

PURDUE FLUIDS SEMINAR SERIES

Exascale direct numerical simulations and on-the-fly reduced order modeling towards zero-carbon fuels for power and transportation

FRIDAY SEPTEMBER 27TH, 2024
2:00PM-3:00PM ARMS 1010



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Abstract

Mitigating climate change while providing the nation's transportation and power generation are important to energy and environmental security. The shift to hydrogen as a clean energy carrier is one of the most promising strategies to reduce CO₂ emissions in the face of increasing energy demand. While hydrogen has a few drawbacks as an energy carrier due to its low energy density, ammonia is simpler to transport and store for extended periods of time, making it an attractive carbon-free energy carrier for off-grid localized power generation and marine shipping. However ammonia has poor reactivity and forms NO_x and N₂O emissions. The poor ammonia reactivity can be circumvented by partial cracking of ammonia to form ammonia/hydrogen/nitrogen blends tailored to match conventional hydrocarbon fuel properties. However, combustion of ammonia/hydrogen/nitrogen blends at high pressure, and in particular, the coupling between turbulence and fast hydrogen diffusion remains poorly understood. Exascale high performance computing provides a unique opportunity for direct numerical simulation (DNS) of turbulent combustion with ammonia/hydrogen blends to investigate pressure effects on the turbulent burning velocity and staged rich-quench-lean combustion as a means to minimize NO emissions. A novel on-the-fly time-dependent reduced order model (ROM) is developed to accelerate DNS of turbulent combustion with high-dimensionality in composition space due to species transport and to mitigate chemical stiffness. The ROM is shown to reduce the computational cost of DNS with complex chemistry by up to two orders of magnitude.

Biography

Jacqueline H. Chen is a Senior Scientist at the Combustion Research Facility at Sandia National Laboratories. She received her B.S. degree in Mechanical Engineering from Ohio State University, her M. S. degree from University of California at Berkeley and her Ph.D. degree from Stanford University. She has contributed broadly to research in turbulent combustion elucidating 'turbulence-chemistry' interactions in combustion through direct numerical simulations. To achieve scalable performance of DNS on heterogeneous computer architectures she leads an interdisciplinary team of computer scientists, applied mathematicians and computational scientists to develop an exascale direct numerical simulation capability for turbulent reactive flows with complex chemistry and multi-physics. She is a member of the National Academy of Engineering and a Fellow of the Combustion Institute and the American Physical Society. She is an Associate Fellow of the AIAA. She is a member of the Council Executive Committee of the American Association for the Advancement of Science and Steering Committee Member of the Engineering Section. She received the Combustion Institute's Bernard Lewis Gold Medal Award in 2018, the Society of Women Engineers Achievement Award in 2018, and the Department of Energy Office of Science Distinguished Scientists Fellow Award in 2020. She served on the Combustion Institute Board of Directors and was past Editor of Journal of Flow, Turbulence and Combustion. She serves on the Department of Energy's Office of Advanced Scientific Computing Research Advisory Committee and Editorial Boards of Physical Review Fluids and Progress in Energy and Combustion.