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HPC IN COMBUSTION: CONTRIBUTIONS TO PHYSICAL UNDERSTANDING AND MODELING

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Abstract. Combustion is a fascinating process occurring over an extended range of temporal and spatial scales. The quest for novel fuel-flexible devices with higher efficiency and reduced emissions leads to new regimes with complex flow-combustion interactions that are poorly understood at the fundamental level. Enabled by advances in computational resources, direct numerical simulations (DNSs) allow for the resolution of all relevant scales, and provide an accurate and complete description, which, together with theory and experiments, can be used to gain physical insights into the interactions of the physicochemical processes from the fundamental and the application level. After briefly discussing our spectral element low Mach number reactive flow solver and its scalabililty on today's HPC architectures, we will present selected examples where high-fidelity simulation were used to complement experiments in single-cylinder optical engines. The generated datasets are also used to validate and tune existing models, establish best practices for engineering-type simulations, and develop a new algebraic model for wall heat transfer in internal combustion engines.

1 Introduction

The availability of numerical methods and tools that can effectively exploit high performance computational resources enables accurate large scale simulations to investigate fundamental as well as practical combustion applications at relatively short turn-around times. This paper presents briefly the computational tool and simulations that benefited from the recent algorithmic improvements in our spectral element massively-parallel code based on Nek5000 [1] for the simulation of low Mach number reactive flows, which have enabled high-fidelity simulations of flows in laboratory-scale internal combustion engines.

2 COMPUTATIONAL APPROACH

2.1 Conservation equations, discretization and solver

Many combustion applications involve flows with strong heat release which are characterized by a large discrepancy between the flow velocity and the speed of sound. These systems are described by the Navier-Stokes equations together with the energy and chemical species conservation equations at the low-Mach number limit together with the equation of state. The formulation allows for acoustic waves to be neglected –thereby facilitating numerical integration– while compressibility effects due to heat release and composition changes are fully accounted for.

The equations are discretized in space using the spectral element method (SEM), a high-order weighted residual method offering not only the rapid convergence and tensor-product efficiency of global spectral methods but also the geometric flexibility of finite elements [2]. Globally, the SEM is based on the decomposition of the domain into E smaller subdomains (spectral elements), and within each element the solution is approximated by N^{th}-order polynomials. Spatial resolution can thus be varied by varying both E and N. It is worth pointing out that, in addition to the solution, the geometry is also described by high-order polynomials. The computational grids use conforming quadrilaterals or hexahedra in 2- and 3-D geometries.

The reactive flow solver employs the high-order splitting scheme of [3], and the discretized equations are advanced in time using a solver that is based on the open source highly-efficient parallel SEM implementation in Nek5000 [1]. Thermodynamic and transport properties as well as the chemical source term are evaluated using CHEMKIN or fuel-specific optimized subroutines. The continuity and momentum equations are integrated with a third-order semi-implicit scheme, while species and energy are advanced implicitly without further splitting using CVODE from the SUNDIALS package [4].

The principal advantage of the spectral element method is that convergence is exponential in N, which implies that significantly fewer grid points per wavelength are required to accurately propagate a signal (or turbulent/flame structure) over the extended times associated with high Reynolds number flow simulations. For the moving geometries encountered in internal combustion engines, mesh motion is accounted for by an arbitrary Langrangian-Eulerian (ALE) implementation. Multiple grids are used to ensure sufficient resolution at all times, and a scalable grid-to-grid spectral interpolation algorithm was developed to interpolate scalar and flow-field data from one mesh to the next, while maintaining the high-order accuracy of the SEM. A high-order splitting scheme is also used in this case, where the hydrodynamic equations are advanced with a backward difference/characteristic-based time-stepping algorithm developed for the ALE method, which allows to overcome the CFL restrictions imposed by standard schemes such as backward difference/extrapolation, an for a significant increase in time step, ensuring numerical stability up to a CFL number equal to 3 [5].

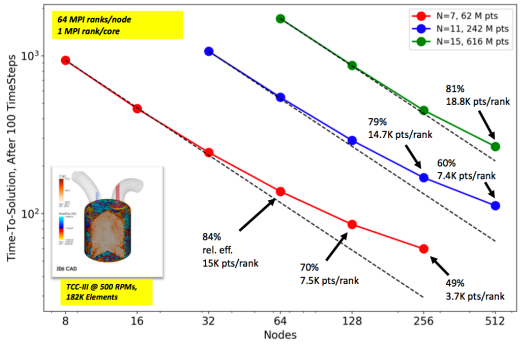


Figure 1: Strong scaling on the ALCF supercomputer Theta [7].

