D7.2 DNS OF REAL-SIZE INTERNAL COMBUSTION ENGINES

VERSION 1.0

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Center of Excellence in Combustion

Change log

Version	Author	Description of Change
V0.1	C. Frouzakis	Editorial changes based on Prof. N. Popivanov's comments
V0.2	C. Frouzakis	Editorial changes based on T. Grenga's comments

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1. Introduction

Although direct numerical simulations (DNS) has been extensively used to study various engine-relevant phenomena in canonical or significantly simplified geometries, only a handful of high-fidelity simulations have been performed to date on laboratory scale engine-like and internal combustion engine (ICE) geometries. These include previous work at ETH Zurich (ETHZ) with the spectral element solver Nek500, which was extended at ETHZ for the simulation low Mach number reactive flows, on CPU HPC systems of the flow and cyclic variability in a valve-piston assembly and wall heat transfer during a compression stroke at 560 rpm (e.g. [1]), the DNS of the compression/expansion stroke in the TU Darmstadt (TUDa) pent-roof engine under motored and fired operation at 800 rpm and throttled conditions [2], the high-resolution multi-cycle LES of the pancake TCC-II engine [3] as well as the DNS of the compression stroke in the TCC-III engine at 800 rpm at Argonne National Laboratory [4]. The planned simulations will extend the application of DNS for ICEs to almost double the engine speed considered to date in order to assess the generality of the findings obtained jointly from DNS and experiments at low engine speed, and simulate multiple cycles initialized from different engine-relevant initial conditions.

2. Methodology, progress and planned simulations

2.1. Aims

The focus is the investigation of (a) the evolution of the momentum and thermal boundary layers and their interaction with the bulk flow field and boundary layer evolution under both non-reactive (motored) and reactive (fired) operation, (b) the interaction of the flame with the flow and the walls, and (c) wall heat transfer phenomena inside the TUDa optical engine.

2.2. Codes

The direct numerical simulations will be performed with the codes that have been developed at ETH Zurich and at Argonne National Laboratory (ANL) based on the open source, spectral element flow solver Nek5000, as well as with NekRS, the new solver targeting both GPU and CPU HPC systems.

The spectral element method (SEM) is based on the decomposition of the computational domain into E smaller subdomains (elements), which can in the general case be curvilinear quadrilaterals or hexahedra that conform to the domain boundaries. Within each element, the geometry and solution are expanded as N^{th}-order polynomials cast in efficient tensor-product form, with values typically in the range N=7-11; the total number of grid points is equal to $E(N+1)^3$, while the number of unique grid points (taking into account that points on the elemental boundaries are shared) is approximately equal to $n=EN^3$. The principal advantage of SEM is that convergence is exponential with N, which implies that significantly fewer grid points per wavelength are required to

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accurately propagate a signal (such as a turbulent/flame structure) over the long times associated with high Reynolds number cold and reactive flow simulations. The solution procedure for solving the governing equations is based on a high-order splitting scheme [5], where the hydrodynamic equations are advanced with a backward difference/characteristic-based (BDF/CHAR), time-stepping algorithm developed for the arbitrary Lagrangian-Eulerian (ALE) method. The BDF/CHAR scheme allows the simulation to overcome CFL restrictions imposed by standard schemes such as backward difference/extrapolation (BDF/EXT). Species and energy equations are integrated using CVODE from the SUNDIALS package.
Nek5000 has demonstrated scalability to leading-edge platforms through the single-program multiple-data (SPMD) era and readily scales to millions of MPI ranks. However, the next generation of Exascale machines will be accelerator-based starting with the more recent advances in GPU architectures. NekRS is written in C++ and the kernels are implemented using the portable Open Concurrent Compute library [6, 7] in order to abstract between different parallel languages. In this way, the MPI+X hybrid parallelism can support seamlessly CUDA, HIP, OPENCL as well as CPUs [8]. It provides access to the standard Nek5000 interface and features (e.g., conjugate heat transfer), which allows users to leverage existing application-specific source code and data files on GPU-based platforms. NekRS is equipped with scalable multilevel solvers. The pressure substep requires a Poisson solve at each step, which is effected through multigrid-preconditioned GMRES iteration coupled with temporal projection to find an optimal initial guess.
Code development and optimization benefits from the work performed in WP4, Tasks 4.1 and 4.3, and WP5, Tasks 5.2 and 5.3.

