Large-Scale Engine Direct Numerical Simulations With NekRS: A Multi-Cycle Database

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ABSTRACT

This paper presents a collection of large-scale engine direct numerical simulations performed with NekRS on JUWELS Booster. Twelve cycles each for two different engine speeds, 1,500 rpm and 2,500 rpm, of the TU Darmstadt engine were calculated, processed and analyzed.

1. Introduction

Internal combustion engines (ICEs) are still the most widespread mobility drive. Due to their enormous spread, even small improvements can lead to significant global savings. Furthermore, the fight against climate change also requires the use of climate-neutral fuels, such as ammonia for the heavy-duty sector. This requires the fastest possible optimizations, which are not possible without the use of simulations.

Due to the extreme conditions and complex/moving geometries, direct numerical simulations (DNSs) of engines are very challenging. This work has calculated twice twelve cycles of the TU Darmstadt ICE at different engine speeds using NekRS on JUWELS Booster.

2. Case setup and numerics

The direct injection engine at TU Darmstadt is a single, optically accessible cylinder with a pent-roof, four-valve head and an inlet port designed to promote tumble flow. The setup is designed to provide well-defined boundary conditions and reproducible operation. The cylinder of the square engine has a bore of $B = 86$ mm, which is typical for a passenger car engine. Detailed information about the engine and the associated test facility can be found in [1], while the engine operating conditions considered here are listed in Tab. 1.

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The multi-cycle DNS was performed using the spectral element solver NekRS/NekCRF [2, 3]. The construction of computational meshes that accurately represent complex ICE geometries is a significant challenge for NekRS due to its requirement for conformal hexahedral meshes. The mesh generation using Coreform Cubit (version 2022.11) involved first filling the cylinder head volume with tetrahedral elements (TETs), which were then divided into four hexahedrons (HEXs) each. The mesh of the lower horizontal plane of the cylinder head was then extruded to the piston to create tensor product element layers capable of accommodating the vertical mesh deformation caused by piston motion while minimizing distortion. The Arbitrary Lagrangian/Eulerian (ALE) formulation [4] was used to account for the mesh deformation resulting from piston motion, with the mesh velocity scaling linearly with the instantaneous piston velocity at the piston and decaying to zero at top dead center (TDC). To compensate for the distortion of the elements as the mesh was compressed, four meshes were constructed with different numbers of spectral elements ranging from $E = 4.8$ to 9.3M. This strategy aimed to maintain good mesh quality throughout the cycle by removing layers as needed. Specifically, the grids were adjusted at different stages: from 600 – 660 crank angle degrees (CAD), $E = 9.3M$ elements were used; from 660 – 690 CAD, the number was reduced

Engine speed [rpm]	Intake p [bar]	Re	No. cycles	OP
1,500	0.95	18,368	12	C
2,500	0.95	30,615	12	E

Table 1
Engine operating conditions (p=pressure; Re =Reynolds number).

