Transforming **ENERGY** Through Computational Excellence

Bringing Low Mach Number Reactive Flow Simulations at the Exascale

Challenge: Reactive flow simulations, including those at a low Mach number, are characterized by large time and space scale separation between the thin, highly reactive chemical reaction fronts and the comparatively slower motion of the flow at scales prescribed by the technological device. The computational resources required to simulate such flows are determined by this scale separation. The extreme scale disparities in practical systems are challenging to simulate, even with exascale resources, and require advanced mathematical and computational algorithms that can exploit key properties of these flows.

Approach: We developed a low Mach number combustion solver called PeleLMeX, tailored for the GPU-based architectures of the U.S. Department of Energy's (DOE) exascale-class computers. The solver uses adaptive mesh refinement (AMR) for scale separation and employs state-of-the-art numerical methods to provide an accurate description of the intricate coupling between fluid mechanics, heat transfer, and chemical reactions. Concurrent, batched, GPU-accelerated iterative linear algebra solvers are used to efficiently evolve the chemical system (through Sundials, a Lawrence Livermore National Laboratory software suite of non-linear and differential/algebraic equation solvers), coupled with a new preconditioning strategy developed at the National Renewable Energy Laboratory to tackle the ill-conditioned projection arising from complex geometries.

Results: PeleLMeX was found to perform very well on the latest DOE GPU-accelerated platforms and is expected to perform equally well on the world's first exascale platform, Frontier, when it comes online later this year. Figure 1 shows the weak scaling performance (i.e., the ability of the solver to handle larger and larger data sets—capturing increasing levels of detail

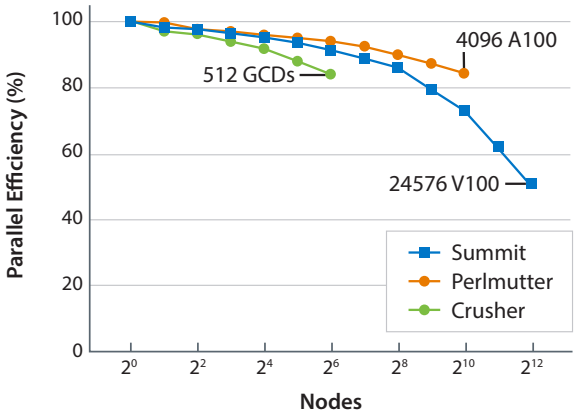

Figure 1. PeleLMeX weak scaling on DOE's GPU-accelerated platforms

over the entire device, with increasing computational power, of PeleLMeX on three supercomputers. The solver is also used by Sandia National Laboratories and other academic partners to study previously out-of-reach, complex physics.

Impact: PeleLMeX's unique capabilities are allowing for reactive flow modeling at unprecedented scales and a reasonable time and cost. The code is currently being extended to tackle more practical, design-oriented simulations by implementing Large Eddy Simulation and data-driven chemical models, providing a fast but accurate tool for engineers considering the emergence of GPU-accelerated platforms. These extensions are critical for enabling the physical insight required to design the next generation of combustion devices as a key component of a renewable energy future.

Pele Suite: **https://github.com/AMReX-Combustion**

PeleLMeX Software: **https://www.osti.gov/biblio/1873317**

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