

**A HIGH-ORDER NAVIER-STOKES SOLVER FOR VISCOUS TOROIDAL
FLOWS**

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Abstract

This thesis details our work in the development and testing of highly efficient solvers for the Navier-Stokes problem in simple toroidal coordinates in three spatial dimensions. In particular, the domain of interest in this work is the region occupied by a fluid between two concentric toroidal shells. The study of this problem was motivated in part by extensions of the study of Taylor-Couette instabilities between rotating cylindrical and spherical shells to toroidal geometries. We note that at higher Reynolds numbers, Taylor-Couette instabilities in cylindrical and spherical coordinates are essentially three dimensional in nature, which motivated us to design fully three-dimensional solvers with a OpenMP parallel numerical implementation suitable for a multi-processor workstation.

We approach this problem using two different time stepping procedures applied to the so-called Pressure Poisson formulation of the Navier-Stokes equations. In the first case, we develop an ADI-type method based on a finite difference formulation applicable for low Reynolds number flows. This solver was more of a pilot study of the problem formulated in simple toroidal coordinates. In the second case - the main focus of our thesis - our main goal was to develop a spectral solver using an explicit fourth order Runge-Kutta time stepping, which is appropriate to the higher Reynolds number flows associated with Taylor-Couette instabilities.

Our spectral solver was developed using a high order Fourier representation in the angular variables of the problem and a high order Chebyshev representation in the radial coordinate between the shells. The solver exhibits super-algebraic convergence in the number of unknowns retained in the problem. Applied to the Taylor-Couette problem, our solver has allowed

us to identify (for the first time, in this thesis) highly-resolved Taylor-Couette instabilities between toroidal shells. As we document in this work, these instabilities take on different configurations, depending on the Reynolds number of the flow and the gap width between shells, but as of now, all of these instabilities are essentially two dimensions. Our work on this subject continues, and we are confident that we will uncover three-dimensional instabilities that have well-known analogues in the cases of cylindrical and spherical shells.

Lastly, a separate physical problem we examine is the flow between oscillating toroidal shells. Again, our spectral solver is able to resolve these flows to spectral accuracy for various Reynolds numbers and gap widths, showing surprisingly rich physical behaviour. Our code also allows us to document the torque required for the oscillation of the shells, a key metric in engineering applications. This problem was investigated since this configuration was recently proposed as a mechanical damping system.

Dedication

jaya śrī rāma ||

From the perch of the shoulders of the giants who came before me, I prostrate to those that have laid the foundation for this work. My shoulders are ready to support those to come in the same way that was done for me.

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Chapter 1

Introduction

1.1 Motivation

Our motivation for this thesis is drawn from two main sources. The first source came to us from the engineering department at York University through the following question: ‘Can an oscillating or rotating fluid in a torus be used as a damping mechanism in spacecraft?’. Spacecraft, marine vessels and other mechanical vehicles require attitude stabilisation devices to maintain a particular orientation. For example, a spacecraft’s attitude can be disturbed by various natural forces such as the Earth’s gravity gradient, solar radiation pressure, aerodynamic forces, and the Earth’s magnetic field [1]. Fluid ring actuators can be used to dissipate these forces since they offer larger torques to the engineer than other shapes of equivalent mass. However, one of the challenges in the development of fluid ring actuators is the complexity of the fluid flow. This piqued our interest from a numerical methods point of view and we decided to pursue our curiosity.

The second source of motivation was that the rotating torus was reminiscent of a similar geometry that generates a remarkable, unexpected, exotic flow, now referred to as Taylor-Couette flow. This phenomenon was first observed and studied in rotating cylinders. Later, Taylor-Couette flow was observed and studied in rotating spheres but there is little literature

that mentions work done in rotating tori. Additionally, understanding flow in a torus may help us understand more complicated flow dynamics in curved pipes as compared to majority of studies that consider flow dynamics in straight pipes which are far easier to model.

Pursuing these ideas and our curiosity would not only uncover unexpected physical behaviour in the flow in a rotating torus but also make novel and interesting contributions to the ever-expanding field of fluid dynamics.

1.2 Taylor-Couette flow

Before we describe Taylor-Couette flow, we first recall key features of Couette flow. Couette flow is fundamental to and extensively studied in fluid mechanics. Its classic description emerges from the motion of a viscous fluid between two, infinitely long, parallel plates with one plate moving only along the surface of the fluid while the other plate remains stationary. The moving plate applies a shearing force to the fluid which results in a linear velocity profile between the plates. If the speed of the moving plate exceeds a particular threshold, then the flow becomes turbulent [2].

Taylor-Couette flow or Taylor-Couette instabilities refer to a series of stable flows that occur between classic Couette flow and turbulence for a sufficiently viscous fluid. The fluid transitions from Couette flow at low speeds to various forms of Taylor-Couette flow at higher speeds and eventually culminates in turbulence once the speed is high enough. Taylor-Couette flow has only been observed in geometries with curvature e.g. cylindrical and spherical geometries and has been studied theoretically and experimentally for over a century with its first modern appearance in physical apparatus documented in Taylor's innovative paper [3].

1.2.1 Cylindrical Taylor-Couette flow

Physical observation

The apparatus needed to physically observe Taylor-Couette flow comprises an incompressible, Newtonian fluid with non-zero viscosity [3] filled between two concentric cylinders. The most common arrangement used to generate Taylor-Couette flow is a stationary outer cylinder in combination with an inner cylinder that is gradually sped up to a constant angular velocity, ω .

For small ω , the flow is laminar (Couette flow). As ω increases, Couette flow transitions into three distinct Taylor-Couette flow patterns before transitioning into turbulence. These Taylor-Couette flows are named Taylor Vortex Flow (TVF), Wavy Vortex Flow (WVF) [4] and Modified Wavy Vortex Flow (MWVF) [5] [6] in order of increasing ω . As ω increases, Couette flow transitions to TVF which then transitions to WVF which then transitions to MWVF which finally transitions to turbulence. TVF, MWF and MWVF are all characterised by bands of toroidal vortices within the gap between the concentric cylinders. An example of a physical experiment demonstrating Taylor-Couette flow is provided by Burkhalter and Koschmieder [7] in Figure 1.1 and Figure 1.2

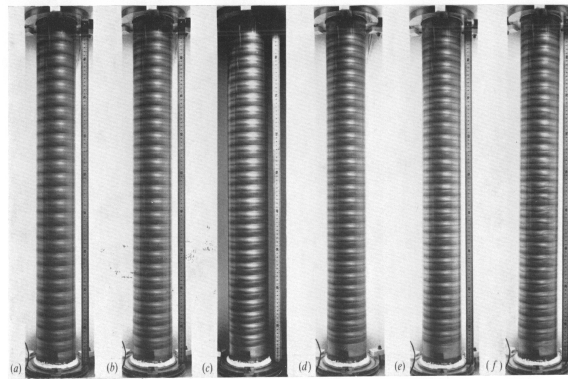


Figure 1.1: Source: J.E. Burkhalter and E.L. Koschmieder (1973)

Figure 1.1 illustrates the evolution of Taylor-Couette flow as the Reynolds number of the fluid is increased from left to right. The flow is seemingly partitioned into several bands of

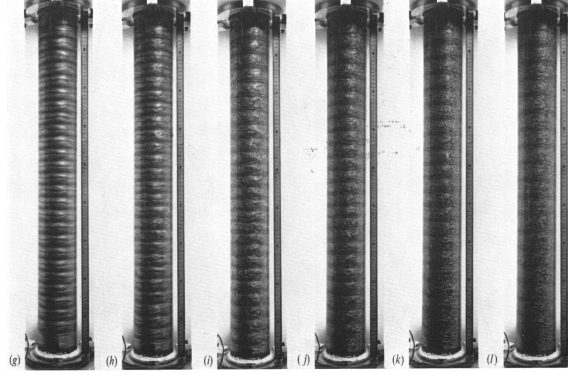


Figure 1.2: Source: J.E. Burkhalter and E.L. Koschmieder (1973)

two-dimensional flow along the height of the cylinder and has been termed as Taylor Vortex Flow. Figure 1.2 illustrates the development of wavy vortices as the Reynolds number is further increased resulting into a three-dimensional flow.

There are numerous other papers documenting physical experiments [8] [9] [10] [11] [12] [13] that illustrate the various stages of Taylor-Couette flow in rotating concentric cylinders while altering physical parameters such as viscosity, gap width and speed of rotation.

Centrifugal instabilities in inviscid flow offer physical insight into the cause of Taylor-Couette flow between two concentric rotating cylinders. In their survey paper on Taylor-Couette flow, Stuart [14] outlines an energy argument [15] introduced by von Kármán which concludes with the observation that centrifugal instabilities occur if the square of the circulation decreases outwards from the centre. In his ground-breaking paper, Taylor [3] established the Taylor number, Ta , as a means of demarcating when instability would develop. The Taylor number is a ratio of the centripetal acceleration to the viscosity of the fluid, $Ta = \frac{\omega^2 r_a d^3}{\nu^2}$. For the rotating concentric cylinders used in Taylor's experiment, the first threshold for instability is at $Ta = 1689$ i.e. when the centripetal acceleration dominates the viscous forces, Taylor-Couette flow develops.

Numerical simulations

Naturally, there have been attempts to replicate the many observed experimental results with numerical simulations. We recall the key ideas used in these numerical simulations [16] [17] [18] that helped shape our work with rotating concentric tori.

Marcus [19] represents the velocity with a combination of Chebyshev coefficients in the radial direction and Fourier coefficients in the angular direction. Another idea present in Marcus' work [20] is to take advantage of symmetry to reduce the computational burden. Another important consideration is how to handle the time-stepping of the Navier-Stokes equations and what terms in the Navier-Stokes equations should be taken at the explicit and implicit time level. These details will be discussed in further detail in subsequent chapters.

1.2.2 Spherical Taylor-Couette flow

Physical observation

Spherical Taylor-Couette flow is less explored and documented than its cylindrical counterpart but there are recorded instances of physical observation of this phenomenon [21]. As in the case of concentric cylinders previously described, we have concentric spheres set up such that the outer sphere is held stationary and the inner sphere is sped up to generate the various characteristic features of Taylor-Couette flow.

Nakabayashi's experiments [22] reported fourteen distinct flow patterns for a particular gap width which were then assigned to four broad categories described below

- laminar flow (basic or intuitive flow)
- laminar toroidal or spiral flow
- wavy or oscillating flow (also called a transition flow)
- turbulence

We note that the Taylor-Couette flows in rotating concentric cylinders and rotating concentric

spheres were mostly generated in thin gaps though there is some work that explores wider gaps [23]. This serves as a starting point for our exploration in rotating concentric tori.

Most recently, Mahloul [24] also experimentally illustrated spherical Taylor-Couette flow and noted that Taylor vortices appeared along the equator and near the poles for rotating concentric spheres with $Ta = 1768$. The Taylor number is larger than the case of the cylinder because of the curvature of the geometry.

Numerical simulations

The first instability of spherical Taylor-Couette flow has also been numerically calculated by Schrauf [25] and appears to be laminar toroidal flow. Many of the techniques and ‘tricks’ used in the development of numerical simulations for the rotating concentric cylinders are used in the development of numerical simulations for the rotating concentric spheres [26] [27] [28] [29] with minor adjustments to account for the geometry. For example, the velocity in the spherical case can be represented entirely spectrally by using Fourier coefficients for the two angular directions in spherical co-ordinates and Chebyshev coefficients for the radial direction.

Similar behaviour is expected and has been observed numerically [30] in the flow between two concentric tori.

1.2.3 Toroidal geometries

Fluid flow in toroidal geometries has also been previously considered. In particular, for our exact geometry of concentric tori and boundary conditions of the inner torus rotating at constant speed while the outer torus is kept stationary, analytic stable steady-state solutions have been found [31]. However, the analytic solutions found give no explicit indication of a bifurcation or the appearance of Taylor-Couette instabilities.

There are instances where the flow inside a single torus was studied both experimentally [32] and numerically. In the case where the torus is spun up to a set speed, a sequence of

bifurcations appear as the Reynolds number is increased which is somewhat analogous to Taylor-Couette flow in other geometries [33]. Additionally, the amount of curvature in the torus appears to influence the critical Reynolds number for which the flow transitions or bifurcates [34]. Finally, there is an instance where the effect of slowing down the fluid inside the torus on the flow near the boundary [35] was examined.

1.3 Navier-Stokes equations

A theoretical exploration of any kind of fluid flow begins with the famous Navier-Stokes equations. They are likely most famous from their appearance in a Millenium Prize problem for which there is a million dollar reward offered by the Clay Mathematics Institute [36]. Currently, there is no mathematical proof that solutions to the Navier-Stokes equations in $\mathbb{R}^3$ both exist and are smooth for any given initial condition (with bounded energy). However, the absence of a rigorous mathematical proof does not deter the effort to find numerical approximations of solutions to the Navier-Stokes equations.

At this point, we impose restrictions on the fluid we want to study to appropriately shape and simplify the Navier-Stokes equations. For a viscous, incompressible, Newtonian fluid with constant density, ρ , and without body forces, the Navier-Stokes equations manifest as

$$\begin{cases} \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\frac{1}{\rho} \nabla p + \nu \nabla^2 \mathbf{u} \\ \nabla \cdot \mathbf{u} = 0 \end{cases} \quad (1.1)$$

where $\mathbf{u}$ is the fluid velocity, p is the fluid pressure and ν is the kinematic viscosity [37].

The Navier-Stokes equations, (1.1), are valid in both $\mathbb{R}^2$ and $\mathbb{R}^3$ and on any open and connected subset, Ω , of these spaces for $t > 0$. The representation of the Navier-Stokes equations in (1.1) is referred to as the classical primitive variables formulation. Physically,

equation (1.1) represents the principle of conservation of momentum and the conservation of mass respectively for a fluid. Equation (1.1) relates a fluid's pressure, p , to its velocity, $\mathbf{u}$ and asserts that a fluid's rate of change of velocity, $\mathbf{u}$, i.e. its acceleration (on the left-hand side) is equivalent to the sum of the forces (one of which is the pressure gradient, ∇p) acting on its particles (on the right-hand side).

1.4 Problem definition

We can now make a precise problem definition for the thesis. We are interested in developing computationally efficient numerical solvers for the Navier-Stokes equations, (1.1), in toroidal co-ordinates to numerically approximate a flow that is impulsively started and has given initial and boundary conditions. Given specific boundary conditions, we anticipate the development and thorough documentation of various forms of Taylor-Couette flow between two concentric tori similar to that found in the flow between rotating concentric cylinders and rotating concentric spheres.

1.4.1 Geometry

The toroidal co-ordinate system or ‘simple’ toroidal coordinates [38] is described by

$$\begin{aligned} x(r, \theta, \phi) &= (R_0 + r \cos \theta) \cos \phi \\ y(r, \theta, \phi) &= (R_0 + r \cos \theta) \sin \phi \\ z(r, \theta, \phi) &= r \sin \theta \end{aligned} \tag{1.2}$$

where r is the polar radius, θ is the polar angle, R_0 is the toroidal radius, ϕ is the toroidal angle, x , y and z are from the usual Cartesian co-ordinate system. For the case of concentric tori, we define r_a and r_b as the inner and outer polar radii respectively. The coordinate ranges are $-\pi < \theta \leq \pi$, $0 \leq r < R_0$ and $0 \leq \phi < 2\pi$.

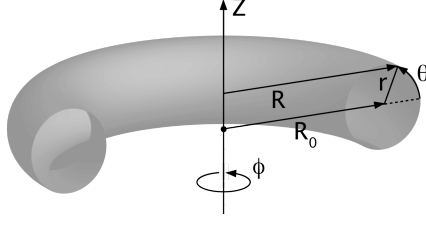


Figure 1.3: Simple toroidal coordinates

1.4.2 Initial, boundary and compatibility conditions

To specify a particular solution to the Navier-Stokes equations, we need initial conditions and boundary conditions. Also, in the case of an impulsively started flow, we must ensure that certain compatibility conditions are upheld (not to be confused with the compatibility conditions needed to ensure that the Poisson equation with Neumann boundary conditions is well-defined).

The initial conditions are simple and shown in (1.3) below for $t = 0$.

$$\mathbf{u}(\mathbf{r}, t = 0) = \mathbf{u}_0(\mathbf{r}), \quad \mathbf{r} \in \Omega \oplus \partial\Omega \quad (1.3)$$

where $\mathbf{u}_0$ is the specified initial velocity, $\mathbf{r}$ represents the generic spatial vector in toroidal co-ordinates, Ω is an open, simply connected and bounded subset of $\mathbb{R}^3$ and $\partial\Omega$ is its boundary.

The boundary conditions are specified by a velocity, $\mathbf{u}_{\partial\Omega}$, on the boundary, $\partial\Omega$, of the domain, Ω , for all $t > 0$ in equation (1.4). Additionally, we assume the boundary is a sufficiently smooth and closed surface.

$$\mathbf{u}(\mathbf{r}, t) = \mathbf{u}_{\partial\Omega}(\mathbf{r}, t), \quad \mathbf{r} \in \partial\Omega, \quad t > 0 \quad (1.4)$$

We now consider the more interesting compatibility conditions that must be satisfied if we want a well-defined problem. The compatibility conditions are motivated by common physical observations in flows. The mathematical statements of the compatibility conditions [39] [40]

[41] are given in (1.5), (1.6) and (1.7) below.

$$\oint_{\partial\Omega} \hat{\mathbf{n}} \cdot \mathbf{u}_{\partial\Omega} dA = 0, \quad t > 0 \quad (1.5)$$

$$\hat{\mathbf{n}} \cdot \mathbf{u}_{\partial\Omega}(\mathbf{r}, 0) = \hat{\mathbf{n}} \cdot \mathbf{u}_0, \quad \mathbf{r} \in \partial\Omega \quad (1.6)$$

$$\nabla \cdot \mathbf{u}_0 = 0, \quad \mathbf{r} \in \Omega \quad (1.7)$$

Equation (1.5) is common and is a mathematical statement of the physical observation that no net flow occurs through the boundary, $\partial\Omega$, for $t > 0$ where $\hat{\mathbf{n}}$ represents the unit normal to $\partial\Omega$. This is commonly referred to as a no-slip boundary condition.

Equation (1.6) is motivated by the physical observation that there must be sufficient continuity between the initial velocity, $\mathbf{u}_0$, and the velocity on the boundary, $\mathbf{u}_{\partial\Omega}$, at $t = 0$. Recall from equation (1.4) that $\mathbf{u}_{\partial\Omega}$ is only defined for $t > 0$ and not at $t = 0$. This is an important and distinguishing condition of impulsively started flows. The mathematical statement in (1.6) asserts that *only* the normal component of the velocity on the boundary, $\mathbf{u}_{\partial\Omega}$ at $t = 0$, must be equal to the normal component of the initial velocity, $\mathbf{u}_0$, on the boundary. In other words, tangential discontinuities do not affect the well-posedness of the equations [40] [42]. This idea has a physical manifestation in the classic Couette flow derived from the impulsively started movement of one of the infinitely long parallel plates. This Couette flow is physically valid despite the tangential discontinuity at the moving plate. However, discontinuities that occur in the normal component of either velocity give rise to an ill-posed problem and requires special treatment so that (1.6) is satisfied. Fortunately, we consider only tangential discontinuities in this thesis.

Finally, (1.7) ensures that the initial velocity, $\mathbf{u}_0$, is divergence-free in the same way the velocity, $\mathbf{u}$, is divergence-free for $t > 0$. Physically, this ensures that mass is conserved also at

$t = 0$. While this is physically obvious, (1.7) is of paramount importance in the theoretical and numerical development of solvers for (1.1) and for its pressure Poisson formulations in particular.

1.4.3 Non-dimensional Navier-Stokes equations

With the initial, boundary and compatibility conditions for (1.1) now clarified, we proceed to non-dimensionalisation to derive the final form of the Navier-Stokes equations needed for the development of its numerical solvers. We define the non-dimensional variables in (1.8) below and distinguish the non-dimensional variables from their dimensional counterparts with hats.

$$\hat{u} = \frac{u}{U}, \quad \hat{v} = \frac{v}{U}, \quad \hat{w} = \frac{w}{U}, \quad \hat{r} = \frac{r}{L}, \quad \hat{t} = \frac{U}{L}t, \quad \hat{p} = \frac{p}{\rho U^2} \quad (1.8)$$

The characteristic velocity, U , is identical for all three velocity components and is defined by $U = \omega R_0$ where ω is the angular velocity of the torus and R_0 is the toroidal radius. The characteristic length, L , is the toroidal radius, R_0 , and implies that $\hat{t} = \omega t$.

We note that alternative choices for the scaling of pressure and length are possible. The expectation of the development of dynamic Taylor-Couette flow [3] justifies our choice for the pressure scale. The alternative pressure scale is more suitable for flows dominated by viscosity and not for dynamic flows. A common choice for the characteristic length in both the rotating concentric cylindrical and rotating concentric spherical cases is the gap width between the cylinders or spheres. We reject this choice for the concentric rotating tori because the toroidal radius, R_0 , is a more natural choice given the geometry. In other words, the expected speed within the toroidal gap is closer to ωR_0 than it is to $\omega \times \text{gap width}$ because of the position of the axis of rotation.

The non-dimensional form of (1.1) is given in (1.9) with the hats omitted for simplicity of presentation.

$$\begin{cases} \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\nabla p + \frac{1}{Re} \nabla^2 \mathbf{u} \\ \nabla \cdot \mathbf{u} = 0 \end{cases} \quad (1.9)$$

where Re is the Reynolds number and is defined by $Re = \frac{UL}{\nu} = \frac{\rho UL}{\mu}$ where $\mu = \nu\rho$ is the dynamic viscosity. With the parameters chosen $Re = \frac{\rho\omega R_0^2}{\mu}$ and it is important to recall this when we consider the results.

Finally, we note that the initial, boundary and compatibility conditions for (1.1) need to be similarly non-dimensionalised. Conveniently, their non-dimensional form is identical to their dimensional form except for (1.7). Equation (1.7) is defined by the divergence for which its non-dimensional form is shown in (1.10) with hats omitted purely for simplicity.

$$\nabla \cdot \mathbf{u} = \frac{\partial u}{\partial r} + \frac{u}{r} + \frac{1}{r} \frac{\partial v}{\partial \theta} + \frac{1}{h_\phi} \left(u \cos \theta - v \sin \theta + \frac{\partial w}{\partial \phi} \right) \quad (1.10)$$

The only difference between (1.7) and (1.10) lies in the h_ϕ term. In the dimensional divergence, $h_\phi = R_0 + r \cos \theta$ while in the non-dimensional divergence, $h_\phi = 1 + r \cos \theta$ instead.

We only consider the non-dimensional form of the Navier-Stokes equations, (1.9), and its initial, boundary and compatibility conditions from this point on. Analytic solutions for (1.9) are notoriously difficult to find so we resort to numerical approximations of the analytic solution instead.

1.5 Thesis structure

We present an outline of the thesis in this section to guide the reader. In Chapter 2, we consider a literature review of two classes of methods used to numerically solve the Navier-Stokes equations: projection methods and pressure Poisson formulations. In Chapters 3 and 4 we present details of the numerical solvers implemented to solve the Poisson equation in both

two and three dimensions. Chapter 5 contains details of the numerical solvers implemented to solve the momentum equations from the Navier-Stokes equations. We present our results from our numerical solvers for two main cases in Chapters 6 and 7. We considered a rotating inner torus with stationary outer torus and both tori oscillating with the same period. Finally, in Chapter 8, we conclude with a summary of our results and their interpretation.

Chapter 2

Literature review

There are numerous ideas regarding numerical solutions of (1.9) in modern literature, an overview of which is presented by Rempfer [43]. We explore two of the more popular and effective classes of numerical methods used to solve some part of the Navier-Stokes equations, (1.9): projection methods and pressure Poisson formulations. These methods were chosen not only for their popularity but also for their application to flow between two concentric rotating tori with an impulsive start. We initially explore projection methods but eventually settle on a particular Poisson formulation for our numerical implementation.

2.1 Projection methods

2.1.1 Overview

Projection methods or fractional step methods [43] constitute a category of numerical solvers dedicated to finding solutions to the entire Navier-Stokes equations. They were pioneered primarily through the independent work of Chorin [44] [45] and Temam [46].

Projection methods became extremely popular in the late 1960s because they circumvented a common issue encountered by the best Navier-Stokes solvers. They decoupled the velocity and

pressure and allowed each quantity to be numerically solved independent of each other [47]. Other popular solvers at the time, such as the famous marker-and-cell method introduced by Harlow and Welch [48], solved a coupled system for the velocity and pressure instead. Solvers for the coupled system are still less computationally efficient than solvers for pressure and velocity independently today.

The main underlying idea on which projection methods are based is illustrated by the famous Hodge decomposition theorem [49].

Theorem 1 (Hodge decomposition). *Every vector-valued function, $v \in L^2(\Omega)$, $\Omega \subset \mathbb{R}^d$, $d = 2, 3$ can be decomposed as*

$$v = \nabla q + \nabla \times \gamma$$

where q and γ are smooth enough in the sense of distributions.

Another interpretation of the Hodge decomposition theorem is that every vector-valued function can be expressed as the sum of a divergence-free part and a curl-free part. This allows us to express the momentum equation from (1.9) as [42]

$$\frac{\partial \mathbf{u}}{\partial t} = Proj[G(\mathbf{u})]$$

where $G(\mathbf{u})$ represents the sum of the advective and diffusive terms and $Proj$ represents the Leray projection [50] onto the space of divergence-free vector fields. In other words, the pressure term is eliminated from the momentum equations and has been replaced with a projection operator instead leaving an equation with only velocity terms. The mathematical details become more complicated from this point and we are mostly interested in the numerical methods that emerge from this mathematical theory. So, we skip ahead to the two main steps of numerical implementations for projection methods listed below.

