International Journal of Heat and Fluid Flow 50 (2014) 287–299

Contents lists available at ScienceDirect

International Journal of Heat and Fluid Flow

journal homepage: www.elsevier.com/locate/ijhff

Accurate prediction of the wall shear stress in rod bundles with the spectral element method at high Reynolds numbers ☆

Justin Walker, Elia Merzari *, Aleksandr Obabko, Paul Fischer, Andrew Siegel

Mathematics and Computer Science Division, Argonne National Laboratory, United States

ARTICLE INFO

Article history:
Received 27 June 2013
Received in revised form 9 August 2014
Accepted 24 August 2014
Available online 18 October 2014

Keywords:
Wall shear stress
Rod bundle flows
Spectral element method
Large eddy simulation

ABSTRACT

Resolving flow near walls is critical to reproducing the high rates of shear that generate turbulence in high Reynolds number, wall-bounded flows. In the present study, we examine the resolution requirements for correctly reproducing mean flow quantities and wall shear stress distribution in a large eddy simulation using the spectral element method. In this method, derivatives are only guaranteed in a weak sense, and the same is true of quantities composed of derivatives, such as the wall shear stress. We are interested in what is required to resolve the wall shear stress in problems that lack homogeneity in at least one direction. The problem of interest is that of parallel flow through a rod bundle configuration. Several meshes for this problem are systematically compared. In addition, we conduct a study of channel flow in order to examine the issues in a canonical flow that contains spanwise homogeneity missing in rod bundle flow. In the case of channel flow, we compare several meshes and subgrid scale models. We find that typical measures of accuracy, such as the law of the wall, are not sufficient for determining the resolution of quantities that vary along the wall. Spanwise variation of wall shear stress in underresolved flows is characterized by spikes—physical points without well-defined derivatives of the velocity—found at element boundaries. These spikes are not particular to any subgrid scale model and are the unavoidable consequence of underresolution. Accurately reproducing the wall shear stress distribution, while minimizing the computational costs, requires increasing the number of elements along the wall (local *h*-refinement) and using very high order ($N = 19$) basis functions (*p*-refinement). We suggest that while these requirements are not easily generalized to grid spacing guidelines, one can apply a general process: construct a mesh that progressively increases elements along any walls, and increase the order of basis functions until the distribution of wall shear stress or any other quantity of interest is smooth.

1. Introduction

Accurate prediction of wall shear stress is critical in the analysis of turbulent wall-bounded flows (Pope, 2000). It is important for the production of correct friction factors, turbulent kinetic energy production, the analysis of heat transfer, and study of fluid–structure interaction. In most flows of engineering interest, the wall shear stress and viscous stresses are nonuniform since they are functions of the velocity derivatives. In order to predict the wall shear stress correctly, the regularity and smoothness of the velocity solution need to be guaranteed. However, in methods that solve the weak form of the Navier–Stokes equation such as the spectral element method (SEM), the space of solutions is usually chosen to be less regular than C^1 so that only weak derivatives are guaranteed to exist, and the derivatives do not have the same strict requirement to converge that the solution does (Deville et al., 2002). While approximations of the convergence of derivatives exist, we are interested in what is seen in practice, especially in the case of underresolved, non-DNS (direct numerical simulation) flows. We aim to provide guidelines to predict wall shear stress in complex engineering flows at realistic Reynolds numbers while maintaining the mesh resolution as coarse as possible. The target problem chosen is the parallel flow in rod bundles.

The prediction of the flow in rod bundles is of fundamental importance in a variety of engineering fields. It is, for instance, relevant for heat transfer applications such as the design of tube and shell heat exchangers as well as nuclear reactor core analysis. In

☆ The submitted manuscript has been created by the University of Chicago as Operator of Argonne National Laboratory ("Argonne") under Contract DE-AC02-06CH11357 with the U.S. Department of Energy. The U.S. Government retains for itself, and others acting on its behalf, a paid-up, nonexclusive, irrevocable worldwide license in said article to reproduce, prepare derivative works, distribute copies to the public, and perform publicly and display publicly, by or on behalf of the Government.
* Corresponding author.
E-mail address: emerzari@anl.gov (E. Merzari).

http://dx.doi.org/10.1016/j.ijheatfluidflow.2014.08.012
0142-727X/

nuclear reactor cores, the heat produced by the nuclear fuel contained within the rods is removed by the coolant flowing through the bundle. To predict with greater accuracy the behavior and the thermal performance of nuclear reactors, one must predict accurately the underlying hydrodynamics.

Rod bundle flows differ significantly from pipe flow and parallel channel flow (Rehme, 1987; Trupp and Azad, 1975; Hooper, 1980). Rod bundles present flow characteristics that are reminiscent of external flows. Viscous dissipation and wall shear stress change azimuthally. Coherent structures might develop in the streamwise direction for particularly tight bundles. Moreover, the flow anisotropy induces secondary flows.

Especially important for nuclear engineering applications is the prediction of the peak fuel temperature and peak fluid temperature. Ideally, one would compute a temperature solution by prescribing a heat flux at the boundary or, even better, by performing a conjugate heat transfer calculation. In cases where that is not possible, the Reynolds analogy can be used to obtain an approximation to the heat transfer from known values of the wall shear stress.