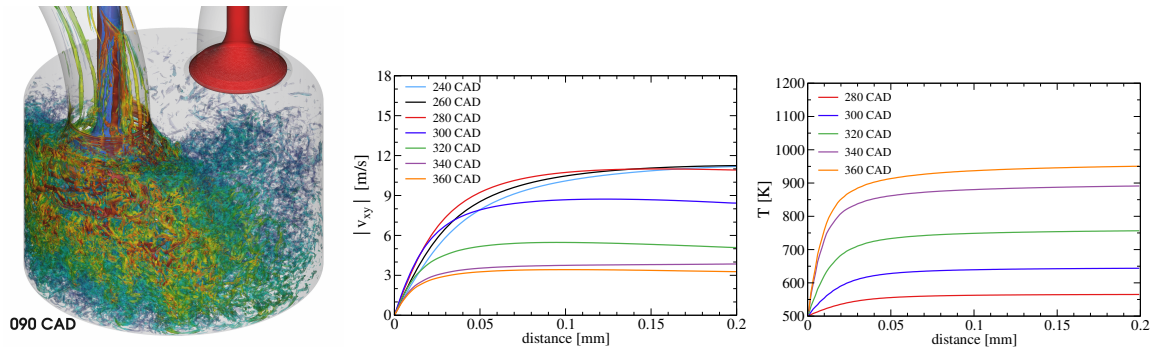
2.2 Parallelization

Parallelism in Nek500 is based on the message passing interface (MPI), and is realized through a domain-decomposition approach in which elements are distributed to processors using a map generated by recursive spectral bisection of the spectral element graph. Element-by-element operator evaluation ensures a high-degree of concurrency. The code has demonstrated very good strong scalability to large numbers of cores with low number of degrees of freedom per process on modern systems (Fig. 1).

3 INTERNAL COMBUSTION ENGINE SIMULATIONS

• **TCC-III engine.** High-order, wall-resolved large eddy simulations captured the in-cylinder flow and heat transfer within the Transparent Combustion Chamber TCC-III experimental engine [6] (Fig. 2). A total of 28 conforming hexahedral grids were generated and used at pre-defined crank-angle degrees (CAD) together with high-order spectral interpolation of the solution between successive meshes. In order to capture the temporally-varying momentum and thermal boundary layers, the normal distance between the walls and the first grid point of less than 10 μm was retained at all times, while the effective resolution in the bulk was between 0.2 and 0.03 mm. The simulation of 34 cycles of the gas exchange process during motored operation at 500 RPM revealed variations in the intake jet penetration and angle from cycle to cycle, and allowed for the characterization and quantification of the in-cylinder, large-scale motion and break down during compression [7].

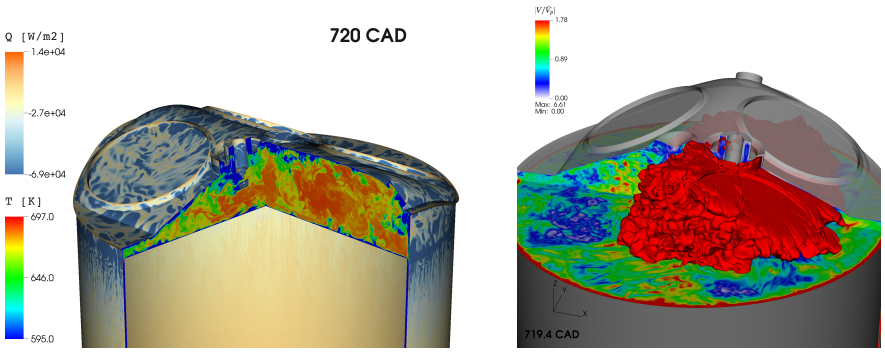
• **Darmstadt engine.** A single cycle was simulated using DNS for the optically accessible single-cylinder research engine of TU Darmstadt (TUD) under motored and fired conditions. In order to maintain the computational costs at affordable levels, a throttled, low turning speed operating point at 800 rpm and 0.4 bar intake pressure was chosen, for which experimental measurements were performed at TUD. For the non-reactive simulations this translates to lower Reynolds number, while for the reactive case, the pressure at spark timing is low enough for the DNS to fully resolve the flame thickness, which decreases strongly with increasing pressure. Two grids were employed in the non-reactive case with 1.6 million and 2.1 spectral elements using 7^{th}-order polynomials, resulting in



(a) (b) (c)

Figure 2: (a) Visualization of the instantaneous vortical flow structures in the TCC engine. (b) Thermal and (c) momentum boundary layers on the cylinder head at different CADs during compression [7].

an average mesh resolution of 40 μm and the first grid point located 5 μm away from the walls. In the fired case, 1.8 million spectral elements and 9^{th}-order polynomials were used, resulting an average resolution of approximately 15 μm in the bulk and 3 μm close to the walls and effectively doubling the resolution of the non-reactive case. Only a tuned global two-step for methane combustion could be afforded at a cost of close to 470 thousand CPU-hr/CAD (compared to about 14,000 CPU-hr/CAD for the motored case). Both simulations were initiated at intake valve closure from a chosen cycled computed using well-resolved multi-cycle large eddy simulations performed with STAR-CD, which were validated against the available experimental data. Instantaneous distributions are shown in Figs. 3(a) and (b) for the non-reactive and the reactive DNS, respectively.



(a) (b)

Figure 3: (a) Instantaneous distribution of heat flux Q on the cylinder walls and temperature inside the single-cylinder TUD engine under motored operation. (b) Flame front (red $T = 1500$ K isosurface) and distribution of velocity magnitude normalized by the mean piston speed under fired operation.

4 CONCLUSIONS

The Nek5000-based numerical code for low Mach number reactive flows exploits the capabilities of modern HPC architectures. The solver's high granularity allows for a significant reduction in the wall-time needed to simulate complex flows in internal combustion engines, while simultaneously increasing the resolution by at least an order of magnitude compared to the current state-of-the-art in scale resolving engine simulations. The generated high-quality dataset enhanced the physical understanding of the complex phenomena and complement commercial and open-source codes for ICE simulation by providing benchmark-type simulations. It has also been used to formulate a novel algebraic wall heat transfer model for wall-modelled LES [9].

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