1. Solve for an auxiliary velocity, $\mathbf{u}^*$, using the momentum equation without the pressure term. This step is also referred to as the prediction step [51] [52] since the auxiliary

velocity, $\mathbf{u}^*$, can be considered a prediction of the velocity at the next time step. Note that the auxiliary velocity, $\mathbf{u}^*$, is not a meaningful physical quantity and is not necessarily divergence-free.

2. Project the auxiliary velocity, $\mathbf{u}^*$, on to the space of divergence-free vector fields to obtain an updated value for the velocity. This projection involves the solution of a Poisson equation. This step is referred to as the correction step since the abstract quantity, $\mathbf{u}^*$, is corrected to a physically meaningful velocity at the next time step that is divergence-free.

2.1.2 First-order methods

The projection methods discussed in this sub-section are called first order because the numerical error is at least $\mathcal{O}(\Delta t)$. On one hand, this forces a large number of time steps to be used to resolve high-accuracy flows. On the other hand, the spatial approximations need not be any more accurate than $\mathcal{O}(\Delta t)$ and this leads to simpler numerical representations and possibly even innovative methods to deal with the notoriously difficult non-linear advection term. The equations used for the prediction and correction stages of the most basic first-order projection method [53] [54] are shown in (2.1) and (2.2) below.

$$\begin{cases} \frac{\mathbf{u}^* - \mathbf{u}^n}{\Delta t} + (\mathbf{u}^n \cdot \nabla) \mathbf{u}^n = \frac{1}{Re} \nabla^2 \mathbf{u}^n \\ \mathbf{u}^* = \mathbf{u}_{\partial\Omega} \quad \text{on} \quad \partial\Omega \end{cases} \quad \textbf{Prediction} \quad (2.1)$$

$$\begin{cases} \frac{\mathbf{u}^* - \mathbf{u}^{n+1}}{\Delta t} = \nabla p^{n+1} \\ \nabla \cdot \mathbf{u}^{n+1} = 0 \\ \mathbf{u}^{n+1} \cdot \hat{\mathbf{n}} = \mathbf{u}_{\partial\Omega}^{n+1} \cdot \hat{\mathbf{n}} \quad \text{on} \quad \partial\Omega \end{cases} \quad \textbf{Correction} \quad (2.2)$$

where $\mathbf{u}^{n+1}$ is the velocity at the next time step, $\mathbf{u}^n$ is the velocity at the current time step and $\mathbf{u}^*$ is the auxiliary or intermediate (non-physical) velocity.

There are a number of comments to be made about the numerical scheme shown in (2.1) and (2.2) before we continue. The most critical issue is the establishment of appropriate boundary conditions for both the prediction and correction stages.

In the prediction stage, the boundary condition for $\mathbf{u}^*$ is quoted [53] as a natural choice for a first order scheme given the boundary condition on $\mathbf{u}$ for (1.9). This is not obvious and is only appropriate if $\mathbf{u}^*$ is close enough to the physical velocity, $\mathbf{u}^*$. In other words, this boundary condition is only appropriate if the time interval is small enough.

The boundary condition for the correction stage is a feature of the projection operator acting on the auxiliary velocity, $\mathbf{u}^*$ [42], and forces the normal component of the prescribed boundary velocity to be equal to the numerically calculated velocity at the next time step, $\mathbf{u}^{n+1}$.

In the correction stage, the auxiliary velocity, $\mathbf{u}^*$, is used to find $\mathbf{u}^{n+1}$. Also, the correction stage makes it obvious that there is an error of $\mathcal{O}(\Delta t)$ associated with this projection method because of the backward difference approximation of the time derivative. This error persists unless $\mathbf{u}^*$ is equal to $\mathbf{u}^{n+1}$ which is not the case in general.

A fully explicit scheme is presented for the prediction stage though this is not mandatory. Fully implicit schemes are notoriously difficult when the non-linear advection term is involved and are generally avoided. A common compromise is to treat the diffusive terms implicitly and to treat the advective terms either explicitly or semi-implicitly [55].

The current form of the correction stage is not yet suitable for a numerical solver. Taking the divergence of the first equation in (2.2), we derive a Poisson equation with Neumann boundary conditions that updates the pressure. Consequently, the correction stage splits into two steps: the pressure update step and the velocity update step. We now have a more computationally meaningful presentation of this projection method in (2.3), (2.4) and (2.5) below [44] [55] [56].

$$\begin{cases} \frac{\mathbf{u}^* - \mathbf{u}^n}{\Delta t} + (\mathbf{u}^n \cdot \nabla) \mathbf{u}^n = \frac{1}{Re} \nabla^2 \mathbf{u}^* \\ \mathbf{u}^* = \mathbf{u}_{\partial\Omega} \quad \text{on} \quad \partial\Omega \end{cases} \quad \text{Auxiliary velocity step} \quad (2.3)$$

$$\begin{cases} \nabla^2 p^{n+1} = \frac{1}{\Delta t} \nabla \cdot \mathbf{u}^* \\ \frac{\partial p^{n+1}}{\partial \mathbf{n}} = 0 \quad \text{on} \quad \partial\Omega \end{cases} \quad \text{Pressure update step} \quad (2.4)$$

$$\mathbf{u}^{n+1} = \mathbf{u}^* - \Delta t \nabla p^{n+1} \quad \text{Velocity update step} \quad (2.5)$$

The most pressing issue now is that there are no boundary conditions explicitly specified for the pressure, p , and they must be deduced instead. Taking the unit normal component of the equations in (2.2), we have the following equation.

$$\frac{\hat{\mathbf{n}} \cdot \mathbf{u}^* - \hat{\mathbf{n}} \cdot \mathbf{u}^{n+1}}{\Delta t} = \hat{\mathbf{n}} \cdot \nabla p^{n+1}$$

We know that $\mathbf{u}^{n+1} \cdot \hat{\mathbf{n}} = \mathbf{u}_{\partial\Omega}^{n+1} \cdot \hat{\mathbf{n}}$ from the correction stage boundary condition and $\mathbf{u}^* = \mathbf{u}_{\partial\Omega}^{n+1}$ from the prediction stage boundary condition resulting in the following boundary condition.

$$\hat{\mathbf{n}} \cdot \nabla p^{n+1} = 0$$

Finally, we need to check that the compatibility condition associated with Poisson equations with Neumann boundary conditions are satisfied for this boundary condition. Gauss' theorem gives us

$$\begin{aligned} 0 &= \int_{\Omega} \frac{1}{\Delta t} \nabla \cdot \mathbf{u}^* dV = \int_{\Omega} \nabla^2 p^{n+1} dV = \int_{\Omega} \nabla \cdot \nabla p^{n+1} dV \\ &= \int_{\partial\Omega} \nabla p^{n+1} \cdot \hat{\mathbf{n}} dS = \int_{\partial\Omega} \frac{\partial p^{n+1}}{\partial n} dS = \int_{\partial\Omega} 0 dS = 0 \end{aligned}$$

However, there are certain numerical issues that must be addressed in the above formulation for the pressure. The first issue is that the error of the numerically calculated pressure is $\mathcal{O}(\Delta t)$. More precisely, Shen [54] [57] proves that the error of the pressure is actually $\mathcal{O}(\Delta t^{\frac{1}{2}})$.

There are several simple ways to deduce that the error on the pressure is at least $\mathcal{O}(\Delta t)$. One way is to closely examine the compatibility condition associated with the Poisson equation that solves for pressure. While we have written a series of equal signs in the proof of compatibility, this is not perfectly precise. In fact, the proof of compatibility holds true *only* if the auxiliary velocity, $\mathbf{u}^*$, is incompressible. However, by its own construction, the projection method states that the auxiliary velocity, $\mathbf{u}^*$, is not necessarily divergence-free; in fact, $\mathbf{u}^*$ is often not divergence-free.

The error of the pressure is also revealed if (2.1) and (2.2) are combined to eliminate the auxiliary velocity, $\mathbf{u}^*$.

$$\frac{\mathbf{u}^{n+1} - \mathbf{u}^n}{\Delta t} + (\mathbf{u}^n \cdot \nabla) \mathbf{u}^n = -\nabla \Psi^{n+1} + \frac{1}{Re} \nabla^2 \mathbf{u}^{n+1} \quad (2.6)$$

where $\Psi^{n+1} = p^{n+1} - \frac{\Delta t}{Re} \nabla^2 p^{n+1}$. The quantity, Ψ^{n+1} , is referred to as a pseudo-pressure and for first order methods, $\Psi^{n+1} \approx p^{n+1}$ to $\mathcal{O}\left(\frac{\Delta t}{Re}\right)$. However, the derivation of the pseudo-pressure, Ψ^{n+1} , is also instrumental in removing or reducing these numerical errors [58].

Not only is there an error of $\mathcal{O}(\Delta t)$ in the pressure, there is also a numerical boundary layer that develops during the calculation of the pressure [59]. The numerical boundary layer is a consequence of the artificial Neumann condition imposed on the pressure and can be deduced [53] by observing

$$\frac{\partial p^{n+1}}{\partial \hat{\mathbf{n}}} = \frac{\partial p^n}{\partial \hat{\mathbf{n}}} = \dots = \frac{\partial p^0}{\partial \hat{\mathbf{n}}} \quad \text{on} \quad \partial \Omega$$

In general, these boundary conditions are not true for the pressure that satisfies the Navier-

Stokes equations. Therefore, the error of $\frac{\partial p^n}{\partial \mathbf{n}}$ on the boundary is $\mathcal{O}(1)$ and gives rise to numerical boundary layers.

Alternatively, it can be viewed as a consequence of advancing the velocity and pressure sequentially in time as opposed to advancing them simultaneously. In other words, the boundary condition for p was derived only after the prediction stage of the projection method [42]. Therefore, the given boundary condition is not exactly applicable to the true pressure, p ; instead it is applicable to the pseudo-pressure, Ψ .

Though somewhat imprecise, we can still use this numerical approximation for the pressure since the numerical approximation for the velocity is no worse than $\mathcal{O}(\Delta t)$ and the larger errors are confined to the boundary. Also, the flow near the boundary may not be as important as flow in the interior of the domain depending on the physical application.

In conclusion, Chorin's first-order scheme can never be better than $\mathcal{O}(\Delta t)$ [54] and is prone to numerical boundary layers. In spite of these limitations, projection methods are still worth pursuing because of their relatively easy computational implementation. As a broad overview of Chorin's scheme, first, $\mathbf{u}^*$ is calculated using $\mathbf{u}^n$, then p is calculated using $\mathbf{u}^*$ and, finally, $\mathbf{u}^{n+1}$ is calculated using both $\mathbf{u}^*$ and p . This is repeated for as many time steps as deemed sufficient or necessary to obtain a suitable numerical solution for both $\mathbf{u}$ and p .

2.1.3 Second-order methods

Improvements to the accuracy of the first-order projection method are attempted by addressing one or more of its weaknesses mentioned in the previous sub-section. Therefore, second-order methods can be classified as follows [53] [60]:

1. those that specify more precise boundary conditions for the auxiliary velocity, $\mathbf{u}^*$
2. those that specify more precise boundary conditions for the pressure, p [61]
3. those that use a pressure increment formulation

We first clarify what is meant by a second-order method. Some literature claims a particular

projection method is second order if only either the velocity or the pressure is accurate to $\mathcal{O}(\Delta t^2)$. This is done to differentiate these methods from Chorin's scheme in which the pressure, velocity and time derivative are all $\mathcal{O}(\Delta t)$. For a projection method to be fully second-order accurate, the approximations to velocity and pressure must be second-order in time. A necessary condition is that the time stepping method be second order consistent, such as in the backwards difference formula [54] shown below

$$\frac{\partial \mathbf{u}}{\partial t} \approx \frac{1}{2\Delta t} (3\mathbf{u}^* - 4\mathbf{u}^n + \mathbf{u}^{n-1})$$

In the presentation of the subsequent second-order schemes, we will keep the time derivative approximation first order for simplicity of presentation. This simplification of the time derivative does not fundamentally change the ideas employed in the development of these second-order schemes. The second-order backward difference approximation of the time derivative means that an additional initial condition is required at the beginning of the numerical scheme. An easy resolution to this issue is to use the solution generated after one (perhaps very small) time step from a projection method that used a first order backward difference approximation for the time derivative as the 'missing' initial condition, $\mathbf{u}^{n-1}$.

Pressure increment formulation

The easiest adjustment to make to Chorin's first-order scheme is to include a pressure increment in the calculation of the auxiliary velocity, $\mathbf{u}^*$. The most famous projection method that employs this idea was proposed by Van Kan [55] [62] [49]. The simplest implementation [54] of a pressure increment formulation is shown in (2.7), (2.8) and (2.9) below.

$$\begin{cases} \frac{\mathbf{u}^* - \mathbf{u}^n}{\Delta t} + (\mathbf{u}^n \cdot \nabla) \mathbf{u}^n + \nabla p^n = \frac{1}{Re} \nabla^2 \mathbf{u}^* \\ \mathbf{u}^* = \mathbf{u}_{\partial\Omega} \quad \text{on} \quad \partial\Omega \end{cases} \quad \text{Auxiliary velocity step} \quad (2.7)$$

$$\begin{cases} \nabla^2 p^{n+1} = \frac{1}{\Delta t} \nabla \cdot \mathbf{u}^* \\ \frac{\partial p^{n+1}}{\partial \mathbf{n}} = 0 \quad \text{on} \quad \partial\Omega \end{cases} \quad \text{Pressure update step} \quad (2.8)$$

$$\mathbf{u}^{n+1} = \mathbf{u}^* - \Delta t \nabla p^{n+1} \quad \text{Velocity update step} \quad (2.9)$$

The inclusion of ∇p^n in (2.7) increases the accuracy [63] of this projection method because the velocity approximation is now $\mathcal{O}(\Delta t)^2$ but the pressure approximation is $\mathcal{O}(\Delta t)$ (the pressure Poisson equation is identical to the one found in the first-order scheme) [54]. However, the numerical boundary layer from the pressure calculations persist. Also, ∇p^n implies that this projection method needs an initial pressure which is not difficult to obtain.

Accurate boundary conditions for pressure

We noted earlier that the boundary condition $\frac{\partial p^{n+1}}{\partial \hat{\mathbf{n}}} = 0$ leads to numerical boundary layers. Recall that this boundary condition was derived by taking the normal component of equation (2.2) and simplified using the idea of zero net flux across the boundary.

Instead, a more consistent boundary condition can be derived by taking the normal component of the momentum equations in (1.9) on the boundary to derive the following equation

$$\frac{\partial p}{\partial \hat{\mathbf{n}}} = \frac{1}{Re} \hat{\mathbf{n}} \cdot \nabla^2 \mathbf{u}$$

In discretised form, the boundary condition can be written as

$$\frac{\partial p^{n+1}}{\partial \mathbf{n}} = \frac{1}{Re} \hat{\mathbf{n}} \cdot \nabla^2 \mathbf{u}^* \quad \text{or} \quad \frac{\partial p^{n+1}}{\partial \hat{\mathbf{n}}} = \frac{1}{Re} \mathbf{n} \cdot \nabla^2 \mathbf{u}^n$$

depending on what terms are taken as implicit or explicit in the chosen numerical scheme.

Using the following vector calculus identity, $\nabla^2 \mathbf{u} = \nabla(\nabla \cdot \mathbf{u}) - \nabla \times (\nabla \times \mathbf{u})$, we can re-write the pressure boundary condition because $0 = \nabla \cdot \mathbf{u}^n \approx \nabla \cdot \mathbf{u}^*$ due to incompressibility as

$$\frac{\partial p}{\partial \hat{\mathbf{n}}} = \frac{1}{Re} \hat{\mathbf{n}} \cdot (-\nabla \times (\nabla \times \mathbf{u}))$$

Therefore, we have a consistent projection method with the aforementioned consistent boundary condition for the pressure.

$$\begin{cases} \frac{\mathbf{u}^* - \mathbf{u}^n}{\Delta t} + (\mathbf{u}^n \cdot \nabla) \mathbf{u}^n + \nabla p^n = \frac{1}{Re} \nabla^2 \mathbf{u}^* \\ \mathbf{u}^* = \mathbf{u}^* \quad \text{on} \quad \partial\Omega \end{cases} \quad \text{Auxiliary velocity step} \quad (2.10)$$

$$\begin{cases} \nabla^2 p^{n+1} = \frac{1}{\Delta t} \nabla \cdot \mathbf{u}^* \\ \frac{\partial p^{n+1}}{\partial \hat{\mathbf{n}}} = \frac{1}{Re} \hat{\mathbf{n}} \cdot (-\nabla \times (\nabla \times \mathbf{u})) \quad \text{on} \quad \partial\Omega \end{cases} \quad \text{Pressure update step} \quad (2.11)$$

$$\mathbf{u}^{n+1} = \mathbf{u}^* - \Delta t \nabla p^{n+1} \quad \text{Velocity update step} \quad (2.12)$$

While this boundary condition is more consistent and removes the numerical boundary layers, it is more difficult and more computationally expensive to implement. This consistent boundary condition is critical to our work because it is explicitly linked to the pressure Poisson reformulations for the Navier-Stokes equations discussed in the next section.

Accurate boundary conditions for the auxiliary velocity

The final shortcoming of Chorin's first-order projection method is the boundary condition used for the auxiliary velocity, $\mathbf{u}^*$. An example of a projection method that addresses this issue is as follows.

$$\begin{cases} \frac{\mathbf{u}^* - \mathbf{u}^n}{\Delta t} + (\mathbf{u}^n \cdot \nabla) \mathbf{u}^n + \nabla p^n = \frac{1}{Re} \nabla^2 \mathbf{u}^* \\ \mathbf{u}^* = \mathbf{u}^* - \Delta t \nabla p^n \quad \text{on } \partial\Omega \end{cases} \quad \text{Auxiliary velocity step} \quad (2.13)$$

$$\begin{cases} \nabla^2 p^{n+1} = \frac{1}{\Delta t} \nabla \cdot \mathbf{u}^* \\ \frac{\partial p^{n+1}}{\partial \mathbf{n}} = 0 \quad \text{on } \partial\Omega \end{cases} \quad \text{Pressure update step} \quad (2.14)$$

$$\mathbf{u}^{n+1} = \mathbf{u}^* - \Delta t \nabla p^{n+1} \quad \text{Velocity update step} \quad (2.15)$$

This method draws inspiration from Kim and Moin [64] who introduced arguably the most famous second-order projection method. Shen [54] quotes the accuracy of the velocity as $\mathcal{O}(\Delta t)^2$ and of the pressure as $\mathcal{O}(\Delta t)^{\frac{3}{2}}$ for the method of Kim and Moin. Additionally, in particular geometries, viz. those with periodicity in at least one dimension [65], Kim and Moin's method becomes second-order accurate in both the velocity and pressure.

At this point, we note that these are all pressure-correction schemes i.e. the pressure is used to correct (or project) the auxiliary velocity on to the space of divergence-free vectors. However, it is also possible to design velocity-correction projection methods [54] though these are less popular.

Velocity-correction projection methods switch the roles of the pressure and velocity in the pressure-correction schemes. In the first sub-step, the convective term is either omitted or treated explicitly. In the second sub-step, the velocity is corrected. From an initial value for the auxiliary velocity, the pressure and physical velocity are solved at the next time step. Then, the auxiliary velocity at the next time step is solved by correcting the physical velocity.

Velocity-correction methods

Velocity-correction methods are similar to pressure-correction schemes and also follow a similar line of development into more accurate schemes. The key difference between velocity-

correction methods and pressure-correction methods is that the order of calculating the auxiliary velocity and pressure is reversed. In pressure-correction schemes, the auxiliary velocity is calculated first and the pressure is subsequently calculated. However, in velocity-correction schemes, the pressure is calculated first and the auxiliary velocity is subsequently calculated.

A simple first-order method (similar to the method proposed by Chorin and Temam) is shown below [54]. The algorithm begins with a known value for the auxiliary velocity, $\mathbf{u}^{*,n}$. Then, the pressure, p^{n+1} , physical velocity, $\mathbf{u}^{n+1}$, and the auxiliary velocity at the next time level, $\mathbf{u}^{*,n+1}$ are calculated in that order. Note that we assign time superscripts to the auxiliary velocity to emphasise how the auxiliary velocity is updated.

$$\begin{cases} \nabla^2 p^{n+1} &= \frac{1}{\Delta t} \nabla \cdot \mathbf{u}^{*,n} + \nabla \cdot [(\mathbf{u}^{*,n} \cdot \nabla) \mathbf{u}^{*,n}] \\ \frac{\partial p^{n+1}}{\partial \mathbf{n}} &= \mathbf{n} \cdot [(\mathbf{u}^{*,n} \cdot \nabla) \mathbf{u}^{*,n}] \quad \text{on } \partial\Omega \end{cases} \quad \text{Pressure update step} \quad (2.16)$$

$$\mathbf{u}^{n+1} = \mathbf{u}^{*,n} + \Delta t \nabla p^{n+1} + \Delta t (\mathbf{u}^{*,n} \cdot \nabla) \mathbf{u}^{*,n} \quad \text{Physical Velocity step} \quad (2.17)$$

$$\begin{cases} \mathbf{u}^{*,n+1} - \frac{\Delta t}{Re} \nabla^2 \mathbf{u}^{*,n+1} = \mathbf{u}^{n+1} \\ \mathbf{u}^{*,n+1} = \mathbf{u}_{\partial\Omega} \quad \text{on } \partial\Omega \end{cases} \quad \text{Auxiliary Velocity update step} \quad (2.18)$$

The similarity between this velocity-correction method and the first-order projection method put forward by Chorin and Temam also extends into their accuracy. The velocity is $\mathcal{O}(\Delta t)$ accurate and the pressure suffers from numerical boundary layers that cause $\mathcal{O}(\Delta t)^{\frac{1}{2}}$ accuracy near the boundary.

Similar to pressure-correction methods, the accuracy of this first-order method can be improved

by again introducing the convection term at time step n in the pressure update step. Recall that the convection term is re-written using the vector identity: $\nabla^2 \mathbf{u} = \nabla(\nabla \cdot \mathbf{u}) - \nabla \times \nabla \times \mathbf{u}$. Note that the first term on the right-hand side of the vector identity is zero because we require the auxiliary velocity to be divergence-free for velocity-correction methods.

$$\begin{cases} \nabla^2 p^{n+1} = \frac{1}{\Delta t} \nabla \cdot \mathbf{u}^{*,n} - \frac{1}{Re} \nabla \times \nabla \times \mathbf{u}^{*,n} + \nabla \cdot [(\mathbf{u}^{*,n} \cdot \nabla) \mathbf{u}^{*,n}] \\ \frac{\partial p^{n+1}}{\partial \mathbf{n}} = \mathbf{n} \cdot [\nabla \cdot [(\mathbf{u}^{*,n} \cdot \nabla) \mathbf{u}^{*,n}]] \quad \text{on } \partial\Omega \end{cases} \quad \text{Pressure update step} \quad (2.19)$$

$$\mathbf{u}^{n+1} = \mathbf{u}^{*,n} - \Delta t \nabla p^{n+1} + \Delta t \nabla \cdot [(\mathbf{u}^{*,n} \cdot \nabla) \mathbf{u}^{*,n}] - \frac{\Delta t}{Re} \nabla \times \nabla \times \mathbf{u}^{*,n} \quad \text{Physical Velocity step} \quad (2.20)$$

$$\begin{cases} \mathbf{u}^{*,n+1} - \frac{\Delta t}{Re} \nabla^2 \mathbf{u}^{*,n+1} - \frac{\Delta t}{Re} \nabla \times \nabla \times \mathbf{u}^{*,n+1} = \mathbf{u}^n \\ \mathbf{u}^{*,n+1} = \mathbf{u}_{\partial\Omega} \quad \text{on } \partial\Omega \end{cases} \quad \text{Auxiliary Velocity update step} \quad (2.21)$$

This is called the rotational form of the velocity-correction method and was introduced by Guermond and Shen [66]. Variants of the rotational form of the velocity-correction method were also introduced by Orzag et. al. [67] [61]. Again, similar to the rotational form of the pressure-correction method i.e. the method that enforced consistent boundary conditions for the pressure, the velocity is $\mathcal{O}(\Delta t)^2$ accurate while the pressure is $\mathcal{O}(\Delta t)^{\frac{3}{2}}$ provided the starter solutions (if needed) are sufficiently accurate.

Third-order methods

Finally, we note that third-order methods have been developed and tested numerically [68] but they involve more complicated boundary conditions and use three time levels of velocity data which can make these methods unwieldy.

2.2 Pressure Poisson formulations

2.2.1 Overview

Pressure Poisson formulations are another class of numerical methods that solve (1.9) and are able to de-couple the velocity, $\mathbf{u}$, and the pressure, p . Perhaps the simplest difference between projection methods and pressure Poisson formulations is that projection methods and fractional step methods are always time discretisations of the Navier-Stokes equations. The idea behind pressure Poisson equations is to perform an ‘index reduction’ on the (continuous) Navier-Stokes equations to obtain a new partial differential equation. The new partial differential equation is an ‘index-1’ version of the Navier-Stokes equations which can then be discretised in time using any method of choice. Another difference between pressure Poisson formulations and projection methods is in the role of the pressure. In projection methods, the pressure was used to correct or project the auxiliary velocity, $\mathbf{u}^*$, onto the true velocity, $\mathbf{u}$. In pressure Poisson formulations, there is no auxiliary velocity that needs correction or projection. Instead, the pressure can be viewed as a function of the velocity, so that, given a pressure, p , at time level n , we can then calculate velocity, $\mathbf{u}$, at time level n . The velocity at time level n is then used to solve for the pressure at time level $n + 1$ and this process is repeated as needed.

