DEPARTMENT OF MECHANICAL & AEROSPACE ENGINEERING
WILLIAM MAXWELL REED SEMINAR SERIES

"First-Principles Simulations of Thermochemical Nonequilibrium."

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Abstract:

Vehicles flying at high speeds can induce strong shock waves, resulting in flight environments rich in coupled flow phenomena, including thermal nonequilibrium, vibrational excitation, and dissociation. To gain molecular-level insight into the thermophysics that drive macroscopic fluid processes, we have incorporated *ab initio* potential energy surfaces in the Direct Molecular Simulation (DMS) method. In this unified framework, energy exchange, chemical reactions, transport, and fluid mechanics naturally arise from a single input. This has enabled us to derive transport properties and generate benchmark numerical solutions from first-principles, and leverage these results to evaluate and refine reduced order models of thermochemical nonequilibrium effects.

Speaker Bio:

Dr. Ashley Verhoff is an Aerospace Engineer in the Aerospace Systems Directorate of the Air Force Research Laboratory (AFRL), where she leads a research team conducting first-principles investigations of thermochemical nonequilibrium effects in high-speed flows. She earned her B.S. in Aerospace Engineering from the University of Cincinnati, and her M.S. and Ph.D. in the same from the University of Michigan. Prior to joining AFRL, Dr. Verhoff worked as an Aerospace Engineer at Blue Origin and as a Project Manager at Radiance Technologies. Her research interests include the development of particle- and continuum-based models for simulating thermochemical nonequilibrium effects and gas-surface interactions, and multi-fidelity approaches for conceptual vehicle design. Dr. Verhoff is also a member of the AIAA Thermophysics Technical Committee, and a Co-Investigator on a Department of Energy INCITE project.

Date: Friday, September 30, 2022
Time: 3:00 PM EST
Place: Whitehall Classroom Building 110
Contact: Dr. Jesse Hoagg

Attendance open to all interested persons

College of Engineering

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