Boulder Fluid and Thermal Sciences Seminar Series

Thursday, March 22, 2018
3:45pm-4:45pm (refreshments at 3:30pm)
Clark Conference Room (ECAD 150), Engineering Center
University of Colorado, Boulder

Incorporating detailed chemistry in reactive-flow simulations by exploiting system stiffness and processor architecture

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Combustion simulations with finite-rate chemistry rely on accurate and efficient methods for solving stiff ordinary differential equations (ODEs). In a typical reacting-flow solver, the ODEs involving chemical kinetics at each spatial location are decoupled by operator splitting, allowing each to be solved concurrently. Efficient ODE solvers must take into account both numerical efficiency as well as the available thread and instruction-level parallelism of the underlying computational hardware being used to perform the simulations, especially on many-core coprocessors. This talk will summarize work on complementary efforts to reduce the computational expense of chemical kinetics on modern processing architectures. First, I will discuss the performance and behavior of exponential and implicit Runge-Kutta integrators implemented for graphics processing units (GPUs). Second, I will compare the performance of explicit Runge-Kutta and implicit Rosenbrock solvers implemented using both single instruction, multiple thread and single instruction, multiple data paradigms executed on multicore CPUs, Many Integrated Core, and GPU processors. Third, I will discuss efforts to intelligently select appropriate integrators based on local stiffness. I will then make overall conclusions based on a synthesis of the results, and identify remaining open questions and directions for future research. Lastly, I will discuss other ongoing research in my group.

Biography: Dr. Kyle Niemeyer is an Assistant Professor 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 interests include computational modeling of reacting and non-reacting fluid flows at various scales and levels of fidelity; analysis, reduction, and validation of chemical kinetic models; and GPU computing. He is also an ardent advocate of open science.