All variations of solvers using the pressure Poisson formulation start by taking the divergence of the conservation of momentum equations [69] [39] in (1.9). Using the incompressibility or zero-divergence condition, we are now presented with the following key equation in (2.22): a Poisson equation for the pressure, p .

$$\nabla^2 p = -\nabla \cdot ((\mathbf{u} \cdot \nabla) \mathbf{u}) \quad (2.22)$$

An important consideration is whether we can generate an equivalent formulation for the Navier-Stokes equations using (2.22). Consider the following set of equations and note that we retain the same initial, boundary and compatibility conditions that accompanied (1.9)

where applicable.

$$\begin{aligned}
\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} &= -\nabla p + \frac{1}{\text{Re}} \nabla^2 \mathbf{u} \\
\nabla^2 p &= -\nabla \cdot ((\mathbf{u} \cdot \nabla) \mathbf{u}) \\
\mathbf{u}(\mathbf{r}, 0) &= \mathbf{u}_0(\mathbf{r}), \quad \mathbf{r} \in \Omega \\
\mathbf{u}(\mathbf{r}, t) &= \mathbf{u}_{\partial\Omega}(\mathbf{r}, t), \quad \mathbf{r} \in \partial\Omega, \quad t > 0
\end{aligned} \tag{2.23}$$

The critical difference between the pressure Poisson formulation in (2.23) and the original statement of the Navier-Stokes equations in (1.9) is that the continuity equation has been replaced with a pressure Poisson equation. The replacement of the continuity equation with the pressure Poisson equation seems natural because we used it to derive the Poisson equation. However, there are issues to resolve in the above formulation before it can be considered equivalent to the Navier-Stokes equations.

2.2.2 Zero divergence boundary condition

The first issue is brought to light if we consider a solution pair, $(\mathbf{U}^*, P^*)$, to the proposed set of equations in (2.23). So,

$$\nabla^2 P^* = -\nabla \cdot ((\mathbf{U}^* \cdot \nabla) \mathbf{U}^*)$$

and

$$\frac{\partial \mathbf{U}^*}{\partial t} + (\mathbf{U}^* \cdot \nabla) \mathbf{U}^* = -\nabla P^* + \frac{1}{\text{Re}} \nabla^2 \mathbf{U}^*$$

Let $\psi = \nabla \cdot \mathbf{U}^*$. Taking the divergence of the momentum equations, we derive

$$\frac{\partial \psi}{\partial t} + \nabla \cdot ((\mathbf{U}^* \cdot \nabla) \mathbf{U}^*) = -\nabla^2 P^* + \frac{1}{\text{Re}} \nabla^2 \psi$$

Using the Poisson equation, the momentum equations simplify into a heat (or diffusion) equation with ψ as the variable in question: $\frac{\partial \psi}{\partial t} = \frac{1}{\text{Re}} \nabla^2 \psi$ with initial conditions specified by (1.7). We recall that the maximum principle for heat equations [70] [71] allows us to deduce that ψ must be zero everywhere *and* zero for all time. This proof is also provided by Gresho et. al. [72]. In other words, we must explicitly enforce the following condition to guarantee equivalence between the original statement of the Navier-Stokes equations and its pressure Poisson formulation.

$$\nabla \cdot \mathbf{u} = 0, \quad \mathbf{r} \in \partial\Omega, \quad t > 0 \quad (2.24)$$

Then, the pressure Poisson formulation of the Navier-Stokes equations with relevant conditions is shown in (2.25) below.

$$\begin{aligned} \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} &= -\nabla p + \frac{1}{\text{Re}} \nabla^2 \mathbf{u} \\ \nabla^2 p &= -\nabla \cdot ((\mathbf{u} \cdot \nabla) \mathbf{u}) \\ \mathbf{u}(\mathbf{r}, 0) &= \mathbf{u}_0(\mathbf{r}), \quad \mathbf{r} \in \Omega \\ \mathbf{u}(\mathbf{r}, t) &= \mathbf{u}_{\partial\Omega}(\mathbf{r}, t), \quad \mathbf{r} \in \partial\Omega, \quad t > 0 \\ \nabla \cdot \mathbf{u} &= 0, \quad \mathbf{r} \in \partial\Omega, \quad t > 0 \end{aligned} \quad (2.25)$$

2.2.3 Pressure boundary conditions

The most obvious issue that remains lies with the boundary conditions. There are now two boundary conditions for the velocity, $\mathbf{u}$, and there are no boundary conditions for pressure, p . In other words, one variable is over-specified and the other variable is under-specified.

One idea to resolve this boundary condition issue is presented by Johnston and Liu [73]. The divergence-free boundary condition is ‘replaced’ by a boundary condition for the pressure Poisson equation. More precisely, the divergence-free boundary condition is enforced by a condition on the pressure equation instead of enforced explicitly as shown in (2.25). The

‘replacement’ pressure boundary condition [74] is shown in (2.26) below.

$$\frac{\partial p}{\partial \hat{\mathbf{n}}} = -\frac{1}{Re} \hat{\mathbf{n}} \cdot (\nabla \times \nabla \times \mathbf{u}) \quad (2.26)$$

We now show how this pressure boundary condition both maintains the divergence-free boundary condition and is suitable for the Poisson equation. Using the identity: $\nabla^2 \mathbf{u} = \nabla(\nabla \cdot \mathbf{u}) - \nabla \times \nabla \times \mathbf{u}$, the normal component of the momentum equations in (2.25) on the boundary may be written as

$$\frac{\partial p}{\partial \mathbf{n}} = \frac{1}{Re} \frac{\partial(\nabla \cdot \mathbf{u})}{\partial \mathbf{n}} - \frac{1}{Re} \mathbf{n} \cdot (\nabla \times \nabla \times \mathbf{u}) \quad \text{on } \partial\Omega, t \geq 0 \quad (2.27)$$

The pressure boundary conditions we actually enforce are consistent with this last expression provided that

$$\frac{\partial \psi}{\partial \mathbf{n}} = 0 \quad \text{on } \partial\Omega, t \geq 0 \quad (2.28)$$

Again, we can use the divergence of the momentum equations to construct a heat-type equation for ψ subject to the boundary conditions $\frac{\partial \psi}{\partial \mathbf{n}} = 0$. Using the initial condition $\psi(t=0) = 0$, the solution must be $\psi = 0$ for $t > 0$. Finally, it is easy to check that the Poisson compatibility condition is also satisfied for (2.26). The updated pressure Poisson formulation is now written as follows.

$$\begin{aligned} \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} &= -\nabla p + \frac{1}{Re} \nabla^2 \mathbf{u} \\ \nabla^2 p &= -\nabla \cdot ((\mathbf{u} \cdot \nabla) \mathbf{u}) \\ \mathbf{u}(\mathbf{r}, 0) &= \mathbf{u}_0(\mathbf{r}), \quad \mathbf{r} \in \Omega \\ \mathbf{u}(\mathbf{r}, t) &= \mathbf{u}_{\partial\Omega}(\mathbf{r}, t), \quad \mathbf{r} \in \partial\Omega, \quad t > 0 \\ \frac{\partial p}{\partial \hat{\mathbf{n}}} &= -\frac{1}{Re} \hat{\mathbf{n}} \cdot (\nabla \times \nabla \times \mathbf{u}) \end{aligned} \quad (2.29)$$

There is another pressure Poisson formulation proposed by Shirokoff and Rosales [75] which is similar to the one put forward by Johnston and Liu. In fact, Shirokoff and Rosales claims that their pressure Poisson formulation was inspired by Johnston and Liu. Again, there is a proof that the pressure boundary condition upholds the zero-divergence boundary condition in [75].

$$\left. \begin{aligned} \frac{\partial \mathbf{u}}{\partial t} - \frac{1}{Re} \nabla^2 \mathbf{u} &= -\nabla p - (\mathbf{u} \cdot \nabla) \mathbf{u} & \text{for } \mathbf{r} \in \Omega \\ \hat{\mathbf{n}} \times (\mathbf{u} - \mathbf{u}_{\partial\Omega}) &= 0 & \text{for } \mathbf{r} \in \partial\Omega \\ \nabla \cdot \mathbf{u} &= 0 & \text{for } \mathbf{r} \in \partial\Omega \end{aligned} \right\}$$

and

$$\left. \begin{aligned} \nabla^2 p &= -\nabla \cdot ((\mathbf{u} \cdot \nabla) \mathbf{u}) & \text{for } \mathbf{r} \in \Omega \\ \hat{\mathbf{n}} \cdot \nabla p &= \hat{\mathbf{n}} \cdot \left(-\mathbf{u}_{\partial\Omega,t} + \frac{1}{Re} \nabla^2 \mathbf{u} - (\mathbf{u} \cdot \nabla) \mathbf{u} \right) & \text{for } \mathbf{r} \in \partial\Omega \end{aligned} \right\}$$

where $\mathbf{u}_{\partial\Omega,t}$ is the tangential component of $\mathbf{u}_{\partial\Omega}$ (not the time derivative).

There are a few more remarks to be made about the boundary conditions and pressure Poisson formulations. The zero-divergence boundary condition is enforced ‘exponentially’ [75] or ‘indirectly’ rather than enforced numerically. Practically, there is no need to incorporate the zero-divergence boundary condition when developing numerical schemes for the pressure Poisson formulation. It does not appear in the code or the matrix structure needed to numerically solve the equations. Instead, the zero-divergence boundary condition is enforced numerically through the boundary condition for the pressure.

With these schemes for the pressure Poisson formulation, we can easily see some of their advantages and disadvantages. One key advantage, especially over the popular projection methods, is that the boundary condition for the pressure is precise. This eliminates errors which causes numerical boundary layers in the projection method [76] [39]. Another advantage is that the pressure is no longer implicitly related to the velocity field and can be recovered through a Poisson solve. On the other hand, a disadvantage is that the boundary conditions are more complicated than those found in the projection method and pose more numerical

challenges.

It should be noted that the crux of the matter is that the zero-divergence boundary condition must be enforced so that the pressure Poisson formulation is equivalent to the Navier-Stokes equations. In fact, it turns out that $\nabla \cdot \mathbf{u} = 0$ and $\hat{\mathbf{n}} \times \mathbf{u} = 0$ are standard boundary conditions for vector Laplacian problems and lead to straightforward variational forms for the Stokes operator (the Leray projection of the Laplacian) at the expense of other difficulties such as complicated boundary conditions for the pressure [77]. However, there are other ideas [73] that can be implemented to ensure that equivalence. We do not elaborate on these here because the current forms of the pressure Poisson formulations are sufficient and suitable for our task of finding efficient numerical solutions to (1.9) in a toroidal geometry.

Finally, we note that projection methods and pressure Poisson formulations are not entirely disconnected. Some projection methods (such as those that implement accurate boundary conditions for the pressure) can be derived from implicit-explicit time stepping schemes of pressure Poisson formulations [60]. We conclude this section by explicitly stating the pressure Poisson formulation in use for this thesis is found in (2.29).

Chapter 3

Poisson Solvers in Two Spatial Dimensions

3.1 Description of the Problem

This chapter concerns itself with the development and testing of solvers for the Poisson problem in toroidal coordinates when the solution is independent of the toroidal angle, ϕ . Efficient Poisson solvers specifically tailored to this coordinate system are not generally available and their development is an important part of this work.

Specifically, we are interested in the Poisson problem in simple toroidal coordinates where there is no variation in the solution in the ϕ -direction. The partial differential equation for unknown $p = p(r, \theta)$ to be solved may be stated as

$$\nabla^2 p = \frac{\partial^2 p}{\partial r^2} + \left(\frac{1}{r} + \frac{\cos \theta}{h_\phi} \right) \frac{\partial p}{\partial r} - \frac{\sin \theta}{r h_\phi} \frac{\partial p}{\partial \theta} + \frac{1}{r^2} \frac{\partial^2 p}{\partial \theta^2} = f(r, \theta) \quad (r, \theta) \subseteq \Omega. \quad (3.1)$$

In what follows we will compute solutions in the domain Ω corresponding to $-\pi \leq \theta < \pi$, $0 < r_a < r < r_b < R_0$. As usual, the quantity $h_\phi = R_0 + r \cos \theta$ is the ϕ scale factor and R_0 is the toroidal radius (see Appendix A for more details). While we do not deal with the

regularity of the solutions in this work, we mention in passing that if the known function, f , is infinitely differentiable (as assumed in this work) together with infinitely differentiable boundary conditions, then we are assured an infinitely differentiable solution, p .

The Poisson equation (3.1) is solved with classic Neumann conditions on the boundaries; i.e.,

$$\frac{\partial}{\partial r}p(r_a, \theta) = h_a(\theta) \quad \text{and} \quad \frac{\partial}{\partial r}p(r_b, \theta) = h_b(\theta), \quad (3.2)$$

where $h_a(\theta)$ and $h_b(\theta)$ are known functions, assumed differentiable. We also apply periodic boundary conditions

$$p(r, 2\pi) = p(r, 0) \quad \text{and} \quad \frac{\partial p}{\partial r}(r, 2\pi) = \frac{\partial p}{\partial r}(r, 0). \quad (3.3)$$

The periodic boundary conditions (3.3) are applied automatically by a Fourier series approach in what follows.

As is well-known, the Neumann problem outlined above is not solvable for arbitrary choices of the right-hand side, $f = f(r, \theta)$, and boundary functions $h_a(\theta)$ and $h_b(\theta)$. Indeed, there is a compatibility or integrability condition that must be satisfied between the boundary conditions and the right-hand side, f . Integrating the partial differential equation (3.1) over the domain Ω and applying Gauss' theorem gives

$$\int_{\Omega} \nabla^2 p \, dA = \oint_{\partial\Omega} \hat{\mathbf{n}} \cdot \nabla p \, d\ell = \oint_{\partial\Omega} \frac{\partial p}{\partial n} d\ell = \int_{\Omega} f(r, \theta) dA, \quad (3.4)$$

where $dA = rh_{\phi} dr d\theta$ and $d\ell = rh_{\phi} d\theta$ are cross-sectional area element and boundary line elements, respectively. Further, we denote $\hat{\mathbf{n}}$ an outward unit normal to the surface (remember that our coordinate system is left-handed so $\hat{\mathbf{e}}_r$ actually points inwards; see Appendix A). It is easy to check that in the three-dimensional case the volume elements is $dV = rh_{\phi} dr d\theta d\phi$ and an element of surface area is $dS = rh_{\phi} d\theta d\phi$. In the two-dimensional case discussed in this section, where there is no variation in the field quantities in the ϕ direction, integrating over the ϕ -coordinate simply produces a multiple of 2π in the integrals. We therefore take

the corresponding cross-sectional area element and boundary line elements in equation (3.4) to be $dA = rh_\phi dr d\theta$ and $d\ell = rh_\phi d\theta$, respectively.

Accounting for the fact that $\hat{\mathbf{e}}_r$ points inwards, the integrals in equation (3.4) may be iterated to yield

$$\begin{aligned} \int_{-\pi}^{\pi} \int_{r_a}^{r_b} \nabla^2 p rh_\phi dr d\theta &= r_a \int_{-\pi}^{\pi} \frac{\partial p}{\partial r}(r_a, \theta)(R_0 + r_a \cos \theta) d\theta \\ &- r_b \int_{-\pi}^{\pi} \frac{\partial p}{\partial r}(r_b, \theta)(R_0 + r_b \cos \theta) d\theta \end{aligned} \quad (3.5)$$

We therefore have the integrability condition (required for the existence of solutions of the Neumann problem)

$$\begin{aligned} \int_{-\pi}^{\pi} \int_{r_a}^{r_b} f(r, \theta) rh_\phi dr d\theta &= r_a \int_{-\pi}^{\pi} \frac{\partial p}{\partial r}(r_a, \theta)(R_0 + r_a \cos \theta) d\theta \\ &- r_b \int_{-\pi}^{\pi} \frac{\partial p}{\partial r}(r_b, \theta)(R_0 + r_b \cos \theta) d\theta \end{aligned} \quad (3.6)$$

In theory, velocity fields we deal with in our Navier-Stokes solvers should produce input functions $f(r, \theta)$ to our Poisson solvers which satisfy the integrability condition (3.6), with each integral in equation (3.6) vanishing. However, small numerical errors resulting in a non-zero divergence may result in this condition not being precisely satisfied. A method for treating this (used in reference [78] and elsewhere) is to instead solve the auxiliary problem [79]

$$\nabla^2 p = f(r, \theta) + C, \quad (3.7)$$

where the constant C may be found (either as part of the overall solution process or explicitly below) so that the Neumann problem is always solvable. If we add the constant C to the integrand on the left-hand side of (3.6) then we can quickly produce the expression

$$\begin{aligned} C &= -\frac{1}{\pi R_0(r_b^2 - r_a^2)} \int_{-\pi}^{\pi} \int_{r_a}^{r_b} f(r, \theta) rh_\phi dr d\theta \\ &+ \frac{r_a}{\pi R_0(r_b^2 - r_a^2)} \int_{-\pi}^{\pi} \frac{\partial p}{\partial r}(r_a, \theta)(R_0 + r_a \cos \theta) d\theta \end{aligned} \quad (3.8)$$

$$- \frac{r_b}{\pi R_0(r_b^2 - r_a^2)} \int_{-\pi}^{\pi} \frac{\partial p}{\partial r}(r_b, \theta) (R_0 + r_b \cos \theta) d\theta, \quad (3.9)$$

which follows from the simple identity

$$\int_{-\pi}^{\pi} \int_{r_a}^{r_b} r h_{\phi} dr d\theta = \pi R_0 (r_b^2 - r_a^2). \quad (3.10)$$

The point of this discussion is not to produce a formula for the constant C to be used in our solution algorithm; rather, we simply demonstrate that a constant can always be found so that the problem is indeed solvable. As stated, our algorithm will find the compatibility constant C as part of our solution process, not as a direct calculation from equation (3.8). In the numerical implementation of Navier-Stokes problems, our expectation is that the value of C will remain small (hopefully near machine precision), but small numerical errors in the divergence will not result in a non-solvable problem as long as we treat the auxiliary problem (3.7).

Another well-known issue with the Neumann problem is that it is not uniquely solvable. Indeed, if p is a solution to the problem then so is $p + a$ where a is an arbitrary constant. This non-uniqueness implies that the matrix corresponding to the discretized Laplace operator with Neumann conditions is singular. In order to remedy this problem we need to specify additional restrictions on the solution. A typical approach (a variation of which we adopt in this work) is to specify that that volume average of the solution vanishes, i.e.,

$$\frac{1}{V} \int_{\Omega} p(r, \theta, \phi) dV = \frac{1}{2R_0\pi^2(r_b^2 - r_a^2)} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \int_{r_a}^{r_b} p(r, \theta, \phi) r h_{\phi} dr d\theta d\phi = 0. \quad (3.11)$$

For solutions dependent only on the cross-sectional variables the last equation reduces to

$$\frac{1}{R_0\pi(r_b^2 - r_a^2)} \int_{-\pi}^{\pi} \int_{r_a}^{r_b} p(r, \theta) r h_{\phi} dr d\theta = 0. \quad (3.12)$$

Our fix to the Poisson problem with Neumann conditions can now be summarized as follows: We solve the auxiliary problem (3.7) together with boundary conditions (3.2) which, in

addition to the solution, introduces a new unknown constant C to be found; this constant C is monitored in our Navier-Stokes solvers and should remain small. The introduction of a new unknown requires an additional equation to be included; this new equation is obtained from a restriction such as (3.12). Together, the inclusion of the new unknown and new equation into the formulation of the Neumann problem results in a non-singular system of equations [78]. These details will be clarified further in the description of our solver below.

3.2 Fourier Representation

Multiplying equation (3.7) by $r^2 h_\phi$ the auxiliary problem can be written in the equivalent form

$$r^2 h_\phi \frac{\partial^2 p}{\partial r^2} + r (h_\phi + r \cos \theta) \frac{\partial p}{\partial r} - r \sin \theta \frac{\partial p}{\partial \theta} + h_\phi \frac{\partial^2 p}{\partial \theta^2} = r^2 h_\phi f(r, \theta) + r^2 h_\phi C. \quad (3.13)$$

We note that the partial differential equation (3.13) is not separable, which is a well-known feature of the Laplace operator in simple toroidal coordinates. Given the periodicity of the problem in the θ -direction, we assume the following Fourier series expansion for the unknown function $p = p(r, \theta)$

$$p(r, \theta) = \sum_{m=-\infty}^{\infty} p_m(r) e^{im\theta}. \quad (3.14)$$

In general, the Fourier coefficient functions $p_m(r)$ are complex-valued. In the case of Fourier representation of real functions $p(r, \theta)$ (as is done in this thesis) we must have $p_{-m}(r) = \text{conjugate}(p_m(r))$ for $m > 0$ and $\text{Imag}(p_0(r)) = 0$. We note that Fourier approximation of smooth periodic functions gives rise to very rapidly convergent algorithms; we will elaborate on this point in more concrete terms shortly. While we determine the functions $p_m(r)$ in equation (3.14) by means of the numerical procedures developed in this chapter, it should be clear that they are related to the solution $p(r, \theta)$ by the discrete Fourier transform:

$$p_m(r) = \frac{1}{2\pi} \int_{-\pi}^{\pi} p(r, \theta) e^{-im\theta} d\theta. \quad (3.15)$$

As indicated, the coefficients $p_m(r)$ remain a function of the radial coordinate, r . A similar expansion is assumed for the right-hand side of (3.13), i.e.,

$$r^2 h_\phi f(r, \theta) = \sum_{m=-\infty}^{\infty} f_m(r) e^{im\theta}. \quad (3.16)$$

To extract equations for the unknown Fourier coefficient functions $p_m(r)$, we substitute the Fourier expansions (3.14) and (3.16) results in (3.13) which gives

$$\sum_{m=-\infty}^{\infty} \mathcal{L}_m^{(0)} p_m(r) e^{im\theta} = \sum_{m=-\infty}^{\infty} f_m(r) e^{im\theta} + r^2 h_\phi C. \quad (3.17)$$

In equation (3.17) we define the ordinary differential operator $\mathcal{L}_m^{(0)}$ as

$$\mathcal{L}_m^{(0)} p_m(r) = r^2 h_\phi p_m''(r) + r(h_\phi + r \cos \theta) p_m'(r) - (imr \sin \theta + m^2 h_\phi) p_m(r) \quad (3.18)$$

Note that the term involving the constant C in equation (3.17) is already in the form of a Fourier series.

Next, we apply standard orthogonality relations to the expression (3.17) to extract a system of ordinary differential equations for $p_m(r)$. Denoting the Kronecker delta symbol as $\delta_{m,n}$, the following (somewhat trivial) identities are easily established:

$$\begin{aligned} \frac{1}{\pi} \int_{-\pi}^{\pi} e^{i(m-n)\theta} d\theta &= 2\delta_{m,n} \\ \frac{1}{\pi} \int_{-\pi}^{\pi} \cos \theta e^{i(m-n)\theta} d\theta &= \delta_{m,n+1} + \delta_{m,n-1} \\ \frac{1}{\pi} \int_{-\pi}^{\pi} \sin \theta e^{i(m-n)\theta} d\theta &= i\delta_{m,n+1} - i\delta_{m,n-1} \end{aligned} \quad (3.19)$$

Multiplying equation (3.17) by $\exp(-in\theta)$, integrating over the range $\theta \in [-\pi, \pi]$ and applying the identities (3.19) leads to a coupled system of ordinary differential equations of the form

$$L_n^{(1)} p_{n-1}(r) + L_n^{(2)} p_n(r) + L_n^{(3)} p_{n+1}(r) = 2f_n(r) + (2r^2 R_0 \delta_{0,n} + r^3 \delta_{1,n} + r^3 \delta_{-1,n}) C, \quad (3.20)$$

where the linear differential operators are given by

$$\begin{aligned}
L_n^{(1)} &= r \left(r^2 \frac{d^2}{dr^2} + 2r \frac{d}{dr} - n(n-1) \right) \\
L_n^{(2)} &= 2R_0 \left(r^2 \frac{d^2}{dr^2} + r \frac{d}{dr} - n^2 \right) \\
L_n^{(3)} &= r \left(r^2 \frac{d^2}{dr^2} + 2r \frac{d}{dr} - n(n+1) \right)
\end{aligned} \tag{3.21}$$

We note that the term on the right-hand side of equation (3.20) associated with the constant C is computed using the identity

$$\frac{1}{\pi} \int_{-\pi}^{\pi} r^2 h_{\phi} e^{-in\theta} d\theta = 2r^2 R_0 \delta_{0,n} + r^3 \delta_{1,n} + r^3 \delta_{-1,n}. \tag{3.22}$$

The boundary conditions are treated by means of Fourier series expansions in a similar manner. The functions in equation (3.2) corresponding to Neumann conditions are expanded as

$$h_a(\theta) = \sum_{n=-\infty}^{\infty} h_n^{(a)} e^{in\theta} \quad \text{and} \quad h_b(\theta) = \sum_{n=-\infty}^{\infty} h_n^{(b)} e^{in\theta}. \tag{3.23}$$

We can therefore see (owing to trigonometric orthogonality) that the Fourier representation of the unknown function $p(r, \theta)$ inherits boundary conditions as follows: in the case of Neumann conditions, we require for all integer indices n

$$p'_n(r_a) = h_n^{(a)} \quad \text{and} \quad p'_n(r_b) = h_n^{(b)}, \tag{3.24}$$

where the prime indicates differentiation.

