

# OpenFOAM & Combustion Simulation



## DeepFlame: An open-source machine learning-empowered CFD package for reacting flow at all speeds based on OpenFOAM-Cantera-Torch coupling

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**Time:** Nov 20, 2022, 10:00 Singapore/Beijing | 02:00 London  
Nov 19, 2022, 21:00 New York

**Host:** Dr. Shangpeng Li (National University of Singapore)

**Register:** [https://nus-sg.zoom.us/webinar/register/WN\\_CJPAzDFRRnCiUzxZPOZ3jQ](https://nus-sg.zoom.us/webinar/register/WN_CJPAzDFRRnCiUzxZPOZ3jQ)



### Abstract

Combustion CFD is among the most demanding tasks for scientific computing. Our community have long been suffering from the dilemma between accuracy and efficiency, particularly for turbulent combustion with detailed chemical kinetics. The emergence of deep learning has brought potentially game-changing methods for combustion modelling. However, deploying deep learning models in combustion codes is non-trivial and requires major refactoring of code structure. To this end, in this talk we introduce DeepFlame v1.0 – a newly released open-source platform for reacting flow simulations based on OpenFOAM-Cantera-PyTorch coupling. A C++/Python hybrid framework is constructed for easy implementation of deep learning algorithms. As a demonstration, we apply the DeePCK method for predicting chemical kinetics (Zhang & Xu et al. CNF 2022) to highlight the potential of deep learning models using the DeepFlame code. Validation is presented via a broad range of canonical cases to assess its accuracy and efficiency. A speed-up of two orders of magnitude is achieved in a simple hydrogen ignition case when performed on a medium-end graphics processing unit (GPU). Further gain in computational efficiency is expected for hydrocarbon and other complex fuels. A similar level of acceleration is obtained on an AI-specific chip – deep computing unit (DCU), highlighting the potential of DeepFlame in leveraging the next-generation computing architecture and hardware.

### About the Speaker

Dr. Zhi X. Chen is an Assistant Professor at Peking University. He received his Ph.D. from University of Cambridge in 2017 and then conducted post-doctoral research at Cambridge, Sandia and DLR in Stuttgart. In 2019 he was recognised by the Royal Academy of Engineering as a Tier-1 Exceptional Talent of the UK and then worked at Robinson College as a Senior Research Fellow before joining Peking University in 2021. He is recipient of several scientific awards, including the 2020 Bernard Lewis Fellowship from the Combustion Institute, and the Best User UK National Supercomputing Service from the EPSRC. He is currently leading the DeepFlame open-source project of the DeepModeling Community (<https://deepmodeling.com>) with the scope to leverage the rapidly growing AI technology for combustion research.

