A Hybrid Approach for Surrogate Modeling of a Methanation Reactor

Luisa Peterson*, Ion Victor Gosea*, Peter Benner*, Kai Sundmacher*

* Max Planck Institute for Dynamics of Complex Technical Systems
Sandtorstr. 1, 39116, Magdeburg, Germany
gosea@mpi-magdeburg.mpg.de

Abstract

Operator inference (OpInf) [1] is an established scientific machine learning approach that enables the construction of reduced-order models by learning the governing dynamics directly from data, bypassing the need for intrusive access to explicit governing equations. A critical challenge in applying OpInf to experimental data is measurement noise, which degrades the finite-difference derivative estimates required for standard regression. To address this issue, we propose a hybrid learning strategy for experimental data-sets that bypasses direct dependence on noisy derivatives.

We treat the latent state as a continuous function approximated by a neural network. This approach is conceptually inspired by DeepMoD [2], which combines PINN and SINDy principles. Here, smoothing and matrix learning occur jointly: the network acts as a differentiable surrogate that filters noise, providing clean time derivatives via automatic differentiation. The OpInf model then serves as a physics-informed regularizer. To ensure robust convergence, we apply a three-stage learning strategy: (1) pre-training the network on data reconstruction (denoising); (2) initializing matrices; and (3) minimizing a composite MSE loss. This formulation decouples the derivative estimation from grid discretization artifacts. The targeted application in this work consists in developing reliable, predictive surrogates for a complex, nonlinear model of a catalytic carbon dioxide methanation reactor [3]. The learned OpInf model serves as the predictive core for optimization-based control. By embedding the reduced-order dynamics as constraints in a nonlinear optimization problem, we aim to maximize reactor performance while adhering to safety limits. We implement the continuous-time optimal control problem using the CasADi framework [4] and solve it via direct multiple shooting with an interior-point solver.

References

[1] B. Kramer, B. Peherstorfer, K. E. Willcox, Learning nonlinear reduced models from data with operator inference, Annual Review of Fluid Mechanics 56 (1) (2024) 521–548 `https://doi.org/10.1146/annurev-fluid-121021-025220`.

[2] G.-J. Both, S. Choudhury, P. Sens, R. Kusters, DeepMoD: Deep learning for model discovery in noisy data, Journal of Computational Physics 428 (2021) 109985 `https://doi.org/10.1016/j.jcp.2020.109985`.

[3] L. Peterson et al., Toward Digital Twins for Power-to-X Processes: Comparing Surrogate Models for a Catalytic CO_2 Methanation Reactor, IEEE Transactions on Automation Science and Engineering 23, (2026) 3469-3483 `https://doi.org/10.1109/TASE.2025.3564637`

[4] A. Wächter, L. T. Biegler, On the implementation of an interior-point filter line-search algorithm for large-scale nonlinear programming, Mathematical Programming 106 (1) (2006) 25–57 https://doi.org/10.1007/s10107-004-0559-y.