SORS/WomenInBSC:"The convergence of exascale computing and data science towards zero-carbon fuels for power generation"

Objectives

Abstract: Mitigating climate change while providing 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 long-haul marine shipping. However ammonia has poor reactivity and forms NOx 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 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. Exascale computing resources are also enabling combined data science and computational workflows. For high-fidelity turbulent reacting flow simulations coupled with detailed chemical kinetics the computational cost and memory use is prohibitively high and methods for chemical species dimensionality reduction are needed. A novel model-driven on-the-fly reduced order surrogate model (ROM) for DNS of reactive flows will be described.

Jacqueline Chen

Short Bio: 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 for the American Association for the Advancement of Science. She received the Combustion Institute's Bernard Lewis Gold Medal Award in 2018, the Society of Women Engineers Achievement Award in 2018, 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 Editorial Boards of Physical Review Fluids and Progress in Energy and Combustion.

Speakers

Speaker: Jacqueline H. Chen. Sandia National Laboratories, Combustion Research Facility
Host: Daniel Mira. CASE - Team leader- Propulsion Technologies Group, BSC
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