

Kyle Niemeyer

Session 1

**Title:** Burning Through Exascale: Reactive Flow Simulation, AI Surrogates, and the Road to Combustion Digital Twins

**Abstract:** The arrival of exascale computing has opened new frontiers for reactive flow simulation, with recent demonstrations of multi-billion-cell turbulent combustion DNS on leadership-class GPU systems. Yet even at exascale, predictive simulation of full combustion devices with detailed chemistry, multi-phase physics, and realistic fuels remains beyond reach—stiff chemical kinetics alone can consume over 90% of wall-clock time. This talk surveys the computational landscape for reactive flows and combustion science over the next five years, focusing on three converging developments. First, the maturation of GPU-native, performance-portable combustion codes and the algorithmic challenges—particularly stiff ODE integration and warp divergence—that continue to limit efficiency on current and emerging architectures. Second, the rapid integration of machine learning surrogates, neural operators, and physics-constrained architectures into HPC workflows, offering algorithmic acceleration on top of hardware gains. Third, the emergence of digital twin frameworks that connect high-fidelity simulation with reduced-order models, data assimilation, and real-time sensing for operational combustion systems. The binding constraints for the next generation of combustion applications are shifting from peak FLOPS to integration challenges: multi-physics coupling at scale, uncertainty quantification across model hierarchies, FAIR data infrastructure for community-scale AI/ML, and a workforce that spans combustion physics, computational science, and GPU computing. The talk concludes with a perspective on what post-exascale systems will need to deliver, not just in raw performance, but in memory architecture, programmability, and AI-readiness, to enable the combustion digital twins and predictive simulation campaigns that the energy transition demands.

**Bio:** Dr. Kyle Niemeyer is Associate Professor of Mechanical Engineering and Associate Head for Undergraduate Programs in the School of Mechanical, Industrial, and Manufacturing Engineering at Oregon State University. He received his PhD in Mechanical Engineering from Case Western Reserve University in 2013. Dr. Niemeyer's research focuses on computational modeling of reacting and non-reacting fluid flows, with a particular interest in numerical methods and high-performance computing. He is also an

ardent advocate of open science, and serves as Associate Editor-in-Chief at the Journal of Open Source Software. He previously served as an AAAS Science and Technology Policy Fellow with the Industrial Efficiency & Decarbonization Office at the US Department of Energy.