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Physics-informed neural networks as reduced simulation models for bioreactor and crystallisation modeling

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By now, simulations have become a very important tool in engineering sciences. However, when applied to engineering problems, they often require large amounts of computation time – even on modern supercomputers. This motivates the growing interest in model order reduction techniques, which approximate full order models at much lower computational costs by drastically reducing the degrees of freedom. Here, the recent break-throughs of deep-learning approaches have drawn the attention towards data-based strategies for constructing reduced models, utilizing, e.g., supervised learning concepts.

While supervised learning algorithms work well for a wide variety of tasks including image recognition and language processing, they often require lots of data – which is mostly sparse in engineering applications – and typically do not include a-priori information about the underlying process – which however is often available. Physics-Informed Neural Networks (PINNs) [1] try to bridge the gap between purely data-driven supervised learning and traditional physics-based modeling by integrating this a-priori knowledge in the form of the governing equations into the learning process.

We aim to employ PINNs as reduced simulation models for predicting the flow field inside bioreactors as well as the crystallisation of polymers. While the first application case is especially challenging regarding the geometry of the reactors and the necessary boundary conditions to precisely model the relevant flow phenomena, the second application case involves complex physical models that govern the dynamics of the crystallisation process. The presented results will show that PINNs qualify as reduced simulation models for complex engineering applications.

REFERENCES

[1] Raissi, M., Perdikaris, P., & Karniadakis, G. E. (2019). Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. *Journal of Computational Physics*, 378, 686–707. https://doi.org/10.1016/j.jcp.2018.10.045