

Model-based emulators and machine learning (ML) methods in nuclear physics

Xilin Zhang (FRIB/MSU)

Emulators as part of computational research in nuclear physics

- Recent years have witnessed success in emulating nuclear bound and continuum states calculations.
- Many other nuclear physics topics (important for FRIB, Jlab, EIC, and astrophysics) are waiting to be explored: nuclear resonances, responses, and reactions, (time-dependent) density functional theory, bridging theory and experiment, and more.
- Synergy between ML and model-driven emulators expands their capability (or one way to achieve physics informed ML).

“Deep learning-based reduced order models (DL-ROMs) have been recently proposed to overcome common limitations shared by conventional reduced order models (ROMs) – built, e.g., through proper orthogonal decomposition (POD) – when applied to **nonlinear time-dependent** parametrized partial differential equations (PDEs).” from Stefania Fresca, Andrea Manzoni (2022) [[2101.11845](https://arxiv.org/abs/2101.11845)]

- In nuclear physics, our recent work combines Gaussian process and model-driven emulators for quantum three-body scattering.

Xilin Zhang, R. Furnstahl (2022) [[2110.04269](https://arxiv.org/abs/2110.04269)]

- The synergy is a new research direction in the field of model order reduction and has great potential in nuclear physics as well.

Jan S. Hesthaven, Cecilia Pagliantini and Gianluigi Rozza (2022)[<https://doi.org/10.1017/S0962492922000058>]

An (incomplete) list of works

- Discrete spectrum:

- Dillon Frame et. al., Phys.Rev.Lett. 121 (2018) 3, 032501 [[1711.07090](#)]
- S. König et. al. , Phys.Lett.B 810 (2020) 135814 [[1909.08446](#)]
- Andreas Ekström and Gaute Hagen, Phys.Rev.Lett. 123 (2019) 25, 252501 [[1910.02922](#)]
- P. Demol et.al., Phys.Rev.C 101 (2020) 4, 041302 [[1911.12578](#)]
- Avik Sarkar and Dean Lee, Phys.Rev.Lett. 126 (2021) 3, 032501 [[2004.07651](#)]
- Sota Yoshida and Noritaka Shimizu, PTEP 2022 (2022) 5, 053D02 [[2105.08256](#)]
- Margarida Companys Franzke et. al., Phys.Lett.B 830 (2022) 137101 [[2108.02824](#)]
- T. Djärv et.al., Phys.Rev.C 105 (2022) 1, 014005 [[2108.13313](#)]
- Pablo Giuliani et. al., [[2209.13039](#)]
- Nuwan Yapa and S. König, Phys.Rev.C 106 (2022) 1, 014309 [[2201.08313](#)]
- Amy L. Anderson et. al., Phys.Rev.C 106 (2022) 3, L031302 [[2206.14889](#)]

- Introduction of model order reduction methods (many good references there):

- J.A. Melendez et. al., J.Phys.G 49 (2022) 10, 102001 [[2203.05528](#)]
- Edgard Bonilla et. al., [[2203.05284](#)]

- Continuum states:

- R.J. Furnstahl et. al., Phys.Lett.B 809 (2020) 135719 [[2007.03635](#)]
- Dong Bai and Zhongzhou Ren, Phys.Rev.C 103 (2021) 1, 014612 [[2101.06336](#)]
- J.A. Melendez et.al., Phys.Lett.B 821 (2021) 136608 [[2106.15608](#)]
- C. Drischler et.al., Phys.Lett.B 823 (2021) 136777 [[2108.08269](#)]
- Xilin Zhang and R.J. Furnstahl, Phys.Rev.C 105 (2022) 6, 064004 [[2110.04269](#)]
- Dong Bai, Phys.Rev.C 106 (2022) 2, 024611