We note that the issue with non-uniqueness of the solution of the system (3.20) in the case of Neumann boundary conditions is strictly related to the differential operators (3.21) associated with index $n = 0$. The discrete versions of these operators in particular will need to be supplemented with additional conditions as they are singular. This point will be expanded upon shortly in the presentation of our algorithm but we note here that the additional

condition in equation (3.12) that guarantees the vanishing of the cross-sectional area integral of the solution (which can be imposed on the problem to ensure uniqueness of the solution) becomes, upon assuming the Fourier expansion (3.14),

$$2R_0 \int_{r_a}^{r_b} p_0(r)rdr + \int_{r_a}^{r_b} p_1(r)r^2dr + \int_{r_a}^{r_b} p_{-1}(r)r^2dr = 0. \quad (3.25)$$

In practice, we have found this condition a little cumbersome to enforce and in this work we adopt a slightly different condition that reads

$$\int_{r_a}^{r_b} p_0(r)dr = 0. \quad (3.26)$$

The implementation of our solver deals with truncations of the infinite Fourier expansions in equations (3.14) and (3.16) and separate problems to be solved for the real and imaginary parts of the unknown functions $p_m(r)$. We will elaborate on these details in what follows. We assume the truncated expansions

$$p(r, \theta) \approx \sum_{m=-N_\theta}^{N_\theta} p_m(r)e^{im\theta} \quad (3.27)$$

and

$$r^2 h_\phi f(r, \theta) \approx \sum_{m=-N_\theta}^{N_\theta} f_m(r)e^{im\theta}. \quad (3.28)$$

As is well-known, these expansions are excellent representations for periodic functions. Specifically, if $p(r, \theta)$ has $q - 1$ continuous θ -derivatives on $[-\pi, \pi)$ but the q th derivative is discontinuous, then the series coefficients are known to possess the asymptotic behaviour

$$p_m(r) \sim \frac{1}{m^{q+1}}$$

for large m . It therefore follows that the truncation error of the expansions (3.27) and (3.28) is $\mathcal{O}(N_\theta^{-q-2})$. In the case of an infinitely differentiable functions $p \in C^\infty[-\pi, \pi)$ and $f \in C^\infty[-\pi, \pi)$ as encountered in the physical cases studies in the thesis, the expansions

(3.27) and (3.28) converge faster than $\mathcal{O}(N_\theta^{-q})$ for any positive integer q i.e. they achieve super-algebraic convergence. This property is a fundamental mathematical pillar on which our methods are constructed. In short, this property ensures an extremely high resolution of the unknowns with very small numbers of Fourier modes N_θ required.

This truncation of the unknowns results in a truncation of the overall problem to be solved. Recall that for a real solution $p(r, \theta)$, $p_0(r)$ is purely real and $p_{-m}(r) = \text{Conjugate}(p_m(r))$. Noting that the compatibility constant C is real, we break up the solution of the system (3.20) into two problems, for the real and imaginary parts as follows. For the real part, we solve

$$\begin{aligned} L_m^{(1)} \text{Real}(p_{m-1}(r)) + L_m^{(2)} \text{Real}(p_m(r)) + L_m^{(3)} \text{Real}(p_{m+1}(r)) \\ = 2\text{Real}(f_m(r)) + (2r^2 R_0 \delta_{0,m} + r^3 \delta_{1,m}) C \end{aligned} \quad (3.29)$$

for $m = 0, 1, \dots, N_\theta$ with $\text{Real}(p_{N_\theta+1}(r)) = 0$ and $\text{Real}(p_{-1}(r)) = \text{Real}(p_1(r))$. This system of equations must be solved with constraint (3.26) subject to boundary conditions

$$\text{Real}(p'_n(r_a)) = \text{Real}(h_n^{(a)}) \quad \text{and} \quad \text{Real}(p'_n(r_b)) = \text{Real}(h_n^{(b)}), \quad (3.30)$$

for $m = 0, 1, \dots, N_\theta$ with Fourier coefficients of the boundary functions $h_n^{(a)}$ and $h_n^{(b)}$ defined as per equation (3.23). For the imaginary part, we solve

$$L_m^{(1)} \text{Imag}(p_{m-1}(r)) + L_m^{(2)} \text{Imag}(p_m(r)) + L_m^{(3)} \text{Imag}(p_{m+1}(r)) = 2\text{Imag}(f_m(r)) \quad (3.31)$$

for $m = 1, 2, \dots, N_\theta$ with $\text{Imag}(p_{N_\theta+1}(r)) = 0$ and $\text{Imag}(p_0(r)) = 0$. This system of equations must be solved with boundary conditions

$$\text{Imag}(p'_n(r_a)) = \text{Imag}(h_n^{(a)}) \quad \text{and} \quad \text{Imag}(p'_n(r_b)) = \text{Imag}(h_n^{(b)}), \quad (3.32)$$

for $m = 1, 2, \dots, N_\theta$. In this way, we only need to solve for half the Fourier coefficients $p_m(r)$;

the other half can easily be deduced by taking the conjugate of the solved half.

We briefly digress to discuss practical issues related to the calculation of the Fourier transform and its inverse. Corresponding to a $(2N_\theta + 1)$ -point equispaced sampling of the function $f_k = f(\theta_k)$ at nodes

$$\theta_k = (k - 1)\Delta\theta, \quad \Delta\theta = \frac{2\pi}{2N_\theta + 1}, \quad k = 1, \dots, 2N_\theta + 1, \quad (3.33)$$

we compute the Discrete Fourier Transform $\hat{f}_k$ for $k = -N_\theta, \dots, N_\theta$ by means of the Fast Fourier Transform [80] in $\mathcal{O}(N_\theta \log N_\theta)$ operations. In particular, in this work, we use numerical routines that have been developed by experts and substantially tested [81].

3.3 Chebyshev Representation

In what follows, we will present a Chebyshev representation of the coupled systems of differential equations (3.29) and (3.31) subject to Neumann boundary conditions and the constraint (3.25). Chebyshev representation of the unknowns will lead to a high-order algorithm for the numerical solution of these equations. Before presenting the details of our Chebyshev representation of the differential equations, we digress briefly to outline important facts pertaining to the representation of functions in Chebyshev series, much of which are contained in the classic reference texts [82] [83].

3.3.1 Chebyshev Series Expansions

The Chebyshev polynomial of the first kind, $T_n(\xi)$, is a polynomial of degree n defined by the relation

$$T_n(\xi) = \cos(n\alpha) \quad \text{when} \quad \xi = \cos \alpha. \quad (3.34)$$

The range of variable ξ is the interval $[-1, 1]$ which allows one to take the range of the corresponding variable α to be the interval $[0, \pi]$, resulting in a one-to-one mapping. It is readily seen from the trigonometric forms that the Chebyshev polynomials must obey the

stable recurrence

$$T_{n+1}(\xi) = 2\xi T_n(\xi) - T_{n-1}(\xi) \quad (3.35)$$

with starting values $T_0(\xi) = 1$ and $T_1(\xi) = \xi$. As is well-known [82] [83] for $n > 0$, the Chebyshev polynomials have the explicit expansion

$$T_n(\xi) = \sum_{k=0}^{\lfloor n/2 \rfloor} \frac{(-1)^k}{2^{2k-n+1}} \frac{n}{n-k} \binom{n-k}{k} \xi^{n-2k} \quad (3.36)$$

with $T_0(\xi) = 1$. As is well-known, the first-kind Chebyshev polynomials are mutually orthogonal on the interval $\xi \in [-1, 1]$ with respect to the weight function $1/\sqrt{1-\xi^2}$. Specifically, they have the following orthogonality relation

$$\int_{-1}^1 \frac{T_n(\xi) T_m(\xi)}{\sqrt{1-\xi^2}} dx = \int_0^\pi \cos(n\alpha) \cos(m\alpha) d\alpha = \begin{cases} \pi & n = m = 0 \\ \pi/2 & n = m > 0 \\ 0 & \text{otherwise} \end{cases} \quad (3.37)$$

The orthogonality relations (3.37) allow us to expand (non-singular) functions defined on the interval $\xi \in [-1, 1]$ in a series of Chebyshev polynomials. Indeed, the Chebyshev series expansion of a function $f(\xi)$ is given by

$$f(\xi) = \sum_{n=0}^{\infty}{}' a_n T_n(\xi), \quad (3.38)$$

where the prime indicates that the coefficient associated with $T_0(\xi)$ is to be halved. Owing to the orthogonality relations (3.37), the coefficients a_n are related to the original function $f(\xi)$ via the Chebyshev transform

$$a_n = \frac{2}{\pi} \int_{-1}^1 \frac{T_n(\xi) f(\xi)}{\sqrt{1-\xi^2}} dx \quad n = 0, 1, 2, \dots \quad (3.39)$$

Indeed, equations (3.38) and (3.39) constitute the Chebyshev transform pair of the function $f(\xi)$. As is well-known, with the change of variables $\xi = \cos \alpha$ we have $T_n(\cos \alpha) = \cos(n\alpha)$ and the Chebyshev expansion (3.38) becomes a cosine series (of an even periodic function) in the θ -variable, while the Chebyshev transform in (3.39) becomes a cosine transform of that function in the α -variable. This observation is important, since it explains how the Chebyshev expansions inherit several properties of Fourier expansions, in particular, the super-algebraic convergence rate of the series when the function $f(\xi)$ is infinitely differentiable.

In the development of numerical schemes for the solution of practical problems, the set of Chebyshev polynomials $T_n(\xi)$ is a natural choice of basis functions to represent an unknown function to be determined. Of course, a truncation of the expansion (3.38) is required:

$$f(\xi) \approx \sum_{n=0}^N a_n T_n(\xi). \quad (3.40)$$

Given the relationship of the Chebyshev series of a function $f(\xi)$ in the ξ -variable to the cosine series of the even periodic function $f(\cos \alpha)$ in the α -variable, it follows that the series coefficients (3.39) may be produced (where necessary) in $\mathcal{O}(N \log N)$ operations by means of a fast cosine transform [80] (also see discussion below). The use of such an expansion is highly advantageous: in the case of an infinitely differentiable function $f \in C^\infty[-1, 1]$, the Chebyshev series (3.40) thus converges faster than $\mathcal{O}(N^{-m})$ for any positive integer m —i.e. it achieves super-algebraic convergence.

We briefly digress to discuss practical issues related to the calculation of the Chebyshev transform and its inverse. Corresponding to an N -point sampling of the function $f_k = f(\xi_k)$ at nodes $\xi_k = \cos(\pi(k-1)/(N-1))$, $k = 1, \dots, N$, we have the DCT-I cosine transform

$$a_k = \frac{1}{2} (f_1 + (-1)^k f_N) + 2 \sum_{j=2}^{N-1} f_j \cos \left(\frac{j(k-1)\pi}{N-1} \right) \quad k = 1, 2, \dots, N. \quad (3.41)$$

After applying the multiplicative factor $1/(N-1)$ to normalize the transform, the results from the DCT-I in equation (3.41) produce approximations to the Chebyshev series coefficients.

Conversely, values of function $f(x_k)$ for $k = 1, \dots, N$ can be reconstructed on the N -point grid by again applying the DCT-I (that is, the DCT-I is the inverse of itself):

$$f_k = \frac{1}{2} \left(a_1 + (-1)^k a_N \right) + 2 \sum_{j=2}^{N-1} a_j \cos \left(\frac{j(k-1)\pi}{N-1} \right) \quad k = 1, 2, \dots, N. \quad (3.42)$$

The inverse transform (3.42) does not need to be normalized. While both the definitions (3.41) and (3.42) show precisely what is computed by the DCT-I, we generally do not directly adapt the summations in these formulas as an $\mathcal{O}(N^2)$ algorithm. Instead both of these quantities are computed using fast $\mathcal{O}(N \log N)$ algorithms; see, for example, details on the fast Fourier transform in [80]. In particular, in this work, we use numerical routines that have been developed by experts and substantially tested [81].

3.3.2 Discretization of Differential Operators

We now turn our attention to producing discrete versions of the differential operators in equation (3.20) which are applicable to functions $p_m(r)$ defined on a Chebyshev grid. For the sake of simplicity in the presentation below, we will approach a description of our methods using a generic function $f(r)$ defined on $r \in [r_a, r_b]$.

First, we transform the variable $r \in [r_a, r_b]$ as follows: Let

$$A = \frac{r_b + r_a}{2} \quad \text{and} \quad B = \frac{r_b - r_a}{2}; \quad (3.43)$$

then $r = A\xi + B$ with $\xi \in [-1, 1]$. A Chebyshev grid with N points in the r -variable is thus defined as

$$r_k = A\xi_k + B = A \cos \left(\frac{(k-1)\pi}{N-1} \right) + B, \quad k = 1, 2, \dots, N. \quad (3.44)$$

Note the reversal in the orientation of the grid with r_k defined such that $r(1) = r_b$ and $r(N) = r_a$. The normalized DCT-I of the discretely sampled function $f_k = f(r_k)$ will then produce the required Chebyshev coefficients a_k used below.

With these definitions in place, we can produce useful results for functions defined as

$$f(r) = \sum_{n=0}^{N-1}{}' a_n T_n(\xi) \quad \text{with} \quad r = A\xi + B. \quad (3.45)$$

As indicated, an N -point sampling on the Chebyshev grid (3.44) produces a polynomial approximation of degree $N - 1$. As before, the prime in the sum indicates that the coefficient associated with $T_0(\xi)$ is to be halved.

In order to compute derivatives of $f(r)$, we proceed as follows. Differentiating the Chebyshev expansion (3.45) results in

$$\frac{d}{dr}f(r) = \frac{1}{A} \frac{d}{d\xi}f(A\xi + B) = \frac{1}{A} \sum_{k=0}^{N-1}{}' c_k T_k(\xi). \quad (3.46)$$

Note that the polynomial approximation for the derivative is one degree less than the original function, and this will be reflected in the calculation of the coefficients c_k below. The coefficient may be determined from the well-known recursion [82, eqn. 2.51]

$$c_{k-1} = c_{k+1} + 2ka_k, \quad k = N - 1, \dots, 1, \quad (3.47)$$

with starting values $c_{N-1} = c_N = 0$. This recursion presents a very efficient method for computing derivatives: one would produce the Chebyshev coefficients a_k in $\mathcal{O}(N \log N)$ operations, compute the coefficients c_k in $\mathcal{O}(N)$ operations and then invert the transform in $\mathcal{O}(N \log N)$ operations to obtain an accurate representation for the derivative at each point on the Chebyshev grid (3.44). In what follows, however, we will need to re-express these operations as a vector-matrix product. Defining the N -element vectors of Chebyshev coefficients

$$\mathbf{a} = [a_0, a_1, a_2, \dots, a_{N-1}]^T \quad (3.48)$$

and

$$\mathbf{c} = [c_0, c_1, c_2, \dots, c_{N-1}]^T \quad (3.49)$$

the coefficients of the derivative of a Chebyshev expansion in equation (3.46) may be produced from the coefficients of the original expansion (3.45) by mean of the vector-matrix product

$$\mathbf{c} = \mathcal{D}\mathbf{a} \quad (3.50)$$

The differentiation matrix, $\mathcal{D}$, has dimensions $N \times N$ and is always upper triangular with a vanishing diagonal and a vanishing last row. Using the recurrence in equation (3.47), it is not difficult to see that if N is odd then the differentiation matrix may be written as

$$\mathcal{D} = \frac{2}{A} \begin{bmatrix} 0 & 1 & 0 & 3 & 0 & 5 & 0 & \dots & 0 & N-2 & 0 \\ & 0 & 2 & 0 & 4 & 0 & 6 & \dots & N-3 & 0 & N-1 \\ & & 0 & 3 & 0 & 5 & 0 & \dots & 0 & N-2 & 0 \\ & & & 0 & 4 & 0 & 6 & \dots & N-3 & 0 & N-1 \\ & & & & 0 & 5 & 0 & \dots & 0 & N-2 & 0 \\ & & & & & \ddots & \ddots & \ddots & \vdots & \vdots & \vdots \\ & & & & & & \ddots & \ddots & \vdots & \vdots & \vdots \\ & & & & & & & 0 & N-3 & 0 & N-1 \\ & & & & & & & & 0 & N-2 & 0 \\ & & & & & & & & & 0 & N-1 \\ & & & & & & & & & & 0 \end{bmatrix}.$$

In a similar way, if N is even then differentiation matrix is

$$\mathcal{D} = \frac{2}{A} \begin{bmatrix} 0 & 1 & 0 & 3 & 0 & 5 & 0 & \dots & N-3 & 0 & N-1 \\ & 0 & 2 & 0 & 4 & 0 & 6 & \dots & 0 & N-2 & 0 \\ & & 0 & 3 & 0 & 5 & 0 & \dots & N-3 & 0 & N-1 \\ & & & 0 & 4 & 0 & 6 & \dots & 0 & N-2 & 0 \\ & & & & 0 & 5 & 0 & \dots & N-3 & 0 & N-1 \\ & & & & & \ddots & \ddots & \ddots & \vdots & \vdots & \vdots \\ & & & & & & \ddots & \ddots & \vdots & \vdots & \vdots \\ & & & & & & & 0 & N-3 & 0 & N-1 \\ & & & & & & & & 0 & N-2 & 0 \\ & & & & & & & & & 0 & N-1 \\ & & & & & & & & & & 0 \end{bmatrix}.$$

The only important distinction between the even and odd cases involves how the matrix is truncated in the last column on the right. We will come back to these definitions shortly in order to define more general differential operators.

Next, given a Chebyshev expansion for the function $f(r)$ in the form (3.45) we seek a representation

$$rf(r) = (A\xi + B)f(A\xi + B) = \sum_{k=0}^{N-1} c_k T_k(\xi). \quad (3.51)$$

If $f(r)$ is represented by a polynomial of degree $N - 1$ then $rf(r)$ will necessarily be a polynomial of degree N . However, as indicated in the sum in equation (3.51) we set the last coefficient $c_N = 0$. This is useful to do since it results in a square matrix for the matrix-vector product representation below, and this has no net effect on our overall algorithm as we later remove the last two rows of these matrices to accommodate boundary conditions. (One might also argue that the very rapid convergence of Chebyshev representations also justifies setting the last coefficient to zero, even in the absence of any procedure we use deleting the last rows of the matrix operators). Using the recurrence (3.35), it is straightforward to derive the

following results:

$$c_k = \frac{A}{2}a_{k-1} + Ba_k + \frac{A}{2}a_{k+1} \quad k = 1, 2, \dots, N-2, \quad (3.52)$$

with $c_0 = Ba_0 + Aa_1$ and $c_{N-1} = Aa_{N-2}/2 + Ba_{N-1}$. In order to recast this as a matrix-vector product (as is required by our method) we again use the coefficient vector definitions (3.48) and (3.49) to obtain

$$\mathbf{c} = \mathcal{R}\mathbf{a} \quad (3.53)$$

The tridiagonal matrix $\mathcal{R}$, which has dimensions $N \times N$, may be written as

$$\mathcal{R} = \frac{1}{2} \begin{bmatrix} 2B & 2A & & & \\ A & 2B & A & & \\ & A & 2B & A & \\ & & \ddots & \ddots & \ddots \\ & & & A & 2B & A \\ & & & & A & 2B \end{bmatrix}.$$

We can now summarize some of the main results of the section required for our numerical method. Consider an N -term Chebyshev expansion of a differentiable function $f(r)$ of the form (3.45) with Chebyshev coefficients stored in the N -element vector (3.48). The Chebyshev coefficients of $L_n^{(1)}f(r)$, $L_n^{(2)}f(r)$ and $L_n^{(3)}f(r)$ (the differential operators defined in equation (3.20)) are given by the vector-matrix products $\mathbf{L}_n^{(1)}\mathbf{a}$, $\mathbf{L}_n^{(2)}\mathbf{a}$ and $\mathbf{L}_n^{(3)}\mathbf{a}$, respectively, where

$$\mathbf{L}_n^{(1)} = \mathcal{R}^3\mathcal{D}^2 + 2\mathcal{R}^2\mathcal{D} - n(n-1)\mathcal{R}, \quad (3.54)$$

$$\mathbf{L}_n^{(2)} = 2R_0\mathcal{R}^2\mathcal{D}^2 + 2R_0\mathcal{R}\mathcal{D} - 2R_0n^2\mathbf{I}, \quad (3.55)$$

and

$$\mathbf{L}_n^{(3)} = \mathcal{R}^3\mathcal{D}^2 + 2\mathcal{R}^2\mathcal{D} - n(n+1)\mathcal{R}. \quad (3.56)$$

Note that we define $\mathbf{I}$ as the $N \times N$ identity matrix in equation (3.55).

3.4 Fully Discrete Representation of the Solution and Resulting Discrete Neumann Problem

With a Fourier representation in the θ -variable and a Chebyshev representation in the r -variable the unknown function $p(r, \theta)$ and $r^2 h_\phi f(r, \theta)$, the left- and right-hand side of the augmented problem (3.13) become

$$p(r, \theta) \approx \sum_{m=-N_\theta}^{N_\theta} \left(\sum_{k=0}^{N_r-1} \hat{p}_{k,m} T_k(\xi) \right) e^{im\theta} \quad (3.57)$$

and

$$r^2 h_\phi f(r, \theta) \approx \sum_{m=-N_\theta}^{N_\theta} \left(\sum_{k=0}^{N_r-1} \hat{f}_{k,m} T_k(\xi) \right) e^{im\theta} \quad (3.58)$$

for $r \in [r_a, r_b]$ and $\theta \in [0, 2\pi)$. Recall that with A and B defined as in (3.43), we have $r = A\xi + B$ for $\xi \in [-1, 1]$. As discussed in preceding sections, if the functions $p(r, \theta)$ and $r^2 h_\phi f(r, \theta)$ are infinitely differentiable in both the r - and θ -variables (as is the case for the problems we examine in this thesis), then the expansions (3.57) and (3.58) will experience super-algebraic convergence in both N_r and N_θ . Such expansions allow us to obtain an extremely high resolution of the solution of the Poisson problem, p , with very small numbers of unknowns.

As detailed in this section, our Poisson solver assumes expansions of the form (3.57) and (3.58) and solves the Poisson Neumann problem for the unknown spectral coefficients $\hat{p}_{k,m}$. Assuming a spatial sampling $p_{k,m} = p(r_k, \theta_m)$ for r_k on the N_r -point Chebyshev grid (3.44) and θ_m on the $2M_\theta + 1$ -point Fourier grid (3.33), the spectral coefficients may be obtained to high accuracy by means of a sequence of normalized Chebyev transforms and Fourier transforms executed in parallel as follows:

PARALLEL DO $k = 1 \dots N_r$

```

DO  $m = 1 \dots 2N_\theta + 1$ 

    FFTIN $m$  =  $p_{k,m}$ 

END DO

EXECUTE FFTFWD(FFTIN, FFTOUT)

DO  $m = 1 \dots 2N_\theta + 1$ 

     $\tilde{p}_{k,m} = \text{FFTOUT}_m / (2N_\theta + 1)$ 

END DO

END PARALLEL DO

PARALLEL DO  $m = 1 \dots 2N_\theta + 1$ 

    DO  $k = 1 \dots N_r$ 

        DCTIN $k$  =  $\tilde{p}_{k,m}$ 

    END DO

    EXECUTE DCTI(DCTIN, DCTOUT)

    DO  $k = 1 \dots N_r$ 

         $\hat{p}_{k,m} = \text{DCTOUT}_k / (N_r - 1)$ 

    END DO

END PARALLEL DO

```

An almost identical algorithm transforms the discretely-sampled function $p_{k,m}$ to $\hat{p}_{k,m}$. In this way, spectral coefficients are obtained from discrete spatial samplings in $\mathcal{O}(N_r N_\theta \log N_r + N_r N_\theta \log N_\theta)$ operations.

The boundary conditions to be enforced in the Neumann case are, for each Fourier mode m

$$\sum_{k=0}^{N_r-1} k^2 \hat{p}_{k,m} \quad (3.59)$$

and

$$\sum_{k=0}^{N_r-1} (-1)^k k^2 \hat{p}_{k,m}. \quad (3.60)$$

The solvability condition (3.26) in the discrete form now simply reads

$$\hat{p}_{0,0} = 0. \quad (3.61)$$

The discrete operators (3.54), (3.55), (3.56) together with the boundary conditions (3.59) and (3.60) and solvability condition (3.61) result in a sparse block tridiagonal system of equations for both the real and imaginary parts of the solution $\hat{p}_{k,m}$ and the compatibility constant C . In the following sections, we give details on the development and implementation of such a sparse matrix solver.

3.5 A Block Tridiagonal Sparse Matrix Solver

The Poisson solver developed in this chapter requires the solution of block tridiagonal linear systems of equations of the form

$$\mathbf{A}\mathbf{x} = \mathbf{z},$$

where

$$\mathbf{x} = [\mathbf{x}_1^T, \mathbf{x}_2^T, \dots, \mathbf{x}_M^T]^T, \quad \mathbf{z} = [\mathbf{z}_1^T, \mathbf{z}_2^T, \dots, \mathbf{z}_M^T]^T,$$

and

$$\mathbf{A} = \begin{bmatrix} \mathbf{A}_1 & \mathbf{B}_1 & & & \\ \mathbf{C}_2 & \mathbf{A}_2 & \mathbf{B}_2 & & \\ & \mathbf{C}_3 & \mathbf{A}_3 & \mathbf{B}_3 & \\ & & \ddots & \ddots & \ddots \\ & & & \mathbf{C}_{M-1} & \mathbf{A}_{M-1} & \mathbf{B}_{M-1} \\ & & & & \mathbf{C}_M & \mathbf{A}_M \end{bmatrix}.$$

Each of the block matrices $\mathbf{A}_2$, $\mathbf{B}_2$ and $\mathbf{A}_k$, $\mathbf{B}_k$, $\mathbf{C}_k$ for $k = 3, \dots, M-1$ have dimension $N \times N$. The block matrices $\mathbf{A}_M$ and $\mathbf{C}_M$ also have dimension $N \times N$. Matrices $\mathbf{C}_1$ and $\mathbf{B}_M$ are not defined. In order to accommodate the augmented Poisson problem described in this chapter, the block matrix $\mathbf{A}_1$ will have dimension $L \times L$, the block matrix $\mathbf{B}_1$ will have dimension $L \times N$ and the block matrix $\mathbf{C}_2$ will have dimension $N \times L$. In the application of our sparse solver to the Poisson problem we will specifically take $L = N + 1$ or $L = N$ (for real and imaginary parts of the solutions, respectively) but we will keep L as a more general dimension in the description of our algorithm below. The column vectors $\mathbf{x}_k$ and $\mathbf{z}_k$ for $k = 2, \dots, M$ have dimension $N \times 1$, while the column vectors $\mathbf{x}_1$ and $\mathbf{z}_1$ have dimension $L \times 1$.