2.3. Methodology

The feasibility of DNS using hexahedral meshes for complex laboratory-scale geometries has been shown in previous work employing a workflow employing large eddy simulations (LES). Multiple engine cycles were computed with a commercial CFD tool using well-resolved wall-modeled LES, and the results were found to be in good agreement with the experimental ensemble-averaged velocity fields on a vertical plane through the axis at low engine speed (800 rpm) and throttled operation (intake pressure 0.4 bar). The cycle that was closest to the measured phase-average behavior provided a realistic initial condition for DNS at inlet valve closure and was used to simulate one motored and one fired compression/expansion stroke [2]. A methodology to map the LES fields from LES onto the DNS grid was developed, which enables both the initialization of the compression stroke for the DNS and furthermore the direct comparability of the LES and DNS results. An efficient mapping algorithm based on the VTK library has been developed for this purpose.
The operating point at 1500 rpm and 0.95 bar intake pressure will be considered in the planned simulations, for which experimental measurements are available at TUDa. Previous LES results for this operating point show a good correspondence between the simulations and the experiments, justifying this choice for DNS. The simulations will almost double the engine speed considered

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to date in order to assess the generality of the findings obtained jointly from DNS and experiments at low engine speed.

Mesh generation

Nek5000 and NekRS require conformal purely hexahedral grids, rendering mesh generation a highly non-trivial task. This is especially true when dealing with the complex geometries of internal combustion engines, such as the TUD engine. In house developed algorithms were used in conjunction with Ansys ICEM CFD and Coreform Cubit to generate the computational grids that accurately represent the complex geometric features of the engine while simultaneously fulfilling the required mesh quality criteria.
Despite decades of research efforts and important advances, automating the generation process for hexahedral meshes for complex geometries is still not possible. It often requires manual intervention resulting in hexahedral mesh generation taking several orders of magnitude longer than tetrahedral mesh generation for the same geometry. One possible solution, which takes advantage of the much faster generation of tetrahedral meshes, is to fill the desired geometry volume with tetrahedral elements (TET) which can then later be split into four hexahedrals (HEX). For this TET-to-HEX approach, grids are generated using the Coreform Cubit, which allows for almost automated generation. However, this method often results in lower quality meshes and does not allow for local refinement. The alternative is to create fully hexahedral meshes from the beginning using a blocking strategy. By decomposing the geometry into several subdomains, the number of elements in different regions can be controlled better and the mesh quality can be significantly improved, albeit at the cost of a very time consuming mesh generation process using the Ansys ICEM CFD software. The merits of both approaches will be assessed in the planned simulations.

ICEM CFD. The creation of the mesh was realized adopting a top-down approach using the block structure definition in ICEM CFD. The mesh generation starts with a block around the volume of the cylinder head which is subsequently divided into smaller blocks in order to capture the complexities of the geometry (Figure 1). The final split contains more than 500 individual blocks which are then associated to the geometry lines and surfaces to produce the final block structure. Certain regions complicate the block meshing, namely the spark plug as well as the outer rim which is used to attach the engine to the test bench. Special effort was put to ensure that the features can be correctly captured resulting in a high quality mesh that can be easily refined according to the resolution requirements.

Coreform Cubit. The grids are constructed by filling the cylinder head volume with TET elements, and subsequently converting each TET to four HEX (Fig. 2). The grid in the remaining part of the cylinder is constructed by extruding the bottom surface mesh to the piston to create tensor-product element layers that can accommodate the vertical mesh deformation resulting from the piston motion while avoiding highly distorted elements. Two layers of elements are added close to the walls in order to ensure that the momentum and thermal boundary layers

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are always fully re-solved. A Laplacian smoother is finally applied to further improve mesh quality.