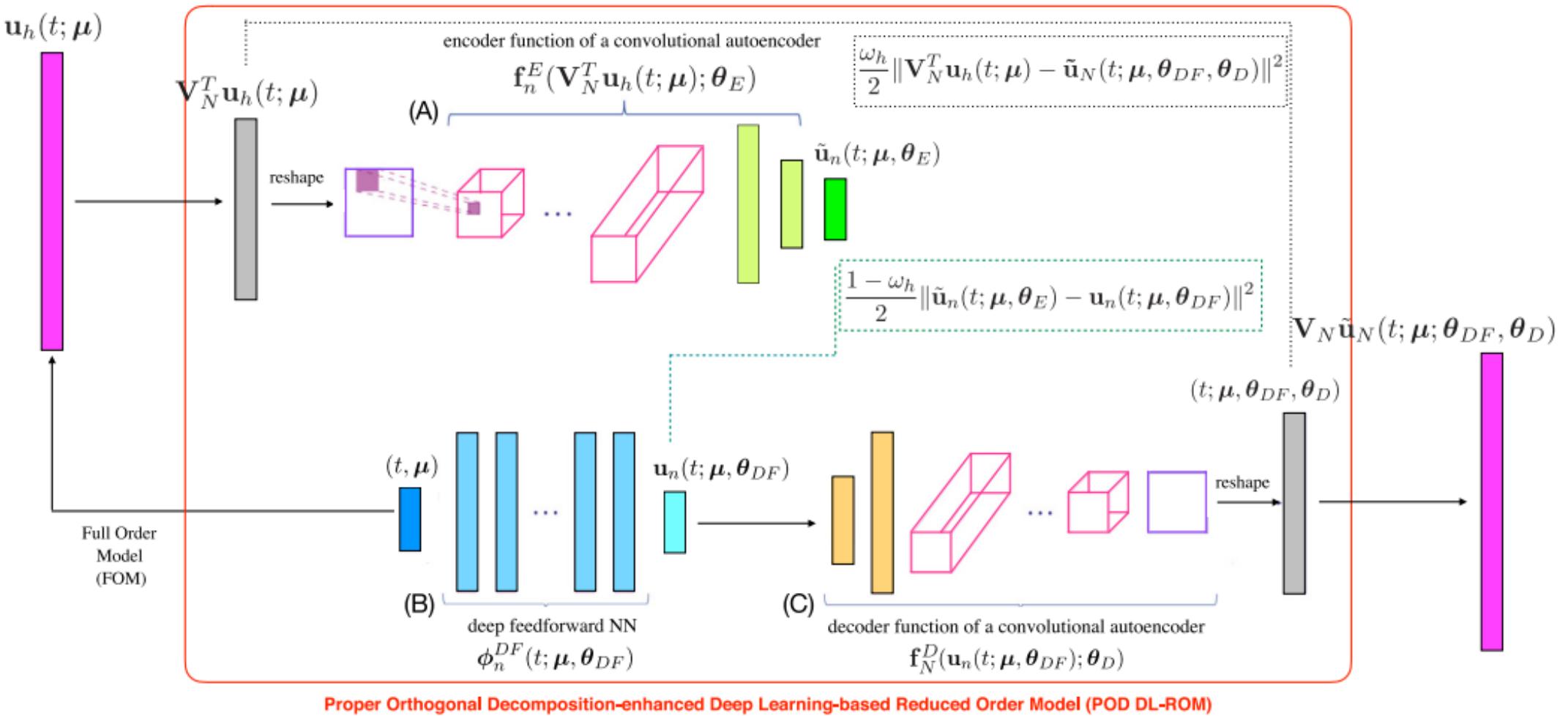


Fig. 1. POD-DL-ROM architecture. Starting from the FOM solution $\mathbf{u}_h(t; \mu)$, the intrinsic coordinates $\mathbf{V}_N^T \mathbf{u}_h(t; \mu)$ are computed, by means of rSVD, and the neural network provides as output $\tilde{\mathbf{u}}_N(t; \mu)$, an approximation of them. The reconstructed solution $\mathbf{u}_h(t; \mu)$ is then recovered through the rPOD basis matrix.