The $L + N(M-1) \times L + N(M-1)$ matrix $\mathbf{A}$ consists of zero elements except for the 3 main block diagonal matrices. The matrix $\mathbf{A}$ has the following $\mathbf{LU}$ factorization:

$$\mathbf{A} = \begin{bmatrix} \mathbf{I} & & & & \\ \mathbf{L}_2 & \mathbf{I} & & & \\ & \mathbf{L}_3 & \mathbf{I} & & \\ & & \ddots & \ddots & \\ & & & \mathbf{L}_{M-1} & \mathbf{I} \\ & & & & \mathbf{L}_M & \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{U}_1 & \mathbf{B}_1 & & & \\ & \mathbf{U}_2 & \mathbf{B}_2 & & \\ & & \ddots & \ddots & \\ & & & \mathbf{U}_{M-2} & \mathbf{B}_{M-2} \\ & & & & \mathbf{U}_{M-1} & \mathbf{B}_{M-1} \\ & & & & & \mathbf{U}_M \end{bmatrix}.$$

In compact notation, we rewrite this last expression as $\mathbf{A} = \mathbf{LU}$. Each of the block matrices $\mathbf{U}_k$ for $k = 2, \dots, M$ and $\mathbf{L}_k$ for $k = 3, \dots, M$ have dimension $N \times N$. The block matrix $\mathbf{U}_1$

has dimension $L \times L$ and the block matrix $\mathbf{L}_2$ has dimension $N \times L$. We also denote $\mathbf{I}$ as the $N \times N$ identity matrix, with the exception of the first (upper left) entry in the global matrix $\mathbf{L}$ above; this identity matrix necessarily has dimension $L \times L$.

Multiplying out the $\mathbf{LU}$ factorization and matching elements with those in the expression for $\mathbf{A}$ leads to the following matrix equations:

$$\mathbf{U}_1 = \mathbf{A}_1 \quad (3.62)$$

For $i = 2, \dots, M$ we have

$$\mathbf{L}_i \mathbf{U}_{i-1} = \mathbf{C}_i \quad (3.63)$$

$$\mathbf{L}_i \mathbf{B}_{i-1} + \mathbf{U}_i = \mathbf{A}_i \quad (3.64)$$

From these equations we derive the following sequence of steps in our factorization phase of the solution procedure:

- (a) Using LAPACK, compute the LU-factorization of block matrix $\mathbf{U}_1 = \mathbf{A}_1$ and determine the rows of $\mathbf{L}_2$ from

$$\mathbf{U}_1^T \mathbf{L}_2^T = \mathbf{C}_2^T.$$

using repeated backsubstitutions with the LU-factorization of $\mathbf{U}_1$. Options in LAPACK allow for the solution of the problem in this form based on the the LU-factorization of $\mathbf{U}_1$ alone; the LU-factorization of $\mathbf{U}_1^T$ is not independently needed. The factorization of $\mathbf{U}_1$ and its pivots should be stored for later use in the substitution phase; see below. Recall that the block matrices in this step have non-standard dimensions but all matrix products are well-defined.

- (b) Determine the matrix $\mathbf{U}_2$ from

$$\mathbf{U}_2 = \mathbf{A}_2 - \mathbf{L}_2 \mathbf{B}_1.$$

Compute the LU factorization of $\mathbf{U}_2$ and store the results. Discard original matrix $\mathbf{U}_2$ if desired.

(c) For $k = 3, \dots, M$ do:

(i) Using the stored factorization for $\mathbf{U}_{k-1}$, compute the rows of $\mathbf{L}_k$ from

$$\mathbf{U}_{k-1}^T \mathbf{L}_k^T = \mathbf{C}_k^T.$$

(ii) Determine the matrix $\mathbf{U}_k$ from

$$\mathbf{U}_k = \mathbf{A}_k - \mathbf{L}_k \mathbf{B}_{k-1}.$$

Compute the LU factorization of $\mathbf{U}_k$ and store the results. Discard the original matrix $\mathbf{U}_k$ if desired.

The block matrices involved in this sequence of steps all have standard dimensions $N \times N$.

Overall, the computational cost of the factorization stage is $\mathcal{O}(L^3) + \mathcal{O}((M-1)N^3)$, the dominant contributions coming from the sequence of LU -factorizations of block matrices $\mathbf{U}_k$, the backsubstitutions to compute $\mathbf{L}_k$ from $\mathbf{U}_{k-1}^T \mathbf{L}_k^T = \mathbf{C}_k^T$ and the matrix-matrix multiplies of $\mathbf{L}_k \mathbf{B}_{k-1}$. The factorization stage is the most expensive part of the solution procedure, but it does not rely on the vector $\mathbf{z}$ and is typically executed only once before repeated use.

Moving on to the details of the forward/backward substitution phase of our solution procedure, we introduce the $L + N(M-1) \times 1$ vector

$$\mathbf{y} = [\mathbf{y}_1^T, \mathbf{y}_2^T, \dots, \mathbf{y}_M^T]^T.$$

The column vectors $\mathbf{y}_k$ for $k = 2, \dots, M$ have dimension $N \times 1$, while the column vector $\mathbf{y}_1$ has dimension $L \times 1$. The forward sweep (i.e. the solution of $\mathbf{L}\mathbf{y} = \mathbf{z}$) produces the following

equations by means of a matrix-vector multiply:

$$\mathbf{y}_1 = \mathbf{z}_1 \quad (3.65)$$

$$\mathbf{L}_k \mathbf{y}_{k-1} + \mathbf{y}_k = \mathbf{z}_k \quad k = 2, \dots, M. \quad (3.66)$$

The backward sweep (i.e. the solution of $\mathbf{U}\mathbf{x} = \mathbf{y}$) then produces the equations

$$\mathbf{U}_k \mathbf{x}_k + \mathbf{B}_k \mathbf{x}_{k+1} = \mathbf{y}_k \quad k = M-1, \dots, 1. \quad (3.67)$$

$$\mathbf{U}_M \mathbf{x}_M = \mathbf{y}_M \quad (3.68)$$

From these equations we can summarize the forward-backward substitution phase of our solution procedure as follows:

- (a) Compute the vector $\mathbf{y}_1 = \mathbf{z}_1$.
- (b) For $k = 2, \dots, M$ compute the vectors $\mathbf{y}_k = \mathbf{z}_k - \mathbf{L}_k \mathbf{y}_{k-1}$.
- (c) Using stored values for the LU factorization of $\mathbf{U}_M$ compute the vector $\mathbf{x}_M$ from

$$\mathbf{U}_M \mathbf{x}_M = \mathbf{y}_M.$$

- (d) For $k = M-1, \dots, 1$, using stored values for the LU factorization of $\mathbf{U}_k$ compute the vector $\mathbf{x}_k$ from

$$\mathbf{U}_k \mathbf{x}_k = \mathbf{y}_k - \mathbf{B}_k \mathbf{x}_{k+1}.$$

Overall, the computational cost of the forward-backward substitution stage is $\mathcal{O}(L^2) + \mathcal{O}((M-1)N^2)$, the dominant contributions coming from the sequence of backsubstitutions to produce $\mathbf{x}_k$ from $\mathbf{U}_k \mathbf{x}_k = \mathbf{y}_k - \mathbf{B}_k \mathbf{x}_{k+1}$ using stored LU-factorizations, as well as the vector-matrix products such as $\mathbf{L}_k \mathbf{y}_{k-1}$ and $\mathbf{B}_k \mathbf{x}_{k+1}$. The forward-backward substitution stage is clearly less expensive than the factorization stage.

3.6 Code Validation

We will use the following non-trivial test case that allows us to examine the convergence rates of our code for potentially highly-oscillatory problems defined on the domain. Using $L = r_b - r_a$ we define the test solution as

$$\begin{aligned} p(r, \theta) = & \left[C_1 e^{\cos(n\theta)} + C_2 e^{\sin(n\theta)} \right] \sin\left(\frac{m\pi}{L}(r_b - r)\right) \\ & + \left[D_1 e^{\cos(n\theta)} + D_2 e^{\sin(n\theta)} \right] \cos\left(\frac{m\pi}{L}(r_b - r)\right), \end{aligned} \quad (3.69)$$

where C_1, C_2, D_1 and D_2 are arbitrary constants. Note that in this test case, the θ -dependence is not trivially resolved by a Fourier representation of the solution and the r -dependence is not trivially resolved with a Chebyshev representation. Differentiating the test solution (3.69) and evaluating that derivative on the boundaries $r = r_a$ and $r = r_b$ produces the needed Neumann boundary conditions for our test case.

$$\frac{\partial p}{\partial r}(r_a, \theta) = -(-1)^m \left(\frac{m\pi}{L}\right) \left[C_1 e^{\cos(n\theta)} + C_2 e^{\sin(n\theta)} \right] \quad (3.70)$$

and

$$\frac{\partial p}{\partial r}(r_b, \theta) = -\left(\frac{m\pi}{L}\right) \left[C_1 e^{\cos(n\theta)} + C_2 e^{\sin(n\theta)} \right]. \quad (3.71)$$

Applying $C_1 = C_2 = 0$ gives classic Neumann conditions (a vanishing function). Applying the ϕ -invariant Laplacian operator in the middle of (3.1) to the test solution in (3.69) gives the data function $f(r, \theta)$ required for the right-hand side of (3.1), hence completing the setup of our test case. The data function may be written as

$$f(r, \theta) = f_c(r, \theta) \cos\left(\frac{m\pi}{L}(r_b - r)\right) + f_s(r, \theta) \sin\left(\frac{m\pi}{L}(r_b - r)\right) \quad (3.72)$$

with

$$f_c(r, \theta) = f_{cc}(r, \theta) e^{\cos(n\theta)} + f_{cs}(r, \theta) e^{\sin(n\theta)} \quad (3.73)$$

and

$$f_s(r, \theta) = f_{sc}(r, \theta)e^{\cos(n\theta)} + f_{ss}(r, \theta)e^{\sin(n\theta)}. \quad (3.74)$$

Finally, the component functions in equations (3.73) and (3.74) are defined as

$$\begin{aligned} f_{cc}(r, \theta) &= -C_1 \left(\frac{m\pi}{L} \right) \frac{R_0 + 2r \cos \theta}{r(R_0 + r \cos \theta)} + D_1 \left[\left(\frac{n}{r} \right)^2 - \left(\frac{m\pi}{L} \right)^2 \right] \\ &+ D_1 \frac{n \sin \theta \sin(n\theta)}{r(R_0 + r \cos \theta)} - D_1 \left(\frac{n}{r} \right)^2 \cos(n\theta) (\cos(n\theta) + 1) \end{aligned} \quad (3.75)$$

$$\begin{aligned} f_{cs}(r, \theta) &= -C_2 \left(\frac{m\pi}{L} \right) \frac{R_0 + 2r \cos \theta}{r(R_0 + r \cos \theta)} + D_2 \left[\left(\frac{n}{r} \right)^2 - \left(\frac{m\pi}{L} \right)^2 \right] \\ &- D_2 \frac{n \sin \theta \cos(n\theta)}{r(R_0 + r \cos \theta)} - D_2 \left(\frac{n}{r} \right)^2 \sin(n\theta) (\sin(n\theta) + 1). \end{aligned} \quad (3.76)$$

$$\begin{aligned} f_{ss}(r, \theta) &= D_2 \left(\frac{m\pi}{L} \right) \frac{R_0 + 2r \cos \theta}{r(R_0 + r \cos \theta)} + C_2 \left[\left(\frac{n}{r} \right)^2 - \left(\frac{m\pi}{L} \right)^2 \right] \\ &- C_2 \frac{n \sin \theta \cos(n\theta)}{r(R_0 + r \cos \theta)} - C_2 \left(\frac{n}{r} \right)^2 \sin(n\theta) (\sin(n\theta) + 1) \end{aligned} \quad (3.77)$$

$$\begin{aligned} f_{sc}(r, \theta) &= D_1 \left(\frac{m\pi}{L} \right) \frac{R_0 + 2r \cos \theta}{r(R_0 + r \cos \theta)} + C_1 \left[\left(\frac{n}{r} \right)^2 - \left(\frac{m\pi}{L} \right)^2 \right] \\ &+ C_1 \frac{n \sin \theta \sin(n\theta)}{r(R_0 + r \cos \theta)} - C_1 \left(\frac{n}{r} \right)^2 \cos(n\theta) (\cos(n\theta) + 1) \end{aligned} \quad (3.78)$$

With $f(r, \theta)$ so defined, the solution to the Poisson Neumann problem with boundary conditions (3.70) and (3.71) must have solution $p(r, \theta)$ given by equation (3.69).

In this section the estimated maximum relative errors e_{max} are given by

$$e_{max} = \frac{\max_{k,m} \left| (p_{k,m}^{(exact)} - \bar{p}^{(exact)}) - (p_{k,m}^{(comp)} - \bar{p}^{(comp)}) \right|}{\max_{k,m} \left| p_{k,m}^{(exact)} - \bar{p}^{(exact)} \right|}, \quad (3.79)$$

N_θ	N_r	$\bar{p}^{(exact)}$	$\bar{p}^{(comp)}$	e_{max}	$ C $
2^4	2^4	3.36×10^{-1}	-1.79×10^{-1}	2.91×10^{-2}	2.11×10^{-2}
	2^5	3.36×10^{-1}	-1.79×10^{-1}	3.11×10^{-2}	1.73×10^{-12}
	2^6	3.36×10^{-1}	-1.79×10^{-1}	3.06×10^{-2}	1.60×10^{-12}
	2^7	3.36×10^{-1}	-1.79×10^{-1}	3.07×10^{-2}	7.62×10^{-13}
2^5	2^4	3.36×10^{-1}	-1.81×10^{-1}	4.21×10^{-4}	2.11×10^{-2}
	2^5	3.36×10^{-1}	-1.81×10^{-1}	5.26×10^{-5}	3.20×10^{-13}
	2^6	3.36×10^{-1}	-1.81×10^{-1}	5.17×10^{-5}	4.68×10^{-13}
	2^7	3.36×10^{-1}	-1.81×10^{-1}	5.18×10^{-5}	1.11×10^{-12}
2^6	2^4	3.36×10^{-1}	-1.81×10^{-1}	4.19×10^{-4}	2.11×10^{-2}
	2^5	3.36×10^{-1}	-1.81×10^{-1}	1.00×10^{-11}	1.15×10^{-12}
	2^6	3.36×10^{-1}	-1.81×10^{-1}	1.00×10^{-11}	1.20×10^{-12}
	2^7	3.36×10^{-1}	-1.81×10^{-1}	9.91×10^{-12}	2.49×10^{-13}
2^7	2^4	3.36×10^{-1}	-1.81×10^{-1}	4.20×10^{-4}	2.11×10^{-2}
	2^5	3.36×10^{-1}	-1.81×10^{-1}	1.68×10^{-13}	2.29×10^{-12}
	2^6	3.36×10^{-1}	-1.81×10^{-1}	4.49×10^{-13}	1.13×10^{-12}
	2^7	3.36×10^{-1}	-1.81×10^{-1}	2.02×10^{-13}	3.07×10^{-13}

Table 3.1: Relative error e_{max} , absolute value of the compatibility constant C and estimated area averages of the solution $\bar{p}$ for various mesh densities. The domain parameters used in this case are $R_0 = 3$, $r_a = 1$ and $r_b = 2$. The parameters defining the test solution are $m = 5$, $n = 7$ and $C_1 = C_2 = D_1 = D_2 = 1$.

where the cross-sectional area average is

$$\bar{p} = \frac{1}{R_0\pi(r_b^2 - r_a^2)} \int_{-\pi}^{\pi} \int_{r_a}^{r_b} p(r, \theta) r h_\phi dr d\theta. \quad (3.80)$$

Values of the cross-sectional average are estimated to high-order using function values on the computational grids for both the computed and exact solutions. In particular our procedure for estimating the double integral uses a high-order trapezoid estimate in the θ -variable followed by a high-order Chebyshev estimate in the r -variable. We stress here that these averages need to be computed so that the computed and test solutions can both be normalized (as per the terms in the error calculation (3.79)) for an apples-to-apples comparison. As discussed earlier in this section, our procedure for computing the solution will in general result in a different average value than the test case (3.69).

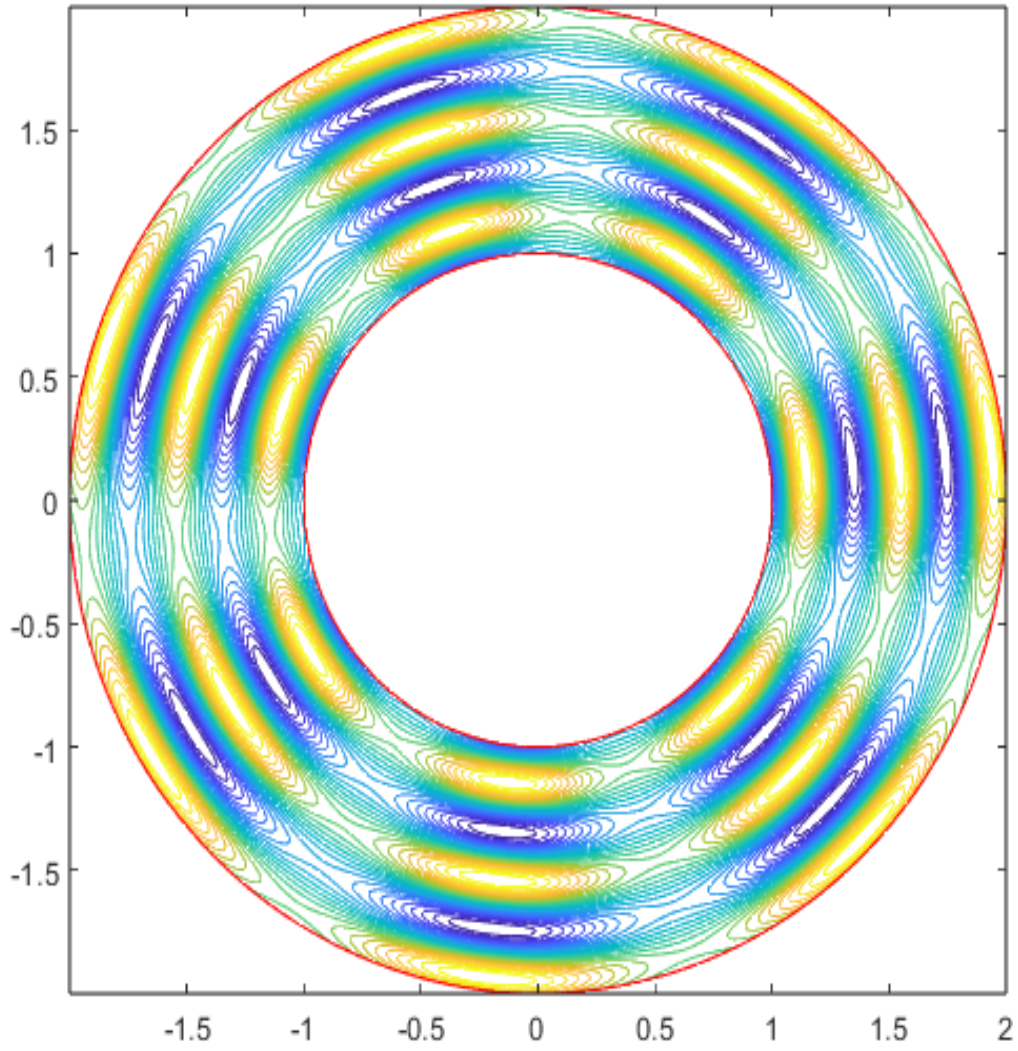


Figure 3.1: Solution contour plot. The domain parameters used in this case are $R_0 = 3$, $r_a = 1$ and $r_b = 2$. The parameters defining the test solution are $m = 5$, $n = 7$ and $C_1 = C_2 = D_1 = D_2 = 1$.

Chapter 4

Poisson Solvers in Three Spatial Dimensions

4.1 Description of the Problem

This chapter concerns itself with the development and testing of solvers for the Poisson problem in toroidal coordinates when the solution $p = p(r, \theta, \phi)$ is a function of all three spatial variables, i.e.,

$$\nabla^2 p = f(r, \theta, \phi). \quad (4.1)$$

The Laplacian operator in toroidal coordinates is defined as

$$\nabla^2 p = \frac{\partial^2 p}{\partial r^2} + \left(\frac{1}{r} + \frac{\cos \theta}{h_\phi} \right) \frac{\partial p}{\partial r} - \frac{\sin \theta}{r h_\phi} \frac{\partial p}{\partial \theta} + \frac{1}{r^2} \frac{\partial^2 p}{\partial \theta^2} + \frac{1}{h_\phi^2} \frac{\partial^2 p}{\partial \phi^2}. \quad (4.2)$$

As usual, the quantity $h_\phi = R_0 + r \cos \theta$ is the ϕ scale factor (see Appendix A for more details). In order to accommodate Neumann boundary conditions, we actually solve the augmented problem below. Much of this chapter is similar in content to the previous chapter and we will omit some of the details here, to avoid duplication.

Our method calls for the solution of the augmented problem

$$\nabla^2 p = f(r, \theta, \phi) + C, \quad (4.3)$$

where the constant C ensures compatibility between the function f and the Neumann boundary conditions, and is found as part of our solution procedure for that case.

4.2 Algorithm Development

We rewrite the original problem in the following equivalent form

$$r^2 h_\phi^2 \frac{\partial^2 p}{\partial r^2} + r h_\phi (h_\phi + r \cos \theta) \frac{\partial p}{\partial r} - r h_\phi \sin \theta \frac{\partial p}{\partial \theta} + h_\phi^2 \frac{\partial^2 p}{\partial \theta^2} + r^2 \frac{\partial^2 p}{\partial \phi^2} = r^2 h_\phi^2 f(r, \theta, \phi) + r^2 h_\phi^2 C \quad (4.4)$$

This operator on the left-hand side of this partial differentiable equation is not separable in the r - and θ -coordinates, but, as we will see, it *is* separable in the ϕ -coordinate which leads to significant efficiencies in our solution procedure. Given the periodicity of the problem in the θ - and ϕ -directions, we assume the following Fourier series expansion for the unknown function $p = p(r, \theta, \phi)$:

$$p(r, \theta, \phi) = \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} p_{m,n}(r) e^{i(m\theta+n\phi)} \quad (4.5)$$

While we determine the functions $p_{m,n}(r)$ in equation (4.5) by means of the numerical procedures developed in this chapter, it should be clear that they are related to the solution $p(r, \theta, \phi)$ by the two dimensional discrete Fourier transform:

$$p_{m,n}(r) = \frac{1}{(2\pi)^2} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} p(r, \theta, \phi) e^{-i(m\theta+n\phi)} d\theta d\phi \quad (4.6)$$

As indicated, the coefficients $p_{m,n}(r)$ remain a function of the radial coordinate, r . A similar expansion is assumed for the right-hand side of (4.4), i.e.,

$$r^2 h_\phi^2 f(r, \theta, \phi) = \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} f_{m,n}(r) e^{i(m\theta+n\phi)}. \quad (4.7)$$

Substitution of the Fourier expansions (4.5) and (4.7) results in

$$\sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} \mathcal{L}_{m,n} p_{m,n}(r) e^{i(m\theta+n\phi)} = \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} f_{m,n}(r) e^{i(m\theta+n\phi)} + r^2 h_\phi^2 C \quad (4.8)$$

where we define the ordinary differential operator $\mathcal{L}_{m,n}$ as

$$\begin{aligned} \mathcal{L}_{m,n} p_{m,n}(r) &= r^2 h_\phi^2 p_{m,n}''(r) + r h_\phi (h_\phi + r \cos \theta) p_{m,n}'(r) \\ &- (imr h_\phi \sin \theta + m^2 h_\phi^2 + n^2 r^2) p_{m,n}(r) \end{aligned} \quad (4.9)$$

We immediately note that this operator is not a function of ϕ so the problem is separable in this coordinate. We also note the symmetry $\mathcal{L}_{m,-n} = \mathcal{L}_{m,n}$, which implies that discrete versions of this operator only need to be constructed for positive n , resulting in substantial memory savings. Specifically, standard trigonometric orthogonality relations in the ϕ -variable lead to the sequence of problems

$$\sum_{m=-\infty}^{\infty} \mathcal{L}_{m,n} p_{m,n}(r) e^{im\theta} = \sum_{m=-\infty}^{\infty} f_{m,n}(r) e^{im\theta} + r^2 h_\phi^2 C \delta_{n,0} \quad (4.10)$$

where we denote the Kronecker delta symbol as $\delta_{m,n}$. The system (4.10) must be solved for all positive and negative integers, n . The case $n = 0$ is singular and is dealt with using the solvers in the previous chapter. In what follows, we assume $n \neq 0$ and drop the second term on the right-hand side of equation (4.10); indeed, compatibility conditions do not need to be considered for these cases.

