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Quasi-DNS capabilities of OpenFOAM for different mesh types

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ABSTRACT

Experimental limitations for certain nuclear reactor safety applications have pushed forward the demand for high fidelity DNS reference solutions for complex geometric configurations such as a T-junction or a spherical pebble bed. The application of traditional high-order DNS codes is limited to simple flow domains such as a periodic box or channel. As a possibility to create reference DNS solutions for more complex geometries, we have assessed the (quasi-)DNS capabilities of the OpenFOAM finite volume CFD solver for both structured hexahedral meshes and arbitrary polyhedral meshes. The feasibility of (quasi-)DNS analyses on polyhedral grids is of main interest, since this may offer the possibility to significantly expand the availability of (quasi-)DNS-quality data on arbitrarily complex geometries. In order to have a basis for the considered assessment, the mutual differences between generally recognized reference DNS data bases for turbulent channel and pipe flows are determined first. Subsequently, the differences between these reference DNS solutions and the present OpenFOAM (quasi-)DNS solutions are quantified for the considered mesh types. We use an existing finite volume CFD method and well known turbulent channel and pipe flow DNS reference cases for the assessments in this paper. New in this paper are the application of this CFD method to (quasi-)DNS analyses using arbitrary polyhedral meshes, and the quantification of respectively the mutual differences between generally recognized reference DNS data bases and the differences between the obtained OpenFOAM (quasi-)DNS data and these reference DNS data bases.

Based on the presented assessment, it is observed that the differences between the OpenFOAM solutions and the considered reference DNS solutions are practically the same as the mutual differences between these reference DNS solutions when structured hexahedral meshes are used. Furthermore, it is observed that the differences as obtained by OpenFOAM on extruded polyhedral meshes are practically the same as those obtained for the structured hexahedral meshes. In contrast, the full polyhedral mesh shows somewhat larger differences near the peaks in the rms velocity profiles, whereas the differences in the bulk flow are again practically the same as those for the hexahedral grids.

1. Introduction

The understanding of the complex heat transport and flow physics occurring in certain nuclear reactor safety applications is a big challenge. Despite several experimental attempts that have been undertaken to understand the complex turbulent flow and heat transfer phenomena in for example T-junction type geometries or pebble bed reactor cores, still a limited amount of data is available to understand these complex phenomena. This limitation is directly related to the difficulty of extracting the required experimental data from such geometric configurations. For such cases, complementary high fidelity Direct or quasi-Direct Numerical Simulation (DNS or q-DNS) is required to provide the data needed for complete understanding of the complex flow and heat transfer phenomena, and for further development and validation of various turbulence modeling approaches.

Within a DNS, all length and time scales of turbulence are fully resolved. Generally, specialized high-order numerical methods are used for this purpose. The application of these high-order numerical methods is generally limited to simple flow domains like a periodic channel or pipe. In this paper, we have determined the DNS capabilities of a finite volume method on unstructured grids using second order spatial and temporal discretisation schemes. Since a priori somewhat lower accuracy can be expected for this numerical method, we have decided to speak about q-DNS capabilities instead of DNS capabilities. It will be explained why we have decided to determine the q-DNS capabilities of the finite volume

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method on hexahedral and arbitrary polyhedral meshes, as used in the OpenFOAM [45] and STAR-CCM+ [40] Computational Fluid Dynamics (CFD) solvers. For OpenFOAM, these capabilities are presented in this paper.

CFD analyses of the turbulent flow and heat transfer are of fundamental importance for specific Nuclear Reactor Safety (NRS) applications. Some of these NRS examples are:

- The primary coolant flow and heat transfer in nuclear fuel rod-bundles (e.g. [2,15,6,5]);
- The turbulent flow and heat transfer in the pebble bed reactor core of high temperature reactors (e.g. [12,37–39]);
- Thermal fatigue resulting from turbulent thermal mixing in T-junction type geometries (e.g. [31,24,23,34,17,46]);
- Pressurized Thermal Shock (PTS) in the Reactor Pressure Vessel (RPV) wall resulting from turbulent thermal mixing of cold emergency core coolant water in the RPV [26].

In these applications, it is not only the mean flow and heat transfer characteristics that are important, but also the flow and temperature fluctuations play a significant role. For instance, the flow oscillations in a rod-bundle can result in flow induced vibrations which may result in structural damage [13,22], and the turbulent temperature fluctuations in T-junctions located in the reactor coolant system can cause thermal fatigue damage [7]. Therefore, accurate predictions of the mean flow and heat transfer characteristics as well as the fluctuations are of significant interest.

