1. Webinar Title

Computational Modeling of High-Pressure Transcritical Flows with Phase Change: Adaptive Tabulation, Neural Networks, and Generative AI

2. Abstract

This seminar presents our advanced computational frameworks for modeling high-pressure transcritical/supercritical flows with multicomponent phase change, addressing the thermodynamic complexities inherent in modern and next-generation propulsion and energy systems. By integrating first-principled real-fluid vapor-liquid equilibrium (VLE) theory with innovative numerical strategies, we characterize the transition from subcritical spray to supercritical fluid, focusing on mixture critical point shifts and phase separation in systems such as multiphase detonation, supercritical carbon dioxide (sCO_2), and sustainable/synthetic aviation fuels (SAF). To overcome the prohibitive computational cost and robustness issue of real-fluid property evaluations, we introduce a synergistic approach combining *in situ* adaptive tabulation (ISAT) with artificial neural network (ANN) architecture to provide order(s) of magnitude acceleration and unprecedented robustness. We demonstrate the deployment of these neural network-aided adaptive tabulation methods in capturing the intricate physics of hypersonic shock-droplet interactions and liquid fuel vaporization at multiphase detonation-relevant conditions (e.g., in liquid-fueled rotating detonation engines), paving a path toward predictive and computationally efficient simulations of high-pressure real-fluid flows. We also demonstrate that GPUs can significantly accelerate real-fluid property evaluations compared to CPUs. Furthermore, we address a key bottleneck in thermodynamic modeling (i.e., unavailability of critical properties of intermediate species) by introducing generative AI models. We specifically highlight a comparative study of transformer-based (SMILES-based BERT) and graph-based (message-passing graph isomorphism networks, GIN) frameworks for predicting the critical properties required for real-fluid equations of state (EOS). Our results demonstrate that while transformers offer superior generalizability for specific parameters like critical pressure, GIN models provide a highly efficient, lightweight alternative with significantly faster inference times and perform on par with transformers on majority of the critical properties.

3. Brief Bio

Dr. Suo Yang is an Associate Professor of Mechanical Engineering at the University of Minnesota. During 2017-2018, He was a Postdoctoral Research Associate of Mechanical & Aerospace Engineering at Princeton University. Dr. Yang received his Ph.D. (2017) and M.S. (2014) degrees in Aerospace Engineering, and another M.S. degree in Computational Science & Engineering (2015), all from the Georgia Institute of Technology. He received a B.S. degree in Mathematics & Applied Mathematics from Zhejiang University in 2011. Dr. Yang's research focuses on the modeling and simulation of turbulent reacting & multiphase flows, including combustion, non-equilibrium plasma, particulate & gas-liquid flows, and hypersonics, with applications in aerospace propulsion & energy systems. He is an awardee of the 2021 DARPA Young Faculty Award (YFA), 2022 ONR Young Investigator (YIP) Award, 2023 DARPA Director's Fellowship Award, 2024 AFOSR Young Investigator (YIP) Award, and 2026 Central States Section of the Combustion Institute (CSSCI) Early Career Award. Dr. Yang has authored over 100 journal articles and refereed conference papers, in which he received 5 Editor's Pick or Featured Article awards from *Physics of Fluids* and *Combustion and Flame*. Dr. Yang is a Senior Member of AIAA and a member of 3 AIAA Technical Committees. He has served as a Technical Discipline Chair or Deputy Chair 5 times for AIAA SciTech Forums. He also actively serves as a reviewer for many top-tier journals for which he received 4 Outstanding Reviewer Awards.