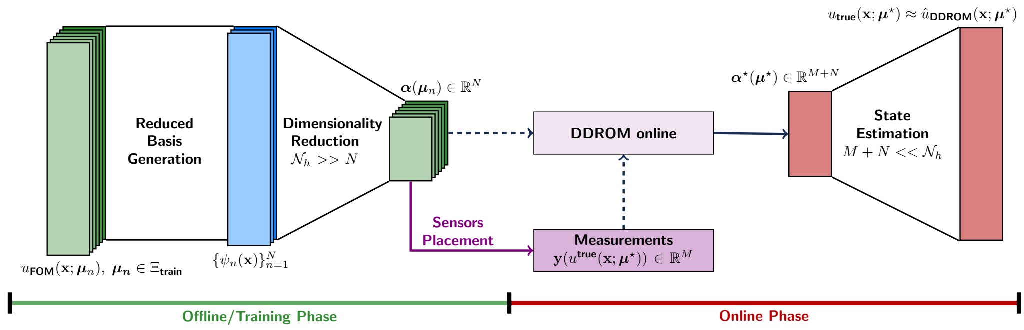

Figure 1: General scheme of DDROM methods (Riva et al., 2024).

All these steps are performed during the offline phase, the online phase aim consists in obtaining in a quick and reliable way a solution of the FOM for an unseen parameter $\mu^\star$, using as input a set of measurements $\mathbf{y} \in \mathbb{R}^M$. The DDROM online takes place which produces a novel set of reduced variables, $\alpha^\star$, and then computing an improved reconstructed state $\hat{u}_{DDROM}$ through a decoding step from the low dimensional state to the high dimensional one.

Up to now, the techniques, reported in the following tables, have been implemented (Cammi et al., 2024; Riva et al., 2024): they have been split into offline and online, including how they connect with Figure 1.

Offline algorithm	Basis Generation	Sensor Placement
Proper Orthogonal Decomposition (POD) (Rozza et al., 2020)	X	
SGreedy (Yvon Maday et al., 2014)		X
Generalised Empirical Interpolation Method (GEIM) (Y. Maday et al., 2015)	X	X

Online algorithm	Input is parameter μ	Input is measurement vector $\mathbf{y}$
POD Projection (Rozza et al., 2020)	X	
POD with Interpolation (PODI) (Demo et al., 2019)	X	
GEIM (Y. Maday et al., 2015)		X
Tikhonov-Regularised (TR)-GEIM (Introini, Cavalleri, et al., 2023)		X
Parameterised-Background Data-Weak (PBDW) (Yvon Maday et al., 2014)		X
Indirect Reconstruction: parameter estimation (Introini, Riva, et al., 2023)		X

This package aims to become a valuable tool for other researchers, engineers, and data scientists working in various fields where multi-physics problems play an important role, and its scope of application is not only restricted to the Nuclear Engineering world. The package also includes tutorials showing how to use the library and its main features, ranging from snapshot generation in dolfinx, import and mapping from OpenFOAM (Weller et al., 1998), to the offline and online phase of each of the aforementioned DDROM algorithms. The case studies are taken from the fluid dynamics and neutronics world, being the most important physics involved in nuclear reactor physics, although the methodologies can be extended to any physics of interest.

Authors contribution with CRediT

- Stefano Riva: Conceptualization, Data curation, Formal analysis, Software, Visualization, Writing – original draft
- Carolina Introini: Conceptualization, Formal analysis, Software, Supervision, Writing – review & editing
- Antonio Cammi: Conceptualization, Project administration, Resources, Supervision, Writing – review & editing

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