Next, to extract a system of ordinary differential equations for $p_{m,n}(r)$, we apply standard orthogonality relations to the expression (4.10). As a result of the dependence of the left-hand

side on θ , this process results in a coupled pentadiagonal system of equations. The following identities are easily established:

$$\frac{1}{\pi} \int_{-\pi}^{\pi} e^{i(m-\ell)\theta} d\theta = 2\delta_{m,\ell} \quad (4.11)$$

$$\frac{1}{\pi} \int_{-\pi}^{\pi} \cos \theta e^{i(m-\ell)\theta} d\theta = \delta_{m,\ell+1} + \delta_{m,\ell-1} \quad (4.12)$$

$$\frac{1}{\pi} \int_{-\pi}^{\pi} \sin \theta e^{i(m-\ell)\theta} d\theta = i\delta_{m,\ell+1} - i\delta_{m,\ell-1} \quad (4.13)$$

$$\frac{1}{\pi} \int_{-\pi}^{\pi} \cos^2 \theta e^{i(m-\ell)\theta} d\theta = \delta_{m,\ell} + \frac{1}{2}\delta_{m,\ell+1} + \frac{1}{2}\delta_{m,\ell-1} \quad (4.14)$$

$$\frac{1}{\pi} \int_{-\pi}^{\pi} \cos \theta \sin \theta e^{i(m-\ell)\theta} d\theta = \frac{i}{2}\delta_{m,\ell+2} - \frac{i}{2}\delta_{m,\ell-2} \quad (4.15)$$

This leads to the following coupled system of ordinary differential equations

$$\begin{aligned} & L_{m,n}^{(1)} p_{m-2,n}(r) + L_{m,n}^{(2)} p_{m-1,n}(r) + L_{m,n}^{(3)} p_{m,n}(r) + L_{m,n}^{(4)} p_{m+1,n}(r) + L_{m,n}^{(5)} p_{m+2,n}(r) \\ &= 2f_{m,n}(r) \end{aligned} \quad (4.16)$$

where the linear differential operators $L_{m,n}^{(k)}$ for $k = 1, \dots, 5$ are given by

$$L_{m,n}^{(1)} = \frac{r^2}{2} \left(r^2 \frac{d^2}{dr^2} + 2r \frac{d}{dr} - (m-1)(m-2) \right) \quad (4.17)$$

$$L_{m,n}^{(2)} = 2rR_0 \left(r^2 \frac{d^2}{dr^2} + \frac{3}{2}r \frac{d}{dr} - \frac{1}{2}(2m-1)(m-1) \right) \quad (4.18)$$

$$L_{m,n}^{(3)} = r^2 (2R_0^2 + r^2) \frac{d^2}{dr^2} + 2r (R_0^2 + r^2) \frac{d}{dr} - ((2R_0^2 + r^2)m^2 + 2r^2n^2) \quad (4.19)$$

$$L_{m,n}^{(4)} = 2rR_0 \left(r^2 \frac{d^2}{dr^2} + \frac{3}{2}r \frac{d}{dr} - \frac{1}{2}(2m+1)(m+1) \right) \quad (4.20)$$

$$L_{m,n}^{(5)} = \frac{r^2}{2} \left(r^2 \frac{d^2}{dr^2} + 2r \frac{d}{dr} - (m+1)(m+2) \right) \quad (4.21)$$

We now obtain a discrete formulation of these operators. Consider an N -term Chebyshev expansion of a differentiable function $f(r)$ of the form (3.45) with Chebyshev coefficients stored in the N -element vector (3.48). The Chebyshev coefficients of $L_{m,n}^{(1)}f(r)$, $L_{m,n}^{(2)}f(r)$,

$L_{m,n}^{(3)}f(r)$, $L_{m,n}^{(4)}f(r)$ and $L_{m,n}^{(5)}f(r)$ are given by the vector- matrix products $\mathbf{L}_{m,n}^{(1)}\mathbf{a}$, $\mathbf{L}_{m,n}^{(2)}\mathbf{a}$, $\mathbf{L}_{m,n}^{(3)}\mathbf{a}$, $\mathbf{L}_{m,n}^{(4)}\mathbf{a}$ and $\mathbf{L}_{m,n}^{(5)}\mathbf{a}$, respectively, where

$$\mathbf{L}_{m,n}^{(1)} = \frac{1}{2}\mathcal{R}^2 \left(\mathcal{R}^2\mathcal{D}^2 + 2\mathcal{R}\mathcal{D} - (m-1)(m-2)\mathbf{I} \right) \quad (4.22)$$

$$\mathbf{L}_{m,n}^{(2)} = 2R_0\mathcal{R} \left(\mathcal{R}^2\mathcal{D}^2 + \frac{3}{2}\mathcal{R}\mathcal{D} - \frac{1}{2}(2m-1)(m-1)\mathbf{I} \right) \quad (4.23)$$

$$\mathbf{L}_{m,n}^{(3)} = \left(2R_0^2\mathcal{R}^2 + \mathcal{R}^4 \right) \mathcal{D}^2 + 2 \left(R_0^2\mathcal{R} + \mathcal{R}^3 \right) \mathcal{D} - (m^2 + 2n^2)\mathcal{R}^2 - 2m^2R_0^2\mathbf{I} \quad (4.24)$$

$$\mathbf{L}_{m,n}^{(4)} = 2R_0\mathcal{R} \left(\mathcal{R}^2\mathcal{D}^2 + \frac{3}{2}\mathcal{R}\mathcal{D} - \frac{1}{2}(2m-1)(m-1)\mathbf{I} \right) \quad (4.25)$$

$$\mathbf{L}_{m,n}^{(5)} = \frac{1}{2}\mathcal{R}^2 \left(\mathcal{R}^2\mathcal{D}^2 + 2\mathcal{R}\mathcal{D} - (m-1)(m-2)\mathbf{I} \right) \quad (4.26)$$

Note that we define $\mathbf{I}$ as the $N \times N$ identity matrix.

4.3 Fully Discrete Representation of the Solution and Resulting Discrete Neumann Problem

With a Fourier representation in the θ - and ϕ -variables and a Chebyshev representation in the r -variable the unknown function $p(r, \theta, \phi)$ and $r^2h_\phi^2f(r, \theta, \phi)$, the right-hand side of the augmented problem (4.4), become

$$p(r, \theta, \phi) \approx \sum_{m=-N_\theta}^{N_\theta} \sum_{n=-N_\phi}^{N_\phi} \left(\sum_{k=0}^{N_r-1} \hat{p}_{k,m,n} T_k(\xi) \right) e^{i(m\theta+n\phi)} \quad (4.27)$$

and

$$r^2h_\phi^2f(r, \theta, \phi) \approx \sum_{m=-N_\theta}^{N_\theta} \sum_{n=-N_\phi}^{N_\phi} \left(\sum_{k=0}^{N_r-1} \hat{f}_{k,m,n} T_k(\xi) \right) e^{i(m\theta+n\phi)} \quad (4.28)$$

for $r \in [r_a, r_b]$, $\phi \in [0, 2\pi)$ and $\theta \in [0, 2\pi)$. Recall that with A and B defined as in (3.43) we have $r = A\xi + B$ for $\xi \in [-1, 1]$. As discussed in preceding sections, if the functions $p(r, \theta, \phi)$ and $r^2h_\phi^2f(r, \theta, \phi)$ are infinitely differentiable in the r -, θ - and ϕ -variables (as is

the case for the problems we examine in this thesis), then the expansions (4.27) and (4.28) will experience super-algebraic convergence in N_r , N_θ and N_ϕ . Such expansions allow us to obtain an extremely high resolution of the solution of the Poisson problem p with very small numbers of unknowns.

As detailed in this section, our Poisson solver assumes expansions of the form (4.27) and (4.28) and solves the Poisson Neumann problem for the unknown spectral coefficients $\hat{p}_{k,m,n}$. Assuming a spatial sampling $p_{k,m,n} = p(r_k, \theta_m, \phi_n)$ for r_k on the N_r -point Chebyshev grid (3.44), θ_m on the $2M_\theta + 1$ -point Fourier grid (3.33), and ϕ_n on the $2M_\phi + 1$ Fourier grid, the spectral coefficients may be obtained to high accuracy by means of a sequence of normalized Chebyshev transforms and Fourier transforms executed in parallel.

The boundary conditions to be enforced in the Neumann case are, for each Fourier mode m and n ,

$$\sum_{k=0}^{N_r-1} k^2 \hat{p}_{k,m,n} \quad (4.29)$$

and

$$\sum_{k=0}^{N_r-1} (-1)^k k^2 \hat{p}_{k,m,n}. \quad (4.30)$$

The discrete operators (4.22), (4.23), (4.24), (4.25) and (4.26) together with the Boundary conditions (4.29) and (4.30) and result in a sparse block pentadiagonal system of equations for both the real and imaginary parts of the solution $\hat{p}_{k,m,m}$. In the following sections give details on the development and implementaton of such a sparse matrix solver.

4.4 A Block Pentadiagonal Sparse Matrix Solver

The Poisson solver developed in this chapter requires the solution of block pentadiagonal linear systems of equations of the form

$$\mathbf{Ax} = \mathbf{z},$$

where

$$\mathbf{x} = [\mathbf{x}_1^T, \mathbf{x}_2^T, \dots, \mathbf{x}_M^T]^T, \quad \mathbf{z} = [\mathbf{z}_1^T, \mathbf{z}_2^T, \dots, \mathbf{z}_M^T]^T,$$

and

$$\mathbf{A} = \begin{bmatrix} \mathbf{A}_1 & \mathbf{B}_1 & \mathbf{C}_1 & & & \\ \mathbf{D}_2 & \mathbf{A}_2 & \mathbf{B}_2 & \mathbf{C}_2 & & \\ \mathbf{E}_3 & \mathbf{D}_3 & \mathbf{A}_3 & \mathbf{B}_3 & \mathbf{C}_3 & \\ & \ddots & \ddots & \ddots & \ddots & \ddots \\ & & \mathbf{E}_{M-2} & \mathbf{D}_{M-2} & \mathbf{A}_{M-2} & \mathbf{B}_{M-2} & \mathbf{C}_{M-2} \\ & & & \mathbf{E}_{M-1} & \mathbf{D}_{M-1} & \mathbf{A}_{M-1} & \mathbf{B}_{M-1} \\ & & & & \mathbf{E}_M & \mathbf{D}_M & \mathbf{A}_M \end{bmatrix}.$$

Each of the block matrices $\mathbf{A}_k$, $\mathbf{B}_k$, $\mathbf{C}_k$, $\mathbf{D}_k$ and $\mathbf{E}_k$, $k = 1, \dots, M$ have dimension $N \times N$. The column vectors $\mathbf{x}_k$ and $\mathbf{z}_k$, $k = 1, \dots, M$ have dimension $N \times 1$. The $NM \times NM$ matrix $\mathbf{A}$ consists of zero elements excepts for the 5 main block diagonal matrices. The matrix $\mathbf{A}$ has the following **LU** factorization:

$$\mathbf{A} = \begin{bmatrix} \mathbf{I} & & & & & \\ \mathbf{L}_2 & \mathbf{I} & & & & \\ \mathbf{M}_3 & \mathbf{L}_3 & \mathbf{I} & & & \\ & \ddots & \ddots & \ddots & & \\ & & \mathbf{M}_{M-1} & \mathbf{L}_{M-1} & \mathbf{I} & \\ & & & \mathbf{M}_M & \mathbf{L}_M & \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{U}_1 & \mathbf{Q}_1 & \mathbf{C}_1 & & & \\ & \mathbf{U}_2 & \mathbf{Q}_2 & \mathbf{C}_2 & & \\ & & \ddots & \ddots & \ddots & \\ & & & \mathbf{U}_{M-2} & \mathbf{Q}_{M-2} & \mathbf{C}_{M-2} \\ & & & & \mathbf{U}_{M-1} & \mathbf{Q}_{M-1} \\ & & & & & \mathbf{U}_M \end{bmatrix}.$$

In compact notation, we rewrite this last expression as $\mathbf{A} = \mathbf{LU}$. Each of the block matrices $\mathbf{L}_k$, $\mathbf{U}_k$, $\mathbf{M}_k$, $\mathbf{Q}_k$, $k = 1, \dots, M$ have dimension $N \times N$. We also denote $\mathbf{I}$ as the $N \times N$ identity matrix.

Multiplying out the **LU** factorization and matching elements with those in the expression for

$\mathbf{A}$ leads to the following matrix equations:

$$\mathbf{U}_1 = \mathbf{A}_1 \quad (4.31)$$

$$\mathbf{Q}_1 = \mathbf{B}_1 \quad (4.32)$$

$$\mathbf{L}_2 \mathbf{Q}_1 + \mathbf{U}_2 = \mathbf{A}_2 \quad (4.33)$$

$$\mathbf{L}_2 \mathbf{C}_1 + \mathbf{Q}_2 = \mathbf{B}_2 \quad (4.34)$$

$$\mathbf{L}_2 \mathbf{U}_1 = \mathbf{D}_2 \quad (4.35)$$

For $i = 3, \dots, M - 1$ we have

$$\mathbf{M}_i \mathbf{C}_{i-2} + \mathbf{L}_i \mathbf{Q}_{i-1} + \mathbf{U}_i = \mathbf{A}_i \quad (4.36)$$

$$\mathbf{L}_i \mathbf{C}_{i-1} + \mathbf{Q}_i = \mathbf{B}_i \quad (4.37)$$

$$\mathbf{M}_i \mathbf{Q}_{i-2} + \mathbf{L}_i \mathbf{U}_{i-1} = \mathbf{D}_i \quad (4.38)$$

$$\mathbf{M}_i \mathbf{U}_{i-2} = \mathbf{E}_i \quad (4.39)$$

Finally the last set of equations is

$$\mathbf{M}_M \mathbf{C}_{M-2} + \mathbf{L}_M \mathbf{Q}_{M-1} + \mathbf{U}_M = \mathbf{A}_M \quad (4.40)$$

$$\mathbf{M}_M \mathbf{Q}_{M-2} + \mathbf{L}_M \mathbf{U}_{M-1} = \mathbf{D}_M \quad (4.41)$$

$$\mathbf{M}_M \mathbf{U}_{M-2} = \mathbf{E}_M \quad (4.42)$$

From these equations we derive the following sequence of steps in our factorization phase of the solution procedure:

- (a) Factor $\mathbf{U}_1 = \mathbf{A}_1$ and determine the rows of $\mathbf{L}_2$ from

$$\mathbf{U}_1^T \mathbf{L}_2^T = \mathbf{D}_2^T.$$

Options in LAPACK allow for the solution of the problem in this form based on the LU-factorization of $\mathbf{U}_1$ alone. The factorization of $\mathbf{U}_1$ and its pivots should be stored for later use in the substitution phase; see below.

- (b) Determine the matrix $\mathbf{Q}_2$ from

$$\mathbf{Q}_2 = \mathbf{B}_2 - \mathbf{L}_2 \mathbf{C}_1.$$

- (c) Using $\mathbf{Q}_1 = \mathbf{B}_1$ Determine the matrix $\mathbf{U}_2$ from

$$\mathbf{U}_2 = \mathbf{A}_2 - \mathbf{L}_2 \mathbf{Q}_1.$$

Compute the LU factorization of $\mathbf{U}_2$ and store the results. Discard $\mathbf{U}_2$?

- (d) For $k = 3, \dots, M - 1$ do:

- (i) Using the stored factorization for $\mathbf{U}_{k-2}$, compute the rows of $\mathbf{M}_k$ from

$$\mathbf{U}_{k-2}^T \mathbf{M}_k^T = \mathbf{E}_k^T.$$

- (ii) Using the stored factorization for $\mathbf{U}_{k-1}$, compute $\mathbf{L}_k$ from

$$\mathbf{U}_{k-1}^T \mathbf{L}_k^T = (\mathbf{D}_k - \mathbf{M}_k \mathbf{Q}_{k-2})^T.$$

- (iii) Determine the matrix $\mathbf{Q}_k$ from

$$\mathbf{Q}_k = \mathbf{B}_k - \mathbf{L}_k \mathbf{C}_{k-1}.$$

- (iv) Determine the matrix $\mathbf{U}_k$ from

$$\mathbf{U}_k = \mathbf{A}_k - \mathbf{L}_k \mathbf{Q}_{k-1} - \mathbf{M}_k \mathbf{C}_{k-2}.$$

Compute the LU factorization of $\mathbf{U}_k$ and store the results. Discard $\mathbf{U}_k$?

(e) Using the stored factorization for $\mathbf{U}_{M-2}$, compute the rows of $\mathbf{M}_M$ from

$$\mathbf{U}_{M-2}^T \mathbf{M}_M^T = \mathbf{E}_M^T.$$

(f) Using the stored factorization for $\mathbf{U}_{M-1}$, compute $\mathbf{L}_M$ from

$$\mathbf{U}_{M-1}^T \mathbf{L}_M^T = (\mathbf{D}_M - \mathbf{M}_M \mathbf{Q}_{M-2})^T.$$

(g) Determine the matrix $\mathbf{U}_M$ from

$$\mathbf{U}_M = \mathbf{A}_M - \mathbf{L}_M \mathbf{Q}_{M-1} - \mathbf{M}_M \mathbf{C}_{M-2}.$$

Compute the LU factorization of $\mathbf{U}_M$ and store the results. Discard $\mathbf{U}_M$?

Moving on to the details of the forward/backward substitution phase of our solution procedure, we introduce the $N \times 1$ vector

$$\mathbf{y} = [\mathbf{y}_1^T, \mathbf{y}_2^T, \dots, \mathbf{y}_M^T]^T.$$

The forward sweep (i.e. the solution of $\mathbf{L}\mathbf{y} = \mathbf{z}$) produces the following equations by means of a matrix-vector multiply on the right-hand side:

$$\mathbf{y}_1 = \mathbf{z}_1 \tag{4.43}$$

$$\mathbf{L}_2 \mathbf{y}_1 + \mathbf{y}_2 = \mathbf{z}_2 \tag{4.44}$$

$$\mathbf{M}_k \mathbf{y}_{k-2} + \mathbf{L}_k \mathbf{y}_{k-1} + \mathbf{y}_k = \mathbf{z}_k \quad k = 3, \dots, M. \tag{4.45}$$

The backward sweep (i.e. the solution of $\mathbf{U}\mathbf{x} = \mathbf{y}$) then produces the equations

$$\mathbf{U}_k \mathbf{x}_k + \mathbf{Q}_k \mathbf{x}_{k+1} + \mathbf{C}_k \mathbf{x}_{k+2} = \mathbf{y}_k \quad k = M-2, \dots, 1. \quad (4.46)$$

$$\mathbf{U}_{M-1} \mathbf{x}_{M-1} + \mathbf{Q}_{M-1} \mathbf{x}_M = \mathbf{y}_{M-1} \quad (4.47)$$

$$\mathbf{U}_M \mathbf{x}_M = \mathbf{y}_M \quad (4.48)$$

From these equations we can summarize the forward-backward substitution phase of our solution procedure as follows:

- (a) Compute the vector $\mathbf{y}_1 = \mathbf{z}_1$.
- (b) Compute the vector $\mathbf{y}_2 = \mathbf{z}_2 - \mathbf{L}_2 \mathbf{y}_1$.
- (c) For $k = 3, \dots, M$ compute the vectors $\mathbf{y}_k = \mathbf{z}_k - \mathbf{L}_k \mathbf{y}_{k-1} - \mathbf{M}_k \mathbf{y}_{k-2}$.
- (d) Using stored values for the LU factorization of $\mathbf{U}_M$ compute the vector $\mathbf{x}_M$ from

$$\mathbf{U}_M \mathbf{x}_M = \mathbf{y}_M.$$

- (e) Using stored values for the LU factorization of $\mathbf{U}_{M-1}$ compute the vector $\mathbf{x}_{M-1}$ from

$$\mathbf{U}_{M-1} \mathbf{x}_{M-1} = \mathbf{y}_{M-1} - \mathbf{Q}_{M-1} \mathbf{x}_M.$$

- (f) For $k = M-2, \dots, 1$, using stored values for the LU factorization of $\mathbf{U}_k$ compute the vector $\mathbf{x}_k$ from

$$\mathbf{U}_k \mathbf{x}_k = \mathbf{y}_k - \mathbf{Q}_k \mathbf{x}_{k+1} - \mathbf{C}_k \mathbf{x}_{k+2}.$$

4.5 Parallel implementation

Several parts of this (and the previous) Poisson solver in three dimensions can run in parallel. We first describe some details of OpenMP and the workstation used to implement the code

and then describe all the instances in which parallel programming is used because this is a key feature of our work.

Open Multi-Processing (OpenMP) is one of the most common programming frameworks used to implement shared-memory parallelism. Shared-memory parallelism assumes that processors have equal access to shared memory [84] covering the whole or a part of the operating memory of a parallel computer [85]. The threads executed in parallel can operate on both the shared data and private data. The workstation used comprised thirty-two processors each with two threads. The model name of the processors is Intel® Xeon® Processor E5-2620 v4 @ 2.10GHz. Finally, we note that using all sixty-four threads is no different to using thirty-two threads because of hardware restrictions. That said, our workstation speeds up the code roughly thirty-two times that without parallel implementation.

The work done and ideas used for the two-dimensional Poisson solver comes into focus when organising the terms on the left-hand side of the three-dimensional Poisson solver.

Recall that the terms on the left-hand side of the two-dimensional Poisson solver could be arranged into a block tri-diagonal matrix. We can construct a similar structure in three dimensions but the extra dimension, which arises from the ϕ variable, requires extra consideration.

For each Fourier mode corresponding to the ϕ variable, we have a block penta-diagonal matrix with each block tri-diagonal. In other words, for each Fourier mode corresponding to the ϕ variable, we have a case similar to the two-dimensional Poisson solver. Each of these block penta-diagonal matrices' LU decomposition can be constructed in parallel according to the aforementioned algorithm. Similarly, the corresponding right-hand side can be constructed in parallel.

We note here that only half the Fourier modes corresponding to the ϕ variable need to be calculated. The remaining Fourier modes can be deduced by the conjugate pairs present in two-dimensional Fourier series (See Appendix B) and further reduces the computational cost.

4.6 Code Validation

To simplify matters, we will use a basic separated trial solution of the form

$$p(r, \theta, \phi) = v(r, \theta) e^{\cos(b\phi)} e^{\sin(q\phi)}, \quad (4.49)$$

where p and q are integers which ensures the 2π -periodicity of the solution in the ϕ -variable.

In this way, the Laplacian acting on our assumed solution becomes

$$\nabla^2 p = \left(f(r, \theta) + \frac{g(\phi)}{h_\phi^2} v(r, \theta) \right) e^{\cos(b\phi)} e^{\sin(q\phi)} \quad (4.50)$$

where

$$g(\phi) = (q \cos(q\phi) - b \sin(b\phi))^2 - b^2 \cos(b\phi) - q^2 \sin(q\phi) \quad (4.51)$$

and

$$\frac{1}{rh_\phi} \frac{\partial}{\partial r} \left(rh_\phi \frac{\partial v}{\partial r} \right) + \frac{1}{r^2 h_\phi} \frac{\partial}{\partial \theta} \left(h_\phi \frac{\partial v}{\partial \theta} \right) = f(r, \theta) \quad (4.52)$$

Clearly, this allows us to recycle the trial solutions from the two dimensional case in the previous chapter. In what follows, we will use for the functions $v(r, \theta)$ the function $p(r, \theta)$ as defined in equation (3.69). Neumann boundary conditions for this test case are:

$$\frac{\partial p}{\partial r}(r_a, \theta, \phi) = -(-1)^m \left(\frac{m\pi}{L} \right) [C_1 e^{\cos(n\theta)} + C_2 e^{\sin(n\theta)}] e^{\cos(b\phi)} e^{\sin(q\phi)} \quad (4.53)$$

and

$$\frac{\partial p}{\partial r}(r_b, \theta, \phi) = - \left(\frac{m\pi}{L} \right) [C_1 e^{\cos(n\theta)} + C_2 e^{\sin(n\theta)}] e^{\cos(b\phi)} e^{\sin(q\phi)}. \quad (4.54)$$

Chapter 5

Velocity solvers

5.1 Description of the problem

A main part of the numerical implementation of either the projection method or the pressure Poisson formulation is the development of a solver that calculates the velocity, $\mathbf{u}$, using the momentum equations with its prescribed initial and boundary conditions. We begin by stating the momentum equations in (5.1) with Dirichlet boundary conditions in (5.2) for a flow that starts from rest.

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} = \frac{1}{Re} \nabla^2 \mathbf{u} \quad (5.1)$$

$$\begin{aligned} \mathbf{u}(r = r_b, \theta, \phi) &= 0 \\ \mathbf{u}(r = r_a, \theta, \phi) &= g(r, \theta) \end{aligned} \quad (5.2)$$

We choose the boundary conditions in (5.2) to reflect the first physical case for which we are interested. The boundary conditions describe a stationary outer torus and an inner torus that is rotated at a fixed angular velocity in the ϕ -direction. However, in general, the boundary

conditions can be any sufficiently continuous function of r , θ and ϕ .

There are two main approaches to solve for the velocity, $\mathbf{u}$, in (5.1): explicit methods and semi-implicit methods. Fully implicit methods are generally avoided because they are notoriously difficult to implement because of the non-linear advection terms.

5.2 Explicit methods

We begin with the explicit methods because they are the simpler of the two approaches. Explicit methods allow us to consider the momentum equations as follows.

$$\frac{\partial \mathbf{u}}{\partial t} = \mathbf{F}(\mathbf{u}, t) \quad (5.3)$$

In discretised form,

$$\frac{\mathbf{u}^{n+1} - \mathbf{u}^n}{\Delta t} = F(\mathbf{u}^n, t^n) \quad (5.4)$$

where n and $n + 1$ indicate the current and next time levels respectively and $\mathbf{F}(\mathbf{u}, t)$ comprises the advection and diffusion terms.

Among the explicit methods, the simplest is the Euler method. However, the Euler method is not only conditionally stable for the momentum equations but also faces additional stability concerns for the moderate to high Reynolds numbers we are interested in investigating.