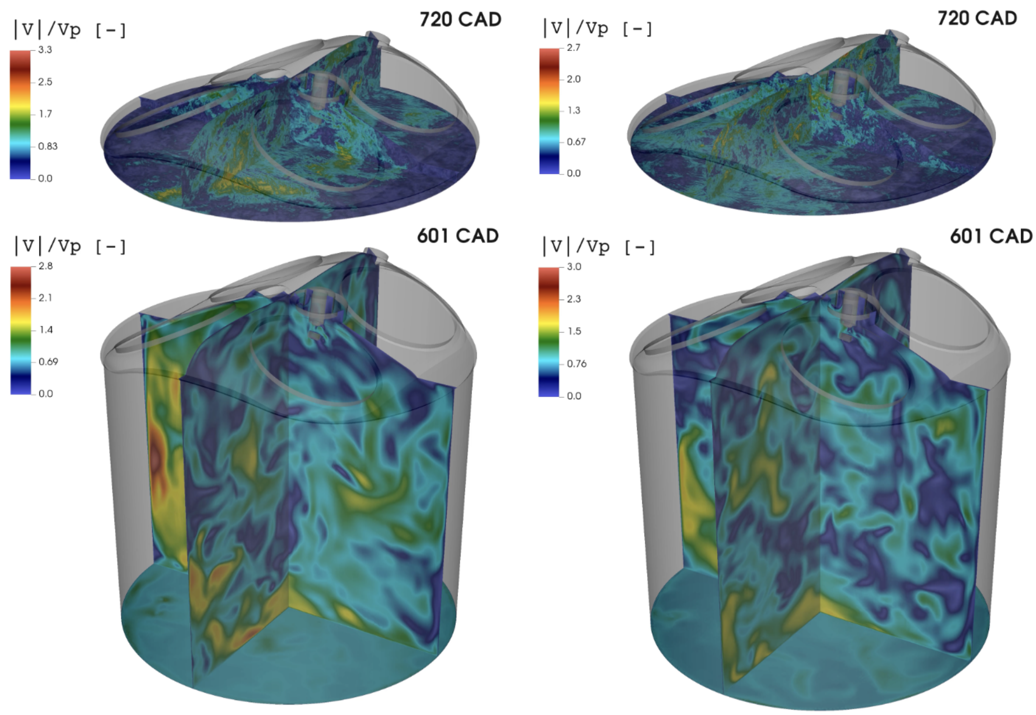

Figure 1: Visualizations of 1,500 rpm (left) and 2,500 rpm (right) for two different CA.

to $E = 6.7M$; from 690 – 710 CAD, it was further reduced to $E = 4.9M$; and from 710–750 CAD, $E = 4.4M$ elements were maintained. A scalable high-order spectral interpolation was used to transition the solution from one grid to the next without compromising the accuracy of the high-order method. Polynomial orders of $N = 7$ and $N = 9$ were chosen for the 1,500 and 2,500 rpm cases, respectively, yielding meshes with 1.5 to 6.8 billion unique grid points. The mesh achieved an average resolution of 30 µm and 23 µm in the bulk, with the first grid point located 3.75 µm and 3 µm away from the wall for 1,500 and 2,500 rpm, respectively.

3. Results and conclusions

Multi-cycle (12 for each engine speed) DNS of a laboratory-scale engine were performed at the practically relevant engine speeds of 1,500 and 2,500 rpm under full-load engine operation (visualizations see Fig. 1. The results confirm previous experimental and numerical findings that the boundary layer (BL) in ICE differs from idealized steady-state turbulent boundary layers, conditions commonly assumed in deriving scaling laws for wall model closures. The large-scale tumble flow generated by the intake process leads to a dynamically changing behavior of the BL, both temporally and locally. Above the piston, the flow undergoes a deceleration-stagnation process, where the tumble vortex hits the piston and then accelerates as the flow diverges from the impact area.

An analysis of the 3D motion of the tumble vortex revealed that the flow also rolls off the cylinder wall, resulting in horizontal vortex structures that are more toward the inlet side at lower heights above the piston and progressively toward the outlet side at higher heights within the cylinder. These structures appear at distances as low as 1 mm from the piston surface during later stages of compression and affect the BL especially at higher engine speeds. As a result, these fluctuations lead to alternating pressure gradients in both the streamwise and spanwise directions, ultimately invalidating the assumption of flow equilibrium. Furthermore, both the BL thickness and the viscous sublayer thickness were found to scale inversely with engine speed and increasing REYNOLDS number *Re* in the bulk, reaching values as low as 0.41 mm and 13 µm, respectively, at the highest engine speed investigated, posing a significant challenge to both numerical and experimental studies in terms of resolution requirements to properly resolve such BL.

The thermal BL was also found to deviate significantly from ideal scaling laws, even at high engine speeds. Similar to the velocity BL, the thickness of the thermal BL was found to scale inversely with engine speed, but to increase with increasing bulk temperature in the cylinder. In contrast, the thermal displacement thickness, which is sometimes used as an approximation of the thermal BL thickness, was found to decrease with increasing bulk temperature. Examination of the heat flux distribution confirmed the similarity between the flow and heat flux patterns and revealed areas of increased heat flux, particularly at locations characterized by strong wall-directed flow caused by the tumble vortex impinging on the piston and cylinder head or the horizontal swirl vortices impinging on the cylinder liner. In addition, significant cyclic variations in the surface-averaged wall heat flux were observed for both operating conditions. An analysis of the cyclic tumble ratio revealed that the cycles in which the tumble ratio reaches lower values near TDC, indicating earlier tumble breakdown, also exhibit higher surface-averaged wall heat fluxes.

These first-of-a-kind simulations [5], resulting in one of the largest databases of ICE flows, represent an important step toward the next generation of ICE simulations using GPU-accelerated HPC platforms. This advancement is critical to improve our understanding and optimization of engine performance under various operating conditions with climate-friendly fuels, and to ensure the practical applicability of the developed technologies in real-world engine designs.

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