Computers & Fluids 116 (2015) 10–16

Contents lists available at ScienceDirect

Computers & Fluids

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

A pencil distributed finite difference code for strongly turbulent wall-bounded flows

Erwin P. van der Poel [a,*], Rodolfo Ostilla-Mónico [a], John Donners [b], Roberto Verzicco [c,a]

[a] Department of Physics, Mesa+ Institute, and J. M. Burgers Centre for Fluid Dynamics, University of Twente, 7500 AE Enschede, The Netherlands
[b] SURFsara, Science Park, 1098 XG Amsterdam, The Netherlands
[c] Dipartimento di Ingegneria Industriale, University of Rome "Tor Vergata", Via del Politecnico 1, Roma 00133, Italy

ARTICLE INFO

Article history:
Received 31 December 2014
Accepted 2 April 2015
Available online 16 April 2015

Keywords:
Finite-difference scheme
Turbulent flows
Rayleigh–Bénard convection
Taylor–Couette flow
Parallelization

ABSTRACT

We present a numerical scheme geared for high performance computation of wall-bounded turbulent flows. The number of all-to-all communications is decreased to only six instances by using a two-dimensional (pencil) domain decomposition and utilizing the favourable scaling of the CFL time-step constraint as compared to the diffusive time-step constraint. As the CFL condition is more restrictive at high driving, implicit time integration of the viscous terms in the wall-parallel directions is no longer required. This avoids the communication of non-local information to a process for the computation of implicit derivatives in these directions. We explain in detail the numerical scheme used for the integration of the equations, and the underlying parallelization. The code is shown to have very good strong and weak scaling to at least 64 K cores.

1. Introduction

Turbulence is known as the "last unsolved problem of classical physics". Direct numerical simulations (DNS) provide a valuable tool for studying in detail the underlying, and currently not fully understood, physical mechanisms behind it. Turbulence is a dynamic and high dimensional process, in which energy is transferred (cascades) from large vortices into progressively smaller ones, until the scale of the energy is so small that they are dissipated by viscosity. DNS requires solving all of the flow scales, and to adequately simulate a system with very large size separation between the largest and the smallest scale, immense computational power is required.

The seminal works on homogeneous isotropic turbulence by Orszag and Patterson [1] and on pressure-driven flow between two parallel plates (also known as channel flow) by Kim et al. [2], while difficult back then, could be performed easily on contemporary smartphones. Computational resources grow exponentially, and the scale of DNS has also grown, both in memory and floating point operations (FLOPS). In approximately 2005, the clock speed of processors stopped increasing, and the focus shifted to increasing the number of processors used in parallel. This presents new challenges for DNS, and efficient code parallelization is now essential to obtaining scientific results.

Efficient parallelization is deeply tied to the underlying numerical scheme. A wide variety of these schemes exist; for trivial geometries, i.e. domains periodic in all dimensions, spectral methods are the most commonly used [3]. However, for the recent DNS of wall-bounded flows, a larger variation of schemes is used. For example, in the present year, two channel flow DNSs at similar Reynolds numbers detailed DNSs were performed using both a finite-difference schemes (FDS) in the case of Ref. [4] or a more complex spectral methods in the case of Ref. [5]. FDS also present several advantages, they are very flexible, allowing for complex boundary conditions and/or structures interacting through the immersed boundary method with relative ease [6]. A commonly asserted disadvantage of low-order FDS is the higher truncation error relative to higher order schemes and spectral methods. However, this is only true in the asymptotic limit where the grid spacing $\Delta x \to 0$ that is commonly not reached. Additionally, aliasing errors are much smaller for lower order schemes [7,8]. Lower-order schemes have been shown to produce adequate first- and second-order statistics, but require higher resolution when compared to spectral methods for high order statistics [9–11]. Because lower-order schemes are computationally very cheap the grid resolution can in general be larger for the same computational cost compared to higher order schemes, although one has to consider the higher memory bandwidth over FLOPS ratio.

* Corresponding author. Tel.: +31 53 489 2470.
E-mail address: e.p.vanderpoel@immend.nl (E.P. van der Poel).

http://dx.doi.org/10.1016/j.compfluid.2015.04.007
0045-7930/© 2015 The Authors. Published by Elsevier Ltd.

In this manuscript, we will detail the parallelization of a second-order FDS based on Verzicco and Orlandi [12] to two wall bounded systems, Rayleigh–Bénard (RB) convection, the flow in a fluid layer between two parallel plates; one heated from below and cooled from above and Taylor–Couette (TC) flow, the flow between two coaxial independently rotating cylinders, although our code can easily extended to any flow that is wall-bounded in one dimension. This FDS scheme has already been used in pure Navier–Stokes simulations [12], with immersed boundary methods [13], for Rayleigh–Bénard convection [14–20] and for Taylor–Couette flow [21,22]. The numerical results have been validated against experimental data numerous times. We will exploit several advantages of the large Re regime and the boundary conditions to heavily reduce communication cost; opening the possibility to achieve much higher driving.

The manuscript is organized as follows: Section 2 describes TC and RB in more detail. Section 3 details the numerical scheme used to advance the equations in time. Section 4 shows that in thermal convection, the Courant–Friedrichs–Lewy (CFL) [23] stability constraints on the timestep due to the viscous terms become less strict than those due to the non-linear terms at high Rayleigh (Reynolds) numbers. Section 5 details a pencil decomposition to take advantage of the new time integration scheme and the choice of data arrangement in the pencil decomposition. Finally, Section 6 compares the computational cost of the existing and the new approach and presents an outlook of what further work can be done to combine this approach with other techniques.