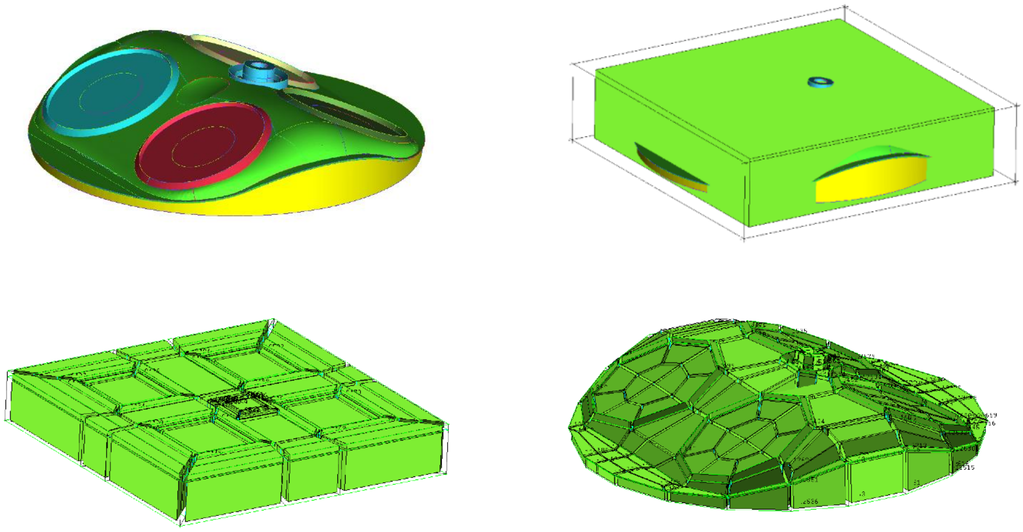

Figure 1: Block meshing using ICEM-CFD.

DNS of Motored operation. The simulations will be performed on (pre-)exascale GPU HPC systems using NekRS enhanced by the implementation of the ALE approach for moving geometries within WP4 and WP5; NekRS has already been shown to perform very efficiently for large-scale simulations on different GPU systems [8]. Multiple grids with E=6 to 8 million spectral elements and polynomial order equal or higher than N=7 resulting in 3.7 to 4.1 billion grid points will be employed during compression to ensure that the small scale structures generated towards the top dead center will remain well resolved. Around the walls, a constant resolution of a few microns will be used in order to fully resolve the boundary layers at all times. Spectral interpolation of the solution from one grid to the next will be used to minimize numerical errors. Three cycles from the LES campaign exhibiting strong variation in the large scale flow structures will be chosen as initial conditions for the DNS to assess the effect of cyclic variability characterizing internal combustion engine operation. Preliminary simulations performed on the JUWELS Buster GPU system at the Jülich Supercomputing Center (JSC) have shown good performance of NekRS.

DNS of Fired operation. A similar workflow will be adopted, where the flow, temperature and species fields from reactive LES at IVC of the cycle that is closest to the mean will be used as initial condition for the DNS. A two-step, six-species global reaction mechanism tuned to match the laminar flame speed and thickness of methane-air flames at the engine conditions will be used first, and depending on performance and availability of computational resources, we will also consider more complex skeletal mechanisms. The mesh in the region around the spark plug will be refined by exploiting the overlapping mesh capability of the

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solvers, which has been found to provide accurate results in the simulation of propagating premixed flames in WP4.

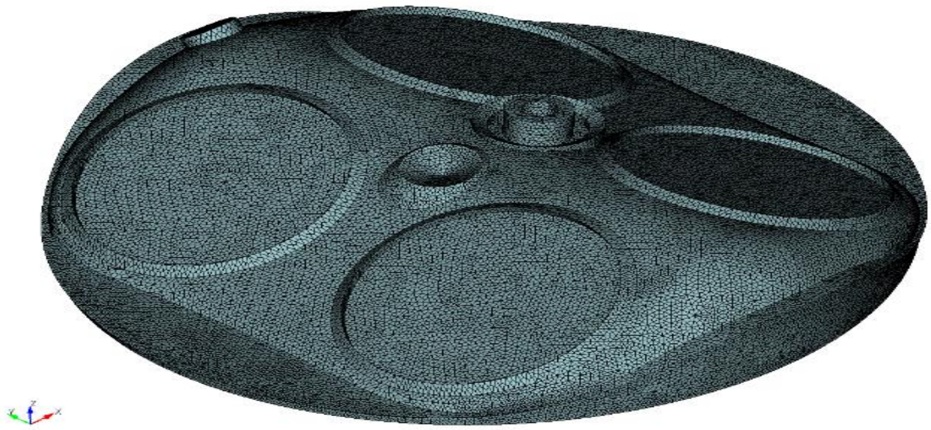

Figure 2: Spectral element skeleton of the fully-conforming hexahedral mesh of the cylinder head after the TET-to-HEX conversion.

2.4. Expected outcomes

The high-fidelity datasets generated by the simulations will provide detailed physical insights on the evolution of the boundary layers and wall heat transfer under motored and fired operation as well as on flame propagation in a realistic internal combustion engine geometry in the presence of large- and small-scale flow variations and its interaction with the engine walls and the piston and flame quenching at relevant pressures and temperatures. The generated data will be post-processed in order to validate commonly used combustion and wall heat transfer models used in large eddy simulations and contribute towards the establishment of best practices in engine CFD.

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