For the considered NRS applications, both Reynolds Averaged Navier–Stokes (RANS) and Unsteady-RANS (e.g. [1,27,28,32]), as well as Large Eddy Simulation (LES) (e.g. [26,31,17]) are used. However, for the considered NRS applications, these CFD approaches need further validation, and potentially also further development. The major problem that hampers further validation of CFD modeling approaches for these NRS applications is the lack of detailed experimental data. Namely, detailed data of the heat transfer with the walls of respectively the fuel bundles and fuel pebbles in the reactor core, the T-junction pipe walls, and the walls of the RPV are lacking. This lack of wall heat transfer data originates from the fact that adiabatic acrylic glass experimental facilities (e.g. the Vattenfall T-junction facility [33], the ROCOM test facility [21,20] have been used in order to have optical access for advanced measurement techniques. Furthermore, it is often very difficult to obtain accurate measurements very close to the walls for these applications. The main reason for this is the finite and often limited spatial resolution in the measurements compared to the required spatial resolution very close to the walls. As a result, no detailed data are available for the velocity and temperature fluctuations very close to the walls. These near wall velocity and temperature fluctuations are of crucial importance in order to understand the fluctuating heat transfer to, for example, the pipe walls in a T-junction in thermal fatigue analyses. Given this situation, complementary DNS or q-DNS data are deemed to be essential in order to:

- understand the considered near wall heat transfer phenomena, and eventually, the heat transfer between the fluid and the walls;
- have complementary reference data for further validation, and potentially further development, of RANS, URANS, and hybrid URANS/LES approaches for application to the considered NRS applications.

Therefore, our eventual aim is to perform DNS or q-DNS analyses for complex geometries like for example a T-junction or a periodic pebble bed. DNS of turbulent flows is generally performed using specialized high-order numerical methods. Traditionally, these methods can be broadly categorized into pseudo-spectral methods and finite difference methods. In pseudo-spectral methods [11], the flow variables are expanded in smooth, mostly orthogonal trial functions, which are defined over the whole computational domain. Typical trial functions are the Fourier series for domains with periodic boundary conditions, or Chebyshev and Legendre polynomials for non-periodic boundary conditions. The spectral method is highly accurate. However, its application is limited to simple domains such as a periodic box or channel (e.g. [19,43,41,10,14].

The order of accuracy of finite difference methods is lower than that of spectral methods. However, it is claimed that spectral-like accuracy for turbulent flows in complex domains can be obtained using the more recent developments based on a combination of compact finite difference schemes on Cartesian meshes together with the immersed boundary method for handling of complex geometries (see e.g. [25,30]).

In principle, the spectral element method can be used also for DNS analyses. In the spectral element method, high-order polynomials are used to approximate the flow variables within the finite element framework in order to obtain spectral accuracy on unstructured meshes. The spectral element method therefore allows the use of complex geometries, while preserving the spectral accuracy.

Complex geometries can be represented using the finite volume method on unstructured meshes. The non-staggered (or: collocated) arrangement of the flow variables is practically preferred for the computation of flows in complex geometries. Therefore, this approach is commonly used in, for example, commercial CFD codes. Generally, concerns have been expressed concerning the suitability of this approach for DNS computations due to the additional damping terms which are introduced in order to prevent pressure–velocity decoupling.

We believe that the selection of a certain numerical method for performing a DNS of a specific application will depend strongly on the complexity of the flow topology. Furthermore, the eventual selection of a certain method will also be influenced by factors such as the availability of CFD solvers to the users and the users' experience with these solvers. For the applications considered here, the walls, and therefore the boundary layers attached to these walls, can have all spatial orientations. We therefore believe that the application of compact finite difference schemes on Cartesian meshes together with the immersed boundary method will result in high near wall mesh resolutions in the entire flow domain. As a result, this method may be sub-optimal for our applications. We therefore expect that a spectral element method or finite volume method on unstructured meshes may be more suitable for our applications. Based on the extensive experience with finite volume methods within our group, we have therefore decided to explore the q-DNS possibilities of this method on hexahedral and arbitrary polyhedral meshes as a first option. Since lower accuracy can be expected for the selected option, we deliberately speak about q-DNS instead of DNS.

The three main objectives of this paper therefore are:

- to determine the mutual differences between generally recognized reference DNS data bases for turbulent channel and pipe flows;
- to quantify the differences between these reference DNS data bases and the present OpenFOAM q-DNS results as obtained on hexahedral and arbitrary polyhedral meshes;
- to assess OpenFOAM's q-DNS capabilities for the applied mesh types based on the obtained differences in the previous step.

The selection of hexahedral and arbitrary polyhedral meshes for the present purpose is based on the following arguments: the q-