2. Rayleigh–Bénard convection and Taylor–Couette flow

RB and TC are paradigmatic models for convective and shear flows, respectively. They are very popular systems because they are mathematically well defined, experimentally accessible and reproduce many of the interesting phenomena observed in applications. A volume rendering of the systems can be seen in Fig. 1. The Reynolds numbers in the common astro- and geo-physical applications are much higher than what can be reached currently in a laboratory. Therefore it is necessary to extrapolate available experimental results to the large driving present in stars and galaxies. This extrapolation becomes meaningless when transitions in scaling behaviour are present, and it is expected that once the Rayleigh number, i.e. the non-dimensional temperature difference, becomes large enough, the boundary layers transition to turbulence. This transition would most likely affect the scaling of interesting quantities. However, experiments disagree on exactly where this transition takes place [24,25]. DNS can be used to understand the discrepancies amongst experiments. However, to reach the high Rayleigh numbers (Ra) of experiments new strategies are required. DNS must resolve all scales in the flow, and the scale separation between the smallest scale and the largest scale grows with Reynolds number. This means larger grids are needed, and the amount of computational work W scales approximately as $W \sim Re^4$ [26].

Simulations of RB commonly imitate the cylindrical geometry most used in experiments. Recently, a DNS with aspect ratio $\Gamma = D/L = 1/3$, where D is the diameter of the plates and L the height of the cell reached $Ra = 10^{12}$ using 1.6 Billion points with a total cost of 2 Million CPU hours [27]. DNS in other geometries have been proposed, such as homogeneous RB, where the flow is fully periodic and a background temperature gradient is imposed. This geometry is easy to simulate [28], but presents exponentially growing solutions and does not have a boundary layer, thus not showing any transition [29]. Axially homogeneous RB, where the two plates of the cylinder are removed, and the sidewalls kept and a background temperature gradient is imposed to drive the flow has also been simulated [30]. This system does not have boundary layers on the plates and does not show the transition. Therefore, it seems necessary to keep both horizontal plates, having at least one wall-bounded direction. The simplest geometry is a parallelepiped box, periodic in both wall-parallel directions, which we will call "rectangular" RB for simplicity. Rectangular RB is receiving more attention recently [31–34], due to possibility to reach higher Ra as compared to more complex geometries. It is additionally the geometry that is closest to natural applications, where there are commonly no sidewalls.

For TC, we have one naturally periodic dimension, the azimuthal extent. The axial extent can be chosen to be either bounded by end-plates, like in experiments, or to be periodic. Axial end-plates have been shown to cause undesired transitions to turbulence if TC is in the linearly stable regime [35], or to not considerably affect the flow if TC is in the unstable regime [36]. Large Re DNS of TC focus on axially periodic TC, bounding the flow only in the radial direction [37,22]. Therefore, the choice of having a single wall-bounded direction for DNS of both TC and RB seems justified.

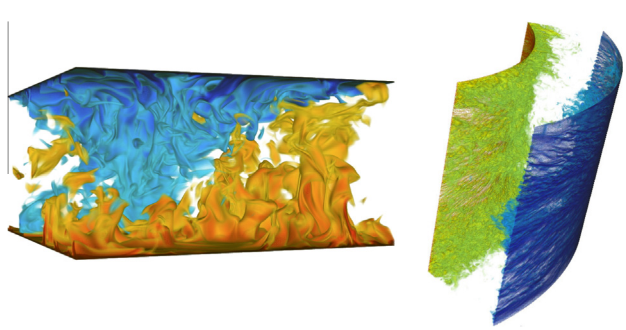

Fig. 1. Left: RB flow for $Ra = 10^8$, $Pr = 1$ and $\Gamma = 2$ in Cartesian coordinates. The horizontal directions are periodic and the plates are subjected to a no-slip and isothermal boundary condition. Red/yellow indicates hot fluid, while (light) blue indicates cold fluid. The small heat carrying structures known as thermal plumes as well as a large scale circulation can be seen in the visualization, highlighting the scale separation in the flow. Right: TC flow with an inner cylinder Reynolds number $Re = 10^5$, a stationary outer cylinder, and a radius ratio $\eta = r_i/r_o = 0.714$. Green fluid has a high angular velocity while blue fluid has a low angular velocity. The smallness of the structures responsible for torque transport, and thus the need for fine meshes, can be appreciated clearly. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

3. Numerical scheme

The code solves the Navier–Stokes equations with an additional equation for temperature in three-dimensional coordinates, either Cartesian or cylindrical. For brevity, we will focus on the RB Cartesian problem, although all concepts can be directly translated to TC in cylindrical coordinates system by substituting the vertical direction for the radial direction, and the two horizontal directions by the axial and azimuthal directions.

The non-dimensional Navier–Stokes equations with the Boussinesq approximation for RB read:

$$\nabla \cdot \mathbf{u} = 0, \tag{1}$$

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \sqrt{\frac{Pr}{Ra}} \nabla^2 \mathbf{u} + \theta \mathbf{e}_x, \tag{2}$$

$$\frac{\partial \theta}{\partial t} + \mathbf{u} \cdot \nabla \theta = \sqrt{\frac{1}{PrRa}} \nabla^2 \theta, \tag{3}$$

where $\mathbf{u}$ is the non-dimensional velocity, p the non-dimensional pressure, θ the non-dimensional temperature and t the non-dimensional time. For non-dimensionalization, the temperature scale is the temperature difference between both plates Δ, the length scale