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IN-SITU DATA ANALYSIS AND VISUALIZATION OF DNS COMBUSTION SIMULATIONS WITH PARAVIEW CATALYST

Minh Bau Luong*, Glendon Holst†, Francisco E. Hernández Pérez*, Hong G. Im*

* Clean Combustion Research Center (CCRC)
4700 King Abdullah University of Science and Technology (KAUST)
Thuwal 23955-6900, Kingdom of Saudi Arabia
e-mail: minhbau.luong@kaust.edu.sa

† KAUST Visualization Core Lab (KVL)
email: glendon.holst@kaust.edu.sa

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Abstract. ParaView Catalyst is adapted to our DNS solver named KARFS to perform in-situ data analysis and visualization for combustion simulations to overcome the IO bottleneck–the gap between IO and computing performance of the high-performance heterogeneous computing architectures. The in-situ integration of modeling, simulation, analysis, and visualization components in KARFS to capture abnormal combustion events, such as super-knock, will be presented.

Towards achieving exascale direct numerical simulation (DNS) of reacting flows, a DNS solver named KARFS (KAUST Adaptive Reacting Flows Solver) has been developed with state-of-the-art programming models for the next-generation high-performance heterogeneous computing architectures of many-core and graphics processing unit (GPU) processors [1]. KARFS is developed in C++ using modern parallel programming patterns, distributed memory parallelism through message passing interface (MPI), and portable on-node parallelism with the Kokkos C++ programming model. KARFS has performance-portable capabilities for multi- and many-core heterogeneous platforms, which is instrumental to meet emerging demands of exascale computing machines. The employed Kokkos framework allows KARFS to straightforwardly utilize the same source code on CPUs and GPUs while maintaining performance comparable to the code that is optimally tuned to either processing unit.

The conventional workflow of simulations performs the computations first and analyzes the output data later. This workflow does not scale on the exascale high-performance computing architectures. Exascale computing features a widening gap between compute power and available input/output (I/O) rates that will impose challenges to save data at a high enough temporal frequency for post-processing. For example, a high frequency of checkpoint data is required to capture extreme short-time-scale detonation events that

places significant stress on the I/O storage system and generates a massive amount of data. In the exascale era, this I/O constraint will be further exacerbated by the difficulty of moving large volumes of data through deep, complex memory hierarchies and across the machine network to hard disks on a heterogeneous supercomputer As such, a new concurrent workflow design, including in-situ massively parallel visualization coupled with analytics, is needed. The in-situ integration between modeling, simulation, analysis, and visualization components must be performed concurrently rather than working independently as they have in the past.

First-principle direct numerical simulation allows unraveling the complex interplay between turbulence and chemical reactions to provide better understanding of the mechanism of detonation development encountered in modern combustion devices under extreme high-load operating conditions, and to develop a reliable predictive model for real-world industrial applications. However, large-scale turbulence, combustion and detonation simulations pose a significant challenge in terms of a wide spectrum of length and time scales, which requires extremely fine spatial and temporal resolutions, and highly intermittent localized phenomena, resulting in an insensitive checkpoint output data and extensive computational resources. Multidimensional simulations of super-knock phenomena in combustion devices face such highly intensive I/O and computational resource requirement [2, 3].

Downsized and boosted technology is being a major development trend for advanced engines. The engines become more compact with a higher power density per volume, and thus provide higher thermal efficiency and cleaner combustion processes that reduce greenhouse CO2 gas as well as NOx and soot emissions. However, the elevated pressure and temperature of the in-cylinder fuel/air mixture under the high-load operating conditions may induce undesired pre-ignition, knock, and even super-knock phenomena [4]. Such abnormal combustion phenomena are also encountered in shock tubes, rapid combustion machines, and gas turbine engines [4].

Super-knock is featured by excessive pressure oscillations and extremely high-pressure spikes that may lead to mechanical failure [4]. The fundamental understanding of the developing super-knock mechanism and a reliable criterion to predict super-knock are needed to prevent destructive operation of combustion devices [5, 6, 7]. High fidelity direct numerical simulations with the capability of fully resolving all temporal and spatial scales and the complex interaction of thermochemistry and turbulence will help address the knocking issues [2, 3]. With the aid of ParaView Catalyst, coupled with our DNS solver, an integrated framework has been set up and deployed, which allows us to capture, visualize and analyze in-situ the highly localized detonation events occurring at sub-nanosecond timescales, as shown representatively in Fig. 1 and Fig. 2.