5.2.1 Fourth order Runge-Kutta method

While there are a myriad of other explicit methods to consider, we restrict our attention to the famous Runge-Kutta fourth-order (RK4) method [86]. The classic RK4 method is more appropriate for (5.1) and has been documented [87] [78] in previous implementations of similar numerical solvers. While the stability of the RK4 method is not unconditional, it is unaffected by higher Reynolds numbers unlike the Euler method. Finally, the RK4 method

is easy to implement numerically while not as computationally taxing as the Euler method and provides sufficient temporal accuracy so as to not render our efforts in spatial accuracy entirely unwarranted. For the differential equation in (5.1), the RK4 method updates the velocity as follows.

$$\mathbf{u}^{n+1} = \mathbf{u}^n + \frac{\Delta t}{6}(k_1 + 2k_2 + 2k_3 + k_4) \quad (5.5)$$

where

$$\begin{aligned} k_1 &= \mathbf{F}(t^n, \mathbf{u}^n) \\ k_2 &= \mathbf{F}\left(t^n + \frac{\Delta t}{2}, \mathbf{u}^n + \frac{1}{2}\Delta t k_1\right) \\ k_3 &= \mathbf{F}\left(t^n + \frac{\Delta t}{2}, \mathbf{u}^n + \frac{1}{2}\Delta t k_2\right) \\ k_4 &= \mathbf{F}(t^n + \Delta t, \mathbf{u}^n + \Delta t k_3) \end{aligned} \quad (5.6)$$

5.3 Semi-implicit methods

Semi-implicit schemes often opt to keep the numerical challenging advective terms at the explicit time level, n , and advance the diffusive terms to the implicit time level, $n + 1$. The resulting discretisation from a semi-implicit scheme can be solved using alternating direction implicit (ADI) techniques.

These ADI techniques are also called time-splitting methods and refer to a set of numerical methods that split the time operator of a given differential equation into two or more pieces. Another interpretation is that these numerical methods perform two or more stages of calculation between the current time step, n , and the next time step, $n + 1$. Time-splitting methods allow multi-dimensional differential equations to be solved with a series of one-dimensional finite difference equations which is more computationally efficient than iterative methods.

McDonough [88] presents three categories of time-splitting methods that may be used for finite difference discretisations of differential equations. They are:

- alternating direction implicit (ADI)
- locally one-dimensional (LOD) [89]
- general Douglas-Gunn (DG)

ADI methods are so named because one dimension is taken as implicit and the other dimensions are taken as explicit in each stage of the split time operator as illustrated by Peaceman and Rachford [90] on the two-dimensional heat equation. In general, ADI methods are developed following three main steps: discretise the differential equation, factor the operator such that each factor contains information along only one dimension and split the factors so that each can be solved for directly [88]. ADI schemes are generally stable and are typically first-order accurate because of how the time operator is factored.

Local one-dimensional methods have the following steps: split the differential equation, then discretise the resulting one-dimensional equations [88]. These methods are treated in detail by Yanenko [91] and mentioned in Briley and McDonald [92].

Douglas-Gunn methods are quite general but can be thought of as following the steps of local one-dimensional methods in reverse: the differential equation is discretised, then split the resulting discretised equations. McDonough [88] provides detailed analysis of these methods with various examples.

5.3.1 Two-dimensional ADI

We begin by describing the simpler two-dimensional problem for the velocity solver as we did for the pressure solver. Not only does it allow us to completely solve the two-dimensional problem but also allows us to transition more easily to the main three-dimensional problem.

Using the expressions from Appendix A, we can write the full version of the momentum equations in two dimensions as follows in (5.7), (5.8), (5.9).

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial r} + \frac{v}{r} \frac{\partial u}{\partial \theta} - \frac{1}{\text{Re}} \left[\nabla^2 u - \frac{u}{r^2} - \frac{u \cos^2 \theta}{H^2} \right] = F_1(r, \theta, t) \quad (5.7)$$

$$\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial r} + \frac{v}{r} \left(\frac{\partial v}{\partial \theta} + u \right) - \frac{1}{\text{Re}} \left[\nabla^2 v - \frac{v}{r^2} - \frac{v \sin^2 \theta}{H^2} \right] = F_2(r, \theta, t) \quad (5.8)$$

$$\frac{\partial w}{\partial t} + u \frac{\partial w}{\partial r} + \frac{v}{r} \frac{\partial w}{\partial \theta} + \frac{w}{H} (u \cos \theta - v \sin \theta) - \frac{1}{\text{Re}} \left[\nabla^2 w - \frac{w}{H^2} \right] = F_3(r, \theta, t) \quad (5.9)$$

where

$$F_1(r, \theta, t) = \frac{v^2}{r} + \frac{w^2 \cos \theta}{H} + \frac{1}{\text{Re}} \left[-\frac{2}{r^2} \frac{\partial v}{\partial \theta} + \frac{v \sin \theta}{H} \left(\frac{\cos \theta}{H} + \frac{1}{r} \right) \right]$$

$$F_2(r, \theta, t) = -\frac{w^2 \sin \theta}{H} + \frac{1}{\text{Re}} \left[\frac{2}{r^2} \frac{\partial u}{\partial \theta} + \frac{u \sin \theta}{H} \left(\frac{\cos \theta}{H} - \frac{1}{r} \right) \right]$$

$$F_3(r, \theta, t) = 0$$

Note that the Laplacian term in (5.7), (5.8), (5.9) must depend only on r and θ for the two-dimensional case. Additionally, the pressure terms have been omitted for simplicity but can easily be included if necessary. We write (5.7), (5.8) and (5.9) in operator form in (5.10), (5.11), (5.12).

$$\frac{\partial u}{\partial t} + L_1 u = F_1 \quad (5.10)$$

$$\frac{\partial v}{\partial t} + L_2 u = F_2 \quad (5.11)$$

$$\frac{\partial w}{\partial t} + L_3 u = F_3 \quad (5.12)$$

with the operators defined as

$$L_1 \equiv u \frac{\partial}{\partial r} + \frac{v}{r} \frac{\partial}{\partial \theta} - \frac{1}{\text{Re}} \left[\nabla^2 - \frac{1}{r^2} - \frac{\cos^2 \theta}{H^2} \right] \quad (5.13)$$

$$L_2 \equiv u \frac{\partial}{\partial r} + \frac{v}{r} \frac{\partial}{\partial \theta} + \frac{u}{r} - \frac{1}{\text{Re}} \left[\nabla^2 - \frac{1}{r^2} - \frac{\sin^2 \theta}{H^2} \right] \quad (5.14)$$

$$L_3 \equiv u \frac{\partial}{\partial r} + \frac{v}{r} \frac{\partial}{\partial \theta} + \frac{1}{H} (u \cos \theta - v \sin \theta) - \frac{1}{\text{Re}} \left[\nabla^2 - \frac{1}{H^2} \right] \quad (5.15)$$

Using a Crank-Nicholson-type scheme (effectively expanding all quantities about a half time step $t_{n+\frac{1}{2}} = t_n + \frac{1}{2}(\Delta t)$), we derive a time-discretised version of equations (5.10), (5.11), (5.12)

$$\frac{u^{n+1} - u^n}{\Delta t} + \frac{1}{2} L_1 (u^{n+1} + u^n) = F_1^{n+\frac{1}{2}} + \mathcal{O}(\Delta t^2)$$

$$\frac{v^{n+1} - v^n}{\Delta t} + \frac{1}{2} L_2 (v^{n+1} + v^n) = F_2^{n+\frac{1}{2}} + \mathcal{O}(\Delta t^2)$$

$$\frac{w^{n+1} - w^n}{\Delta t} + \frac{1}{2} L_3 (w^{n+1} + w^n) = F_3^{n+\frac{1}{2}} + \mathcal{O}(\Delta t^2)$$

In a more useful form,

$$\left(1 + \frac{\Delta t}{2} L_1 \right) u^{n+1} = \left(1 - \frac{\Delta t}{2} L_1 \right) u^n + (\Delta t) F_1^{n+\frac{1}{2}} + \mathcal{O}(\Delta t^2) \quad (5.16)$$

$$\left(1 + \frac{\Delta t}{2} L_2\right) v^{n+1} = \left(1 - \frac{\Delta t}{2} L_2\right) v^n + (\Delta t) F_2^{n+\frac{1}{2}} + \mathcal{O}(\Delta t^2) \quad (5.17)$$

$$\left(1 + \frac{\Delta t}{2} L_3\right) w^{n+1} = \left(1 - \frac{\Delta t}{2} L_3\right) w^n + (\Delta t) F_3^{n+\frac{1}{2}} + \mathcal{O}(\Delta t^2) \quad (5.18)$$

We decompose the operators defined in equations (5.13), (5.14), (5.15) as

$$\begin{aligned} L_1 &\equiv L_1^{(r)} + L_1^{(\theta)} \\ L_2 &\equiv L_2^{(r)} + L_2^{(\theta)} \\ L_3 &\equiv L_3^{(r)} + L_3^{(\theta)} \end{aligned} \quad (5.19)$$

where

$$\begin{aligned} L_1^{(r)} &\equiv u \frac{\partial}{\partial r} - \frac{1}{\text{Re}} \left[\frac{\partial^2}{\partial r^2} + \left(\frac{1}{r} + \frac{\cos \theta}{H} \right) \frac{\partial}{\partial r} - \frac{1}{r^2} - \frac{\cos^2 \theta}{H^2} \right] \\ L_1^{(\theta)} &\equiv \frac{v}{r} \frac{\partial}{\partial \theta} - \frac{1}{\text{Re}} \left[-\frac{\sin \theta}{rH} \frac{\partial}{\partial \theta} + \frac{1}{r^2} \frac{\partial^2}{\partial \theta^2} \right] \\ L_2^{(r)} &\equiv u \frac{\partial}{\partial r} + \frac{u}{r} - \frac{1}{\text{Re}} \left[\frac{\partial^2}{\partial r^2} + \left(\frac{1}{r} + \frac{\cos \theta}{H} \right) \frac{\partial}{\partial r} - \frac{1}{r^2} - \frac{\sin^2 \theta}{H^2} \right] \\ L_2^{(\theta)} &\equiv \frac{v}{r} \frac{\partial}{\partial \theta} - \frac{1}{\text{Re}} \left[-\frac{\sin \theta}{rH} \frac{\partial}{\partial \theta} + \frac{1}{r^2} \frac{\partial^2}{\partial \theta^2} \right] \\ L_3^{(r)} &\equiv u \frac{\partial}{\partial r} + \frac{1}{H} (u \cos \theta - v \sin \theta) - \frac{1}{\text{Re}} \left[\frac{\partial^2}{\partial r^2} + \left(\frac{1}{r} + \frac{\cos \theta}{H} \right) \frac{\partial}{\partial r} - \frac{1}{H^2} \right] \\ L_3^{(\theta)} &\equiv \frac{v}{r} \frac{\partial}{\partial \theta} - \frac{1}{\text{Re}} \left[-\frac{\sin \theta}{rH} \frac{\partial}{\partial \theta} + \frac{1}{r^2} \frac{\partial^2}{\partial \theta^2} \right] \end{aligned} \quad (5.20)$$

Note that $L_i^{(r)}$ contains terms that have a r -derivative as well as terms independent of either a r - or θ - derivative. However, $L_i^{(\theta)}$ only contains terms that have a θ -derivative. The independent terms can also be found in $L_i^{(\theta)}$ if defined appropriately with no drawback if desired. Equations (5.16), (5.17), (5.18) can now be written in (5.21).

$$\begin{aligned}
\left[1 + \frac{\Delta t}{2} (L_1^{(r)} + L_1^{(\theta)})\right] u^{n+1} &= \left(1 - \frac{\Delta t}{2} L_1\right) u^n + (\Delta t) F_1^{n+1/2} + O(\Delta t)^2 \\
\left[1 + \frac{\Delta t}{2} (L_2^{(r)} + L_2^{(\theta)})\right] v^{n+1} &= \left(1 - \frac{\Delta t}{2} L_2\right) v^n + (\Delta t) F_2^{n+1/2} + O(\Delta t)^2 \\
\left[1 + \frac{\Delta t}{2} (L_3^{(r)} + L_3^{(\theta)})\right] w^{n+1} &= \left(1 - \frac{\Delta t}{2} L_3\right) w^n + (\Delta t) F_3^{n+1/2} + O(\Delta t)^2
\end{aligned} \tag{5.21}$$

Each operator in (5.21) can be factored in a similar way. For example,

$$1 + \frac{\Delta t}{2} (L_1^{(r)} + L_1^{(\theta)}) = \left(1 + \frac{\Delta t}{2} L_1^{(r)}\right) \left(1 + \frac{\Delta t}{2} L_1^{(\theta)}\right) - \frac{(\Delta t)^2}{4} L_1^{(r)} L_1^{(\theta)}$$

The system (5.21) can now be written as

$$\begin{aligned}
\left(1 + \frac{\Delta t}{2} L_1^{(r)}\right) \left(1 + \frac{\Delta t}{2} L_1^{(\theta)}\right) u^{n+1} &= \left(1 - \frac{\Delta t}{2} L_1\right) u^n + (\Delta t) F_1^{n+1/2} + O(\Delta t)^2 \\
\left(1 + \frac{\Delta t}{2} L_2^{(r)}\right) \left(1 + \frac{\Delta t}{2} L_2^{(\theta)}\right) v^{n+1} &= \left(1 - \frac{\Delta t}{2} L_2\right) v^n + (\Delta t) F_2^{n+1/2} + O(\Delta t)^2 \\
\left(1 + \frac{\Delta t}{2} L_3^{(r)}\right) \left(1 + \frac{\Delta t}{2} L_3^{(\theta)}\right) w^{n+1} &= \left(1 - \frac{\Delta t}{2} L_3\right) w^n + (\Delta t) F_3^{n+1/2} + O(\Delta t)^2
\end{aligned} \tag{5.22}$$

Finally, we can derive an ADI solver for the momentum equations in (5.23).

$$\begin{aligned}
\left(1 + \frac{\Delta t}{2} L_1^{(r)}\right) u^{n+1/2} &= \left(1 - \frac{\Delta t}{2} L_1\right) u^n + (\Delta t) F_1^{n+1/2} \\
\left(1 + \frac{\Delta t}{2} L_1^{(\theta)}\right) u^{n+1} &= u^{n+1/2} \\
\left(1 + \frac{\Delta t}{2} L_2^{(r)}\right) v^{n+1/2} &= \left(1 - \frac{\Delta t}{2} L_2\right) v^n + (\Delta t) F_2^{n+1/2} \\
\left(1 + \frac{\Delta t}{2} L_2^{(\theta)}\right) v^{n+1} &= v^{n+1/2} \\
\left(1 + \frac{\Delta t}{2} L_3^{(r)}\right) w^{n+1/2} &= \left(1 - \frac{\Delta t}{2} L_3\right) w^n + (\Delta t) F_3^{n+1/2} \\
\left(1 + \frac{\Delta t}{2} L_3^{(\theta)}\right) w^{n+1} &= w^{n+1/2}
\end{aligned} \tag{5.23}$$

The following presentation is made with finite difference approximations and equispaced grids for r and θ in mind. We have spoken about Chebyshev grids for r and discrete Fourier transforms for θ (and ϕ) in the development of the Poisson solver. It is also possible to use these spectral representations within the ADI framework for the velocity solver. However, the ADI methods presented here are more suitable for first-order projection methods which also shares an error of $\mathcal{O}(\Delta t)$ and is part of our early work on the Navier-Stokes solver.

We can now spatially discretise the L_1 , L_2 and L_3 operators using the already established shorthand for finite difference operators. Note that the $L_k^{(\theta)}$ operators are the same for $k = 1, 2, 3$ in (5.24), (5.25), (5.26).

$$L_1^{(r)} u_{i,j}^{n+1/2} = \left[\frac{u_{i,j}^n}{2(\Delta r)} \delta_r^* - \frac{1}{\text{Re}} \left(\frac{\delta_r^2}{(\Delta r)^2} + \frac{1}{2(\Delta r)} \left(\frac{1}{r_i} + \frac{\cos \theta_j}{H_{i,j}} \right) \delta_r^* \right. \right. \\ \left. \left. - \frac{1}{r_i^2} - \frac{\cos^2 \theta_j}{H_{i,j}^2} \right) \right] u_{i,j}^{n+1/2} + O(\Delta r)^2 \quad (5.24)$$

$$L_1^{(\theta)} u_{i,j}^{n+1} = \left[\frac{v_{i,j}^n}{2r_i(\Delta \theta)} \delta_\theta^* - \frac{1}{\text{Re}} \left(-\frac{\sin \theta_j}{2(\Delta \theta)r_i H_{i,j}} \delta_\theta^* + \frac{1}{r_i^2(\Delta \theta)^2} \delta_\theta^2 \right) \right] u_{i,j}^{n+1} + O(\Delta r)^2$$

$$L_2^{(r)} v_{i,j}^{n+1/2} = \left[\frac{u_{i,j}^n}{2(\Delta r)} \delta_r^* + \frac{u_{i,j}^n}{r_i} - \frac{1}{\text{Re}} \left(\frac{\delta_r^2}{(\Delta r)^2} + \frac{1}{2(\Delta r)} \left(\frac{1}{r_i} + \frac{\cos \theta_j}{H_{i,j}} \right) \delta_r^* \right. \right. \\ \left. \left. - \frac{1}{r_i^2} - \frac{\sin^2 \theta_j}{H_{i,j}^2} \right) \right] v_{i,j}^{n+1/2} + O(\Delta r)^2 \quad (5.25)$$

$$L_2^{(\theta)} v_{i,j}^{n+1} = \left[\frac{v_{i,j}^n}{2r_i(\Delta \theta)} \delta_\theta^* - \frac{1}{\text{Re}} \left(-\frac{\sin \theta_j}{2(\Delta \theta)r_i H_{i,j}} \delta_\theta^* + \frac{1}{r_i^2(\Delta \theta)^2} \delta_\theta^2 \right) \right] v_{i,j}^{n+1} + O(\Delta r)^2$$

$$\begin{aligned}
L_3^{(r)} w_{i,j}^{n+1/2} &= \left[\frac{u_{i,j}^n}{2(\Delta r)} \delta_r^* + \frac{1}{H_{i,j}} \left(u_{i,j}^n \cos \theta_j - v_{i,j}^n \sin \theta_j \right) \right. \\
&\quad \left. - \frac{1}{\text{Re}} \left(\frac{\delta_r^2}{(\Delta r)^2} + \frac{1}{2(\Delta r)} \left(\frac{1}{r_i} + \frac{\cos \theta_j}{H_{i,j}} \right) \delta_r^* - \frac{1}{H_{i,j}^2} \right) \right] w_{i,j}^{n+1/2} + O(\Delta r)^2 \quad (5.26) \\
L_3^{(\theta)} w_{i,j}^{n+1} &= \left[\frac{v_{i,j}^n}{2r_i(\Delta \theta)} \delta_\theta^* - \frac{1}{\text{Re}} \left(-\frac{\sin \theta_j}{2(\Delta \theta)r_i H_{i,j}} \delta_\theta^* + \frac{1}{r_i^2(\Delta \theta)^2} \delta_\theta^2 \right) \right] w_{i,j}^{n+1} + O(\Delta r)^2
\end{aligned}$$

We can simplify the discrete operators and express them in their tri-diagonal form in (5.27), (5.28), (5.29), (5.30) below.

$$L_k^{(\theta)} \alpha_{i,j} = A_{i,j}^{(\theta)} \alpha_{i,j-1} + B_{i,j}^{(\theta)} \alpha_{i,j} + C_{i,j}^{(\theta)} \alpha_{i,j+1} \quad (5.27)$$

where

$$\begin{aligned}
A_{i,j}^{(\theta)} &= -\frac{1}{r_i(\Delta \theta)} \left[\frac{1}{2} v_{i,j}^n + \frac{1}{\text{Re}} \left(\frac{\sin \theta_j}{2H_{i,j}} + \frac{1}{r_i(\Delta \theta)} \right) \right] \\
B_{i,j}^{(\theta)} &= \frac{2}{r_i^2(\Delta \theta)^2 \text{Re}} \\
C_{i,j}^{(\theta)} &= \frac{1}{r_i(\Delta \theta)} \left[\frac{1}{2} v_{i,j}^n + \frac{1}{\text{Re}} \left(\frac{\sin \theta_j}{2H_{i,j}} - \frac{1}{r_i(\Delta \theta)} \right) \right]
\end{aligned}$$

$$L_1^{(r)} \phi_{i,j} = A_{i,j}^{(r,1)} \phi_{i-1,j} + B_{i,j}^{(r,1)} \phi_{i,j} + C_{i,j}^{(r,1)} \phi_{i+1,j} \quad (5.28)$$

where

$$\begin{aligned}
A_{i,j}^{(r,1)} &= -\frac{1}{(\Delta r)} \left[\frac{1}{2} u_{i,j}^n + \frac{1}{\text{Re}} \left(\frac{1}{(\Delta r)} - \frac{1}{2} \left(\frac{1}{r_i} + \frac{\cos \theta_j}{H_{i,j}} \right) \right) \right] \\
B_{i,j}^{(r,1)} &= \frac{1}{\text{Re}} \left(\frac{2}{(\Delta r)^2} + \frac{1}{r_i^2} + \frac{\cos^2 \theta_j}{H_{i,j}^2} \right) \\
C_{i,j}^{(r,1)} &= \frac{1}{(\Delta r)} \left[\frac{1}{2} u_{i,j}^n - \frac{1}{\text{Re}} \left(\frac{1}{(\Delta r)} + \frac{1}{2} \left(\frac{1}{r_i} + \frac{\cos \theta_j}{H_{i,j}} \right) \right) \right]
\end{aligned}$$

$$L_2^{(r)} \phi_{i,j} = A_{i,j}^{(r,2)} \phi_{i-1,j} + B_{i,j}^{(r,2)} \phi_{i,j} + C_{i,j}^{(r,2)} \phi_{i+1,j} \quad (5.29)$$

where

$$\begin{aligned} A_{i,j}^{(r,2)} &= A_{i,j}^{(r,1)} = -\frac{1}{(\Delta r)} \left[\frac{1}{2} u_{i,j}^n + \frac{1}{\text{Re}} \left(\frac{1}{(\Delta r)} - \frac{1}{2} \left(\frac{1}{r_i} + \frac{\cos \theta_j}{H_{i,j}} \right) \right) \right] \\ B_{i,j}^{(r,2)} &= \frac{1}{r_i} u_{i,j}^n + \frac{1}{\text{Re}} \left(\frac{2}{(\Delta r)^2} + \frac{1}{r_i^2} + \frac{\sin^2 \theta_j}{H_{i,j}^2} \right) \\ C_{i,j}^{(r,2)} &= C_{i,j}^{(r,1)} = \frac{1}{(\Delta r)} \left[\frac{1}{2} u_{i,j}^n - \frac{1}{\text{Re}} \left(\frac{1}{(\Delta r)} + \frac{1}{2} \left(\frac{1}{r_i} + \frac{\cos \theta_j}{H_{i,j}} \right) \right) \right] \end{aligned}$$

$$L_3^{(r)} \phi_{i,j} = A_{i,j}^{(r,3)} \phi_{i-1,j} + B_{i,j}^{(r,3)} \phi_{i,j} + C_{i,j}^{(r,3)} \phi_{i+1,j} \quad (5.30)$$

where

$$\begin{aligned} A_{i,j}^{(r,3)} &= A_{i,j}^{(r,1)} = -\frac{1}{(\Delta r)} \left[\frac{1}{2} u_{i,j}^n + \frac{1}{\text{Re}} \left(\frac{1}{(\Delta r)} - \frac{1}{2} \left(\frac{1}{r_i} + \frac{\cos \theta_j}{H_{i,j}} \right) \right) \right] \\ B_{i,j}^{(r,3)} &= \frac{1}{H_{i,j}} \left(u_{i,j}^n \cos \theta_j - v_{i,j}^n \sin \theta_j \right) + \frac{1}{\text{Re}} \left(\frac{2}{(\Delta r)^2} + \frac{1}{H_{i,j}^2} \right) \\ C_{i,j}^{(r,3)} &= C_{i,j}^{(r,1)} = \frac{1}{(\Delta r)} \left[\frac{1}{2} u_{i,j}^n - \frac{1}{\text{Re}} \left(\frac{1}{(\Delta r)} + \frac{1}{2} \left(\frac{1}{r_i} + \frac{\cos \theta_j}{H_{i,j}} \right) \right) \right] \end{aligned}$$

5.3.2 Test case

We now present a test case used in the validation of our solvers for equations (5.7), (5.8), (5.9). The test functions we assume for velocities u , v and w below obey the appropriate Dirichlet boundary conditions but are not formal solutions to the Navier-Stokes equations. As such, operating on these assumed forms with each of the above equations will produce a residual function; we label these residuals G_1 , G_2 and G_3 . Our plan is to use the residual

functions computed below in order to reproduce the assumed velocities using our numerical solvers.

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial r} + \frac{v}{r} \frac{\partial u}{\partial \theta} - \frac{1}{Re} \left[\nabla^2 u - \frac{u}{r^2} - \frac{u \cos^2 \theta}{h_{\phi,i,j}^2} \right] - F_1(r, \theta, t) = G_1(r, \theta, t) \quad (5.31)$$

$$\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial r} + \frac{v}{r} \left(\frac{\partial v}{\partial \theta} + u \right) - \frac{1}{Re} \left[\nabla^2 v - \frac{v}{r^2} - \frac{v \sin^2 \theta}{h_{\phi,i,j}^2} \right] - F_2(r, \theta, t) = G_2(r, \theta, t) \quad (5.32)$$

$$\frac{\partial w}{\partial t} + u \frac{\partial w}{\partial r} + \frac{v}{r} \frac{\partial w}{\partial \theta} + \frac{w}{H} (u \cos \theta - v \sin \theta) - \frac{1}{Re} \left[\nabla^2 w - \frac{w}{h_{\phi,i,j}^2} \right] - F_3(r, \theta, t) = G_3(r, \theta, t) \quad (5.33)$$

With c and d as positive integers, β as a real constant and $L = r_b - r_a$, we assume the following test functions

$$u(r, \theta) = e^{\cos(n\theta)} \sin \left(\frac{c\pi}{L} (r_b - r) e^{-\beta^2 t} \right) \quad (5.34)$$

$$v(r, \theta) = e^{\sin(n\theta)} \sin \left(\frac{c\pi}{L} (r_b - r) e^{-\beta^2 t} \right) \quad (5.35)$$

$$w(r, \theta) = u(r, \theta) - r \cos \theta - r \sin \theta \quad (5.36)$$

Note that u and v both vanish on the domain boundaries at $r = r_a$ and $r = r_b$, while the values of w lie on an inclined plane and are in general non-zero, as in our applications to be studied as part of this work.