RANS models developed for internal flows do not usually fare well for rod bundles because of a combination of the previous points (Baglietto and Ninokata, 2005; Merzari et al., 2008). Accounting for more physics and reasonable tuning leads to better results. However, a more general approach such as large eddy simulation (LES) is desirable to lead to better predictability and freedom in exploring the design space (Merzari and Ninokata, 2011). In LES the large scales of turbulence are resolved while the small scale contribution to dissipation is modeled. Wall-resolved LES presents significant advantages when considering conjugate heat transfer calculations. Moreover, it permits exploring the physics of near-wall turbulence, which dramatically influences heat transfer. Traditionally, wall-resolved LES has been limited to relatively low Reynolds numbers since the computational cost scales superlinearly with the Reynolds number. One of the purposes of the present work is to test such methodology at Reynolds numbers of engineering interest and to verify how coarse the grid can be. As part of the Center for the Exascale Simulation of Advanced Reactors (CESAR) (CESAR Team, 2012) effort, increasingly large simulations are planned comprising full reactor cores, and accessing the minimal computational requirements is of fundamental importance.

The code used for all the calculations performed for the present work is Nek5000 (Fischer, 1997; Fischer et al., 2008), a code developed at Argonne National Laboratory and the target CFD code of CESAR. Nek5000 has demonstrated excellent parallel performance on petascale level machines when at least 20,000 collocation points are allocated per MPI process. Nek5000 solves the incompressible Navier–Stokes equations in the weak form using the spectral element method, a higher-order method in space.

In the present paper we explore the computational requirements to perform LES simulations at high Reynolds numbers in rod bundles using Nek5000. We study two cases: parallel flow around a single rod in an infinite array and channel flow. The objective is to be able to perform full bundle simulations at the Reynolds numbers encountered in prototype reactors ($\sim$70,000) with the least amount of computational effort possible while maintaining excellent accuracy for both velocity distribution and wall shear stress. This implies operating LES at the limit of underresolution, where the method does not guarantee a smooth solution of the derivatives. An approach to locally increase the resolution was found to be required in order to correctly resolve the wall shear stress. In fact, in order to achieve accurate prediction of wall shear stress in an LES, resolution requirements are greater than what is needed for other measures of accuracy such as the law of the wall.

Preliminary results for a 37-rod bundle simulation, performed by using the resolution guidelines described in the present work, are shown in Fig. 1. The grid resolution studies presented in this work have been performed on an infinite array (Fig. 1d) for simplicity and reduced computational cost.

In Section 2, the computational methodology is summarized. In Section 3 the issues concerning wall shear stress are described in more detail. Section 4 contains a systematic study of the effects of underresolution on the mean flow quantities in the case of channel flow. Section 5 focuses on the target case, the parallel flow in rod bundles. The results of several calculations are compared and conclusions drawn about best practices.

2. Methodology

Calculations were performed by using the spectral element code Nek5000 (Fischer et al., 2008). Nek5000 solves the incompressible Navier–Stokes equations.

In this study the incompressible Navier–Stokes equations are solved in their standard Cartesian form:

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{1}{\mathrm{Re}} \frac{\partial^2 u_i}{\partial x_j \partial x_j} \tag{1a}$$

$$\frac{\partial u_i}{\partial x_i} = 0 \tag{1b}$$

along with appropriate boundary conditions. All variables have been nondimensionalized by a characteristic length δ and bulk velocity scale U_b; Re is the Reynolds number.

The domain and equations are discretized following the form of the spectral element method. The spectral element method solves the Navier–Stokes equations on a given domain by discretizing the solution space into elements such that the global solution is composed of piecewise polynomial functions with compact support. The problem is solved as a variational problem in what is known as weak form (Deville et al., 2002). (More details are given in Section 3.) Lagrangian polynomial functions of up to the 23rd degree have been used to discretize the velocity field in each element in the present work. In the generalized, weighted residual framework, the present spectral-element method can be classified as a Galerkin method where the test functions and the basis functions for each element are Lagrange polynomials evaluated on Gauss–Lobatto–Legendre collocations points for the velocity. The pressure is solved with the same order polynomials as the velocity (P_N-P_N formulation).

Eqs. (1a) and (1b) are integrated in time by using a characteristic scheme as described by Maday et al. (1990). This method avoids the Courant–Friedrichs–Lewy (CFL) stability constraint in typical semi-implicit timestepping implementations, allowing greater time steps with CFL values in the range of 3–4.

In all problems considered here, periodic boundary conditions are applied in the streamwise direction. A dynamic forcing term is calculated at each time step to ensure a fixed flow rate.

The LES calculations carried out in this study use the stabilizing filter of Fischer and Mullen (2001). In this method, the solution at each time step is explicitly filtered. The filter operator F_α is defined as

$$F_\alpha := \alpha I_{N-1} + (1-\alpha)\mathbf{I} \tag{2}$$

where $\mathbf{I}$ is the identity operator and I_N is the interpolation operator at the $N+1$ GLL nodes. This filter has the desirable property that it preserves the spectral convergence of SEM. As $N \to \infty$, the interpolation error goes to zero exponentially.

Note that in Sections 4 and 5 of this paper we decompose the x component of velocity as $\tilde{u} = U + u$, where U is the mean component and u is the fluctuating component, and use $\bar{\cdot}$ to indicate averaging. Similarly, the y and z components of velocity are denoted by $\tilde{v} = V + v$ and $\tilde{w} = W + w$, respectively.