The homogeneous ignition delay time, τ_{ig}^{0}, and equilibrium pressure, P_e, of the ethanol/air mixture at the initial conditions, temperature T_0 of 1200 K, pressure P_0 of 35 atm, and equivalence ratio ϕ_0 of 1.0 are 75 μs, and 99 atm, respectively. Other relevant ideal one-dimensional detonation parameters associated with this initial condition are the von Neumann pressure, P_{VN} of 315 atm, Chapman–Jouguet pressure, P_{CJ} of 185 atm, and

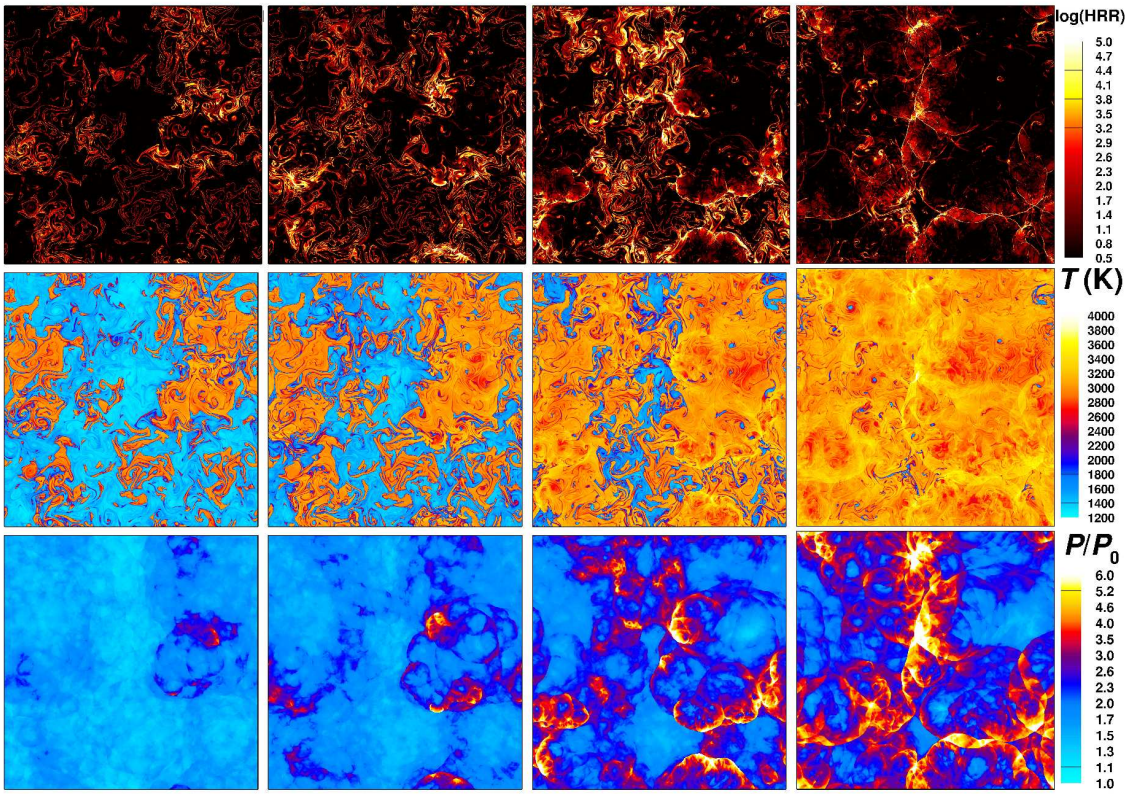

Figure 1: Instantaneous isocontours of heat release rate (top row), temperature (middle row), and pressure (bottom row) for a case labeled as G_5^1 (the most energetic length scale of temperature and turbulent field, l_T of of 5 mm and l_e of 1 mm, turbulent velocity fluctuation u' of 83.3 m/s, and the ratio of the ignition delay time to turbulent time scale τ_{ig}/τ_t of 5.0) with increasing time from left to right [3].

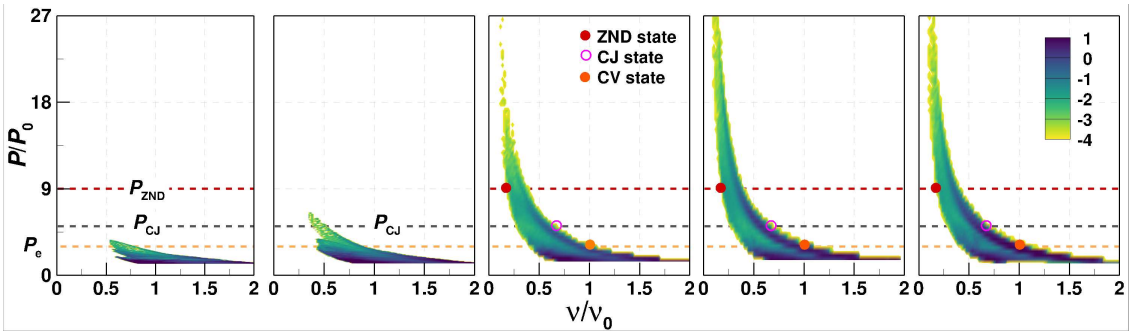

Figure 2: The joint probability density function (PDF) of the normalized pressure-specific volume (in log scale) [2].

Chapman–Jouguet speed, V_{CJ} of 1836 m/s. Further details will be provided in the presentation.

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