Application of CFD, Machine Learning, and Shape Optimization to flow chemistry applications

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Mixing reactors are used in chemical synthesis, polymerisation or pharmaceutical manufacturing. Computational fluid dynamics (CFD) simulations for these reactors are expensive, and solutions obtained are specific to the particular flow and geometry condition, making the evaluations based on various geometries for design improvements challenging. To overcome this challenge, we will aim to build faster machine-learning based surrogate models with the focus is on handling high-dimensional simulation data for complex reactor geometrical parameters. The proposed model will leverage advanced deep learning techniques, specifically graph neural networks (GNNs) and specialised convolutional neural network (CNN) autoencoders. GNNs are chosen for their ability to capture geometric and topological information effectively, making them suitable for representing complex geometrical features in fluid dynamics. On the other hand, CNN autoencoders are expected to learn a compressed representation of fluid dynamics, facilitating efficient simulation of high-dimensional data. This approach aims to significantly improve computational efficiency and accuracy in fluid dynamics simulations, especially in scenarios with varying flow rates, and geometric configurations. The project's success will be measured by the surrogate model's ability to outperform traditional CFD methods in terms of computational efficiency and accuracy, as well as its robustness and flexibility in handling different fluid flow scenarios.