From Simulation to AI: Physics-Informed Neural Networks for Chemical Kinetics in Turbulent Hydrogen Swirling Flames

Supervised by: Umair Ahmed[*] (email: umair.ahmed@newcastle.ac.uk)
Co-Supervised by: Xinyi Chen[*] (email: xinyi.chen@newcastle.ac.uk)
[*]School of Engineering, Newcastle University, Newcastle upon Tyne, NE1 7RU

This project investigates the ability of physics-informed neural networks (PINNs) for reliable prediction of chemical kinetics in turbulent hydrogen swirling flames. Hydrogen combustion is a key pathway toward net-zero energy systems, as it eliminates carbon-based greenhouse gas emissions. However, hydrogen-air flames exhibit fundamentally different thermochemical behaviour from hydrocarbon fuels, including strong differential diffusion and increased susceptibility to flame instabilities, flashback, and extinction, particularly under swirling conditions relevant to gas turbines. The proposed research builds on an ongoing EPSRC project that has generated **large-scale high-fidelity direct numerical simulation (DNS) databases** of reacting low-swirl hydrogen-air flames across a range of mixture compositions, swirl and Reynolds numbers (as shown in Fig. 1). While DNS provides unparalleled physical insight, it is extremely computationally expensive and therefore impractical for routine engineering design. The resulting datasets contain fully resolved flow, transport, and chemical reaction fields and are **several terabytes in size**, making them ideal for training and benchmarking data-driven models. This project therefore aims to **develop machine learning based surrogate models** capable of accurately representing chemical reaction source terms for complex real-world type reactive flows. Predictive capabilities of pretrained open-source neural networks (https://github.com/tianhanz/DNN-Models-for-Chemical-Kinetics) with soft or hard physical constraints, will be first evaluated using the available DNS datasets. Building on this analysis, new PINN models will then be trained on **high-performance computing (HPC) GPU resource available on Bede**.

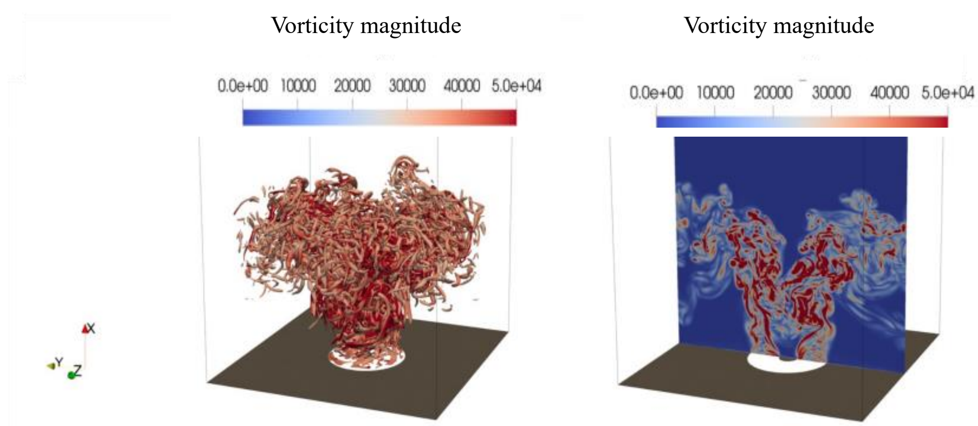

Figure1: Swirling flow simulations showing the turbulent flow structure (left) and vortex strength (right).

High-performance computing is central to this project. The DNS datasets are several terabytes in size and require **parallel data processing** and **GPU-accelerated machine learning workflows**. The student will use the **Bede HPC system** to access, process, and analyse these large datasets and to train physics-informed neural networks at scale. Through this work, the student will gain experience with **research software engineering** and **research data management best practices**, including handling large HDF5 simulation datasets, building reproducible data-analysis pipelines, and using Git version control for collaborative scientific workflows. Neural network models will be developed and trained using modern machine-learning frameworks such as PyTorch, with training executed on GPU nodes via SLURM-based HPC workflows. The project will provide hands-on training in computational fluid dynamics, combustion modelling, machine learning, and large-scale scientific computing, equipping the student with practical skills in Python, GPU-accelerated training, and HPC-based data analysis.