5.3.3 Code validation

Our primary tool for code validation is the relative error between the numerical solution and the exact solution provided by test case in the previous section. To avoid division by zero, which occurs because of the particular functions we chose for the test case, we define the relative error by dividing the absolute error by the maximum of value of the exact solution for each velocity u , v and w .

We document the effect of reducing the grid step size in each direction on the relative error in the following tables. We run the code from $t = 0$ to $t = 1$ with a time grid of 2000 points and a θ -grid of 5121 points.

r -points	θ -points	Rel. error for u	Rel. error for v	Rel. error for w
11	5121	0.106460522844456	0.101824626276425	0.076270617581738
21	5121	0.026321900279580	0.024914298988916	0.017846947910836
41	5121	0.006680960712242	0.006272113397171	0.004582719651107
81	5121	0.001982730651815	0.001779468949894	0.001462409238713

Table 5.1: Effect of varying r -grids on relative error

r -points	θ -points	Rel. error for u	Rel. error for v	Rel. error for w
321	11	0.207313094229894	0.191982767125024	0.167691204174861
321	21	0.070092401694405	0.066154271614073	0.051866160209083
321	41	0.019749601924173	0.015429834002836	0.014100270415165
321	81	0.005114953239386	0.004190573123548	0.003701662510889

Table 5.2: Effect of varying θ -grids on relative error

As expected, doubling the points in both the r - and θ - grids reduces the error by a factor of (approximately) four. We omit the effect of varying the time grid on the relative error because it is too computationally taxing to use extremely fine grids for r and θ .

5.3.4 Three-dimensional ADI

The development of an ADI numerical solver for the full three-dimensional momentum equations is similar to that of the ADI numerical solver for the two-dimensional equations.

The main difference is that there is an additional intermediate step to account for the additional variable, ϕ . Consequently, we omit many of the steps that were shown in the two-dimensional case to avoid needless repetition. We begin by summarising the momentum equations in (5.37).

$$\begin{aligned}\frac{\partial u}{\partial t} + L_1 u &= F_1 \\ \frac{\partial v}{\partial t} + L_2 v &= F_2 \\ \frac{\partial w}{\partial t} + L_3 w &= F_3\end{aligned}\tag{5.37}$$

where

$$\begin{aligned}L_1 &= u \frac{\partial}{\partial r} + \frac{v}{r} \frac{\partial}{\partial \theta} + \frac{w}{h_{\phi,i,j}} \frac{\partial}{\partial \phi} - \frac{1}{Re} \left(\nabla^2 - \frac{1}{r^2} - \frac{\cos^2 \theta}{h_{\phi,i,j}^2} \right) \\ L_2 &= u \frac{\partial}{\partial r} + \frac{v}{r} \frac{\partial}{\partial \theta} + \frac{u}{r} + \frac{w}{h_{\phi,i,j}} \frac{\partial}{\partial \phi} - \frac{1}{Re} \left(\nabla^2 - \frac{1}{r^2} - \frac{\sin^2 \theta}{h_{\phi,i,j}^2} \right) \\ L_3 &= u \frac{\partial}{\partial r} + \frac{v}{r} \frac{\partial}{\partial \theta} + \frac{w}{h_{\phi,i,j}} \frac{\partial}{\partial \phi} + \frac{1}{h_{\phi,i,j}} (u \cos \theta - v \sin \theta) - \frac{1}{Re} \left(\nabla^2 - \frac{1}{h_{\phi,i,j}^2} \right)\end{aligned}$$

and

$$\begin{aligned}F_1 &= \frac{v^2}{r} + \frac{w^2 \cos \theta}{h_{\phi,i,j}} + \frac{1}{Re} \left[-\frac{2}{r^2} \frac{\partial v}{\partial \theta} + \frac{v \sin \theta}{h_{\phi,i,j}} \left(\frac{\cos \theta}{h_{\phi,i,j}} + \frac{1}{r} \right) - \frac{2 \cos \theta}{h_{\phi,i,j}^2} \frac{\partial w}{\partial \phi} \right] \\ F_2 &= -\frac{w^2 \sin \theta}{h_{\phi,i,j}} + \frac{1}{Re} \left[\frac{2}{r^2} \frac{\partial u}{\partial \theta} + \frac{u \sin \theta}{h_{\phi,i,j}} \left(\frac{\cos \theta}{h_{\phi,i,j}} - \frac{1}{r} \right) + \frac{2 \sin \theta}{h_{\phi,i,j}^2} \frac{\partial w}{\partial \phi} \right] \\ F_3 &= \frac{1}{Re} \frac{1}{h_{\phi,i,j}^2} \left(2 \cos \theta \frac{\partial u}{\partial \phi} - 2 \sin \theta \frac{\partial v}{\partial \phi} \right)\end{aligned}$$

Splitting the operator as we have already demonstrated, we derive new operators using L_1 ,

L_2 and L_3 . Note that each equation in the ADI formulation is effectively a solver for a one-dimensional advection-diffusion equation and that the $L_p^{(\theta)}$ and $L_p^{(\phi)}$ operators are the same for $p = 1, 2, 3$.

$$\begin{aligned}
\left(1 + \frac{\Delta t}{2} L_1^{(r)}\right) u^{n+1/3} &= \left(1 - \frac{\Delta t}{2} L_1\right) u^n + (\Delta t) F_1^{n+1/3} \\
\left(1 + \frac{\Delta t}{2} L_1^{(\theta)}\right) u^{n+2/3} &= u^{n+1/3} \\
\left(1 + \frac{\Delta t}{2} L_1^{(\phi)}\right) u^{n+1} &= u^{n+2/3} \\
\\
\left(1 + \frac{\Delta t}{2} L_2^{(r)}\right) v^{n+1/3} &= \left(1 - \frac{\Delta t}{2} L_2\right) v^n + (\Delta t) F_2^{n+1/3} \\
\left(1 + \frac{\Delta t}{2} L_2^{(\theta)}\right) v^{n+2/3} &= v^{n+1/3} \\
\left(1 + \frac{\Delta t}{2} L_2^{(\phi)}\right) v^{n+1} &= v^{n+2/3} \\
\\
\left(1 + \frac{\Delta t}{2} L_3^{(r)}\right) w^{n+1/3} &= \left(1 - \frac{\Delta t}{2} L_3\right) w^n + (\Delta t) F_3^{n+1/3} \\
\left(1 + \frac{\Delta t}{2} L_3^{(\theta)}\right) w^{n+2/3} &= w^{n+1/3} \\
\left(1 + \frac{\Delta t}{2} L_3^{(\phi)}\right) w^{n+1} &= w^{n+2/3}
\end{aligned} \tag{5.38}$$

where

$$\begin{aligned}
L_1^{(r)} &\equiv u \frac{\partial}{\partial r} - \frac{1}{Re} \left[\frac{\partial^2}{\partial r^2} + \left(\frac{1}{r} + \frac{\cos \theta}{h_{\phi,i,j}} \right) \frac{\partial}{\partial r} - \frac{1}{r^2} - \frac{\cos^2 \theta}{h_{\phi,i,j}^2} \right] \\
L_1^{(\theta)} &\equiv \frac{v}{r} \frac{\partial}{\partial \theta} - \frac{1}{Re} \left[-\frac{\sin \theta}{r h_{\phi,i,j}} \frac{\partial}{\partial \theta} + \frac{1}{r^2} \frac{\partial^2}{\partial \theta^2} \right] \\
L_1^{(\phi)} &\equiv \frac{w}{h_{\phi,i,j}} \frac{\partial}{\partial \phi} - \frac{1}{Re} \frac{1}{h_{\phi,i,j}^2} \frac{\partial^2}{\partial \phi^2} \\
\\
L_2^{(r)} &\equiv u \frac{\partial}{\partial r} + \frac{u}{r} - \frac{1}{Re} \left[\frac{\partial^2}{\partial r^2} + \left(\frac{1}{r} + \frac{\cos \theta}{h_{\phi,i,j}} \right) \frac{\partial}{\partial r} - \frac{1}{r^2} - \frac{\sin^2 \theta}{h_{\phi,i,j}^2} \right] \\
L_2^{(\theta)} &\equiv \frac{v}{r} \frac{\partial}{\partial \theta} - \frac{1}{Re} \left[-\frac{\sin \theta}{r h_{\phi,i,j}} \frac{\partial}{\partial \theta} + \frac{1}{r^2} \frac{\partial^2}{\partial \theta^2} \right] \\
L_2^{(\phi)} &\equiv \frac{w}{h_{\phi,i,j}} \frac{\partial}{\partial \phi} - \frac{1}{Re} \frac{1}{h_{\phi,i,j}^2} \frac{\partial^2}{\partial \phi^2}
\end{aligned}$$

$$\begin{aligned}
L_3^{(r)} &\equiv u \frac{\partial}{\partial r} + \frac{1}{h_{\phi,i,j}} (u \cos \theta - v \sin \theta) - \frac{1}{Re} \left[\frac{\partial^2}{\partial r^2} + \left(\frac{1}{r} + \frac{\cos \theta}{h_{\phi,i,j}} \right) \frac{\partial}{\partial r} - \frac{1}{h_{\phi,i,j}^2} \right] \\
L_3^{(\theta)} &\equiv \frac{v}{r} \frac{\partial}{\partial \theta} - \frac{1}{Re} \left[-\frac{\sin \theta}{r h_{\phi,i,j}} \frac{\partial}{\partial \theta} + \frac{1}{r^2} \frac{\partial^2}{\partial \theta^2} \right] \\
L_3^{(\phi)} &\equiv \frac{w}{h_{\phi,i,j}} \frac{\partial}{\partial \phi} - \frac{1}{Re} \frac{1}{h_{\phi,i,j}^2} \frac{\partial^2}{\partial \phi^2}
\end{aligned}$$

We can simplify the discrete operators and express them in their tri-diagonal form in (5.39), (5.40), (5.41), (5.42), (5.43).

$$L_p^{(\theta)} \alpha_{i,j,k} = A_{i,j,k}^{(\theta)} \alpha_{i,j-1,k} + B_{i,j,k}^{(\theta)} \alpha_{i,j,k} + C_{i,j,k}^{(\theta)} \alpha_{i,j+1,k} \quad (5.39)$$

where

$$A_{i,j,k}^{(\theta)} = -\frac{v_{i,j,k}^n}{2r_i \Delta \theta} - \frac{1}{Re} \left[\frac{\sin \theta_j}{2\Delta \theta r_i h_{\phi,i,j}} + \frac{1}{r_i^2 (\Delta \theta)^2} \right]$$

$$B_{i,j,k}^{(\theta)} = \frac{1}{Re} \frac{2}{r_i^2 (\Delta\theta)^2}$$

$$C_{i,j,k}^{(\theta)} = \frac{v_{i,j,k}^n}{2r_i \Delta\theta} - \frac{1}{Re} \left[-\frac{\sin \theta_j}{2\Delta\theta r_i h_{\phi,i,j}} + \frac{1}{r_i^2 (\Delta\theta)^2} \right]$$

$$L_p^{(\phi)} \alpha_{i,j,k} = A_{i,j,k}^{(\phi)} \alpha_{i,j,k-1} + B_{i,j,k}^{(\phi)} \alpha_{i,j,k} + C_{i,j,k}^{(\phi)} \alpha_{i,j,k+1} \quad (5.40)$$

where

$$A_{i,j,k}^{(\phi)} = -\frac{w_{i,j,k}^n}{2H_{i,j} \Delta\phi} - \frac{1}{Re} \frac{1}{h_{\phi,i,j} (\Delta\phi)^2}$$

$$B_{i,j,k}^{(\phi)} = \frac{1}{Re} \frac{2}{h_{\phi,i,j}^2 (\Delta\phi)^2}$$

$$C_{i,j,k}^{(\phi)} = \frac{w_{i,j,k}^n}{2H_{i,j} \Delta\phi} - \frac{1}{Re} \frac{1}{h_{\phi,i,j} (\Delta\phi)^2}$$

$$L_1^{(r)} \alpha_{i,j,k} = A_{i,j,k}^{(r)} \alpha_{i-1,j,k} + B_{i,j,k}^{(r)} \alpha_{i,j,k} + C_{i,j,k}^{(r)} \alpha_{i+1,j,k} \quad (5.41)$$

where

$$A_{i,j,k}^{(r,1)} = \left(-\frac{u_{i,j,k}^n}{2\Delta r} - \frac{1}{Re} \left[\frac{1}{(\Delta r)^2} - \frac{1}{2\Delta r} \left(\frac{1}{r_i} + \frac{\cos \theta_j}{h_{\phi,i,j}} \right) \right] \right)$$

$$B_{i,j,k}^{(r,1)} = \left(\frac{1}{Re} \left[\frac{2}{(\Delta r)^2} + \frac{1}{r_i^2} + \frac{\cos^2 \theta_j}{h_{\phi,i,j}^2} \right] \right)$$

$$C_{i,j,k}^{(r,1)} = \left(\frac{u_{i,j,k}^n}{2\Delta r} - \frac{1}{Re} \left[\frac{1}{(\Delta r)^2} + \frac{1}{2\Delta r} \left(\frac{1}{r_i} + \frac{\cos \theta_j}{h_{\phi,i,j}} \right) \right] \right)$$

$$L_2^{(r)} \alpha_{i,j,k} = A_{i,j,k}^{(r)} \alpha_{i-1,j,k} + B_{i,j,k}^{(r)} \alpha_{i,j,k} + C_{i,j,k}^{(r)} \alpha_{i+1,j,k} \quad (5.42)$$

where

$$A_{i,j,k}^{(r,2)} = \left(-\frac{u_{i,j,k}^n}{2\Delta r} - \frac{1}{Re} \left[\frac{1}{(\Delta r)^2} - \frac{1}{2\Delta r} \left(\frac{1}{r_i} + \frac{\cos \theta_j}{h_{\phi,i,j}} \right) \right] \right)$$

$$B_{i,j,k}^{(r,2)} = \left(\frac{u_{i,j,k}}{r_i} + \frac{1}{Re} \left[\frac{2}{(\Delta r)^2} + \frac{1}{r_i^2} + \frac{\sin^2 \theta_j}{h_{\phi,i,j}} \right] \right)$$

$$C_{i,j,k}^{(r,2)} = \left(\frac{u_{i,j,k}^n}{2\Delta r} - \frac{1}{Re} \left[\frac{1}{(\Delta r)^2} + \frac{1}{2\Delta r} \left(\frac{1}{r_i} + \frac{\cos \theta_j}{h_{\phi,i,j}} \right) \right] \right)$$

$$L_3^{(r)} \alpha_{i,j,k} = A_{i,j,k}^{(r)} \alpha_{i-1,j,k} + B_{i,j,k}^{(r)} \alpha_{i,j,k} + C_{i,j,k}^{(r)} \alpha_{i+1,j,k} \quad (5.43)$$

where

$$A_{i,j,k}^{(r,3)} = \left(-\frac{u_{i,j,k}^n}{2\Delta r} - \frac{1}{Re} \left[\frac{1}{(\Delta r)^2} - \frac{1}{2\Delta r} \left(\frac{1}{r_i} + \frac{\cos \theta_j}{h_{\phi,i,j}} \right) \right] \right)$$

$$B_{i,j,k}^{(r,3)} = \left(\frac{1}{H_{i,j}} (u_{i,j,k} \cos \theta_j - v_{i,j,k} \sin \theta_j) + \frac{1}{Re} \left[\frac{2}{(\Delta r)^2} + \frac{1}{h_{\phi,i,j}^2} \right] \right)$$

$$C_{i,j,k}^{(r,3)} = \left(\frac{u_{i,j,k}^n}{2\Delta r} - \frac{1}{Re} \left[\frac{1}{(\Delta r)^2} + \frac{1}{2\Delta r} \left(\frac{1}{r_i} + \frac{\cos \theta_j}{h_{\phi,i,j}} \right) \right] \right)$$

5.3.5 Test case

For our test problem, we choose to solve the following equations

$$\frac{\partial u}{\partial t} - \frac{1}{\text{Re}} \nabla^2 u - F_1(r, \theta, \phi, t) = G_1(r, \theta, t) \quad (5.44)$$

$$\frac{\partial v}{\partial t} - \frac{1}{\text{Re}} \nabla^2 v - F_2(r, \theta, t) = G_2(r, \theta, \phi, t) \quad (5.45)$$

$$\frac{\partial w}{\partial t} - \frac{1}{\text{Re}} \nabla^2 w - F_3(r, \theta, t) = G_3(r, \theta, \phi, t) \quad (5.46)$$

where G_1 , G_2 and G_3 is found from the following assumed solutions i.e. by substituting the assumed solutions into the momentum equations, we get residuals which are labelled as G_1 , G_2 and G_3

$$\begin{aligned} u(r, \theta, \phi, t) &= e^{\cos(n\theta)} \sin\left(\frac{m\pi(r_b - r)}{r_b - r_a}\right) e^{\cos(n\phi)} e^{-\alpha t} \\ v(r, \theta, \phi, t) &= e^{\cos(n\theta)} \sin\left(\frac{m\pi(r_b - r)}{r_b - r_a}\right) e^{\sin(n\phi)} e^{-\alpha t} \\ w(r, \theta, \phi, t) &= e^{\sin(n\theta)} \sin\left(\frac{m\pi(r_b - r)}{r_b - r_a}\right) e^{\sin(n\phi)} e^{-\alpha t} \end{aligned} \quad (5.47)$$

5.3.6 Code validation

Our primary tool for code validation is the relative error between the numerical solution and the exact solution provided by test case in the previous section. To avoid division by zero, which occurs because of the particular functions we chose for the test case, we define the relative error by dividing the absolute error by the maximum of value of the exact solution for each velocity u , v and w .

We document the effect of reducing the grid step size in each direction on the relative error

in the following tables. We run the code from $t = 0$ to $t = 1$ with a time grid of 2000 points and a θ -grid of 5121 points.

r -points	θ -points	ϕ -points	Rel. error for u	Rel. error for v	Rel. error for w
11	161	161	0.00827352261	0.00655397711	0.00902934606
21	161	161	0.00209115465	0.00169817955	0.00235992228
41	161	161	0.00072844189	0.00066557112	0.00079131803

Table 5.3: Effect of varying r -grids on relative error

r -points	θ -points	ϕ -points	Rel. error for u	Rel. error for v	Rel. error for w
321	11	161	0.02263747449	0.02560349211	0.02797228615
321	21	161	0.00650398354	0.00791665451	0.00747405341
321	41	161	0.00148236519	0.00178189294	0.00158785158

Table 5.4: Effect of varying θ -grids on relative error

r -points	θ -points	ϕ -points	Rel. error for u	Rel. error for v	Rel. error for w
321	161	11	0.00454893653	0.00723080930	0.02366458290
321	161	21	0.00121426434	0.00201633017	0.00655242034
321	161	41	0.00046585527	0.00061707877	0.00140172642

Table 5.5: Effect of varying ϕ -grids on relative error

As expected, doubling the points in both the r -, θ - and ϕ - grids reduces the error by a factor of (approximately) four. We omit the effect of varying the time grid on the relative error because it is too computationally taxing to use extremely fine grids for r , θ and ϕ .

Chapter 6

Results: Rotating only the inner torus

In this chapter, we will see the numerical results obtained from combining the two main parts together to numerically study the flow between two concentric tori. The results presented in this chapter are obtained by implementing a pressure Poisson formulation to solve for the pressure and a RK4 method to solve for the velocity. In order to guarantee appropriate smoothness of the solution in a neighborhood of $t = 0$ (and hence preserve the high-order accuracy of the solutions for $t > 0$) we do not use impulsively-started boundary conditions. Instead, we make use of a smooth 'spin-up' function $f(t; 0, t_1)$ which smoothly transitions the velocities on the boundary from rest at $t = t_0 = 0$ to the maximum steady values at $t = t_1$. The time t_1 where boundary velocity reaches its maximum value is called the 'spin-up time'. A full description of the spin-up function is presented in Appendix C. With these considerations in mind, the boundary conditions enforced in this chapter are

$$\mathbf{u}(r, \theta, \phi, t) = \begin{cases} (0, 0, (1 - f(t; 0, t_1))(1 + r_a \cos \theta)), & r = r_a \\ (0, 0, 0), & r = r_b \end{cases} \quad (6.1)$$

In our simulations, we experimented with the following parameters:

- the number of grid points used for the Chebyshev grid in the radial direction, N_r

- the number of grid points used for the Fourier coefficients in the θ direction, N_θ
- the number of grid points used for the Fourier coefficients in the ϕ direction, N_ϕ
- the Reynolds number, Re
- the final time at which the flow is observed, t_{end}
- the inner polar radius, r_a
- the outer polar radius, r_b
- toroidal radius, R_0
- the spin-up time, t_1

Recall that we use $R_0 = 1$ and that $r_a < r_b < R_0$ in all cases because R_0 is the characteristic length used in the non-dimensionalisation of the Navier-Stokes equations.

Our simulations have revealed two distinct kinds of flows. The first kind of flow observed is the physically intuitive expectation from such a setup. The main component of the flow is in the ϕ -direction with negligible contributions from both the r - and θ - components of velocity. This occurs at lower Reynolds numbers and at lower speeds of rotation.

The second kind of flow is observed at higher Reynolds numbers and is of much greater interest. The second kind of flow is comprised of two unique sections. On the outer sides of the torus, i.e. the regions where the speed is greatest, we observe the development of ‘fingers’ or bands of flow that alternate between high and low speed within a certain polar angle. Outside of this polar angle, the flow resembles that which was described in the first case.

After several trial runs, we found a set of parameters that illustrates an exciting and unexpected narrative starring these two distinct flows.

6.1 Increasing Reynolds number

We begin by examining the effect of increasing the Reynolds number while keeping all other parameters fixed. All relevant parameters for the various flows simulated in this section are summarised in Table 6.1 below. Note that the final column contains hyperlinks to the relevant sub-section in this and subsequent similar tables.

For each case, we have the following types of figures (though not all of them are presented for brevity)

- Profile of each velocity component, u , v and w , and their corresponding contour plots for $\phi = 0$ generated using MATLAB. This is sufficient to understand the flow throughout the entire geometry since there is no ϕ -dependence in the flow for this set of parameters.
- Cross-sections of the tori along the plane where $\phi = 0$ which illustrate the speed of each component of the flow at each point between the two tori generated using Paraview
- Profile of the pressure, p , and divergence, $\nabla \cdot \mathbf{u}$, along with their corresponding contour plots for $\phi = 0$ generated using MATLAB.

There are a few remarks regarding the following figures. We have magnified the gap between the tori in the subsequent plots purely for visual effect; magnification does not change the fundamental features of the flow. We have observed the flow at larger values of t_{end} to ensure that a steady-state flow has been reached even at 100s.

None of the simulations presented in this chapter and the next exceeded a run time of approximately one week. As one would expect, the simulations with $N_r = 30$ took the most time. The time step was chosen through a combination of analysis and experimentation. We began by defining the time in terms of the maximum value possible from the Courant-Friedrichs-Lewy condition shown below.

$$\Delta t = \frac{(\Delta x)_{\min}}{u_{\max}}$$

where $(\Delta x)_{\min}$ is the smallest possible spatial step from the r -, θ - and ϕ - grids and $u_{\max}$ chosen from the boundary conditions to maximise Δt . However, this definition sometimes forced simulations to end prematurely with NaN values appearing in the velocity components. This means that the Courant number of 1 was inappropriate for some sets of parameters. At this point, we resorted to a process of trial and error to determine the number of time steps needed for a particular set of parameters. For a given number of time steps, we ensured that symmetry was preserved and that the divergence was low enough allowing a maximum of only 0.01.

As usual, the bottleneck in Navier-Stokes solvers is the Poisson solver. The velocity update is simply a collection of various field quantities all of which are less expensive than the Poisson solve because of the use of Fourier and Chebyshev series. For instance, the computational time to compute and invert a two-dimensional Fourier series is $\mathcal{O}(N_\theta N_\phi \log(N_\theta N_\phi))$ and the calculation of a derivative in Fourier space is merely a inexpensive multiplication. However, we need to invert $N_r \times N_r$ matrices by construction of the block penta-diagonal matrix using Chebyshev series. Therefore, the computational time of the Poisson solve, and thus, the entire solver, is $\mathcal{O}(N_r^2 N_\theta N_\phi)$. In physical time, we observed that an increase as small as five radial points nearly doubles the computational run time.

N_r	N_θ	N_ϕ	Re	t_{end}	r_a	r_b	R_0	Spin-up	Sub-section	Figures
20	200	40	5000	100s	0.25	0.28	1.0	50s	Case 1	6.1, 6.2, 6.3, 6.4
20	200	40	8000	100s	0.25	0.28	1.0	50s	Case 2	6.5, 6.6, 6.7, 6.8
30	200	40	15000	100s	0.25	0.28	1.0	50s	Case 3	6.9, 6.10, 6.11, 6.12
30	200	40	20000	100s	0.25	0.28	1.0	50s	Case 4	6.13
30	200	40	30000	100s	0.25	0.28	1.0	50s	Case 5	6.15

Table 6.1: Parameters used to study the effect of increasing Reynolds number

6.1.1 Case 1, $r_a = 0.25$, $r_b = 0.28$, $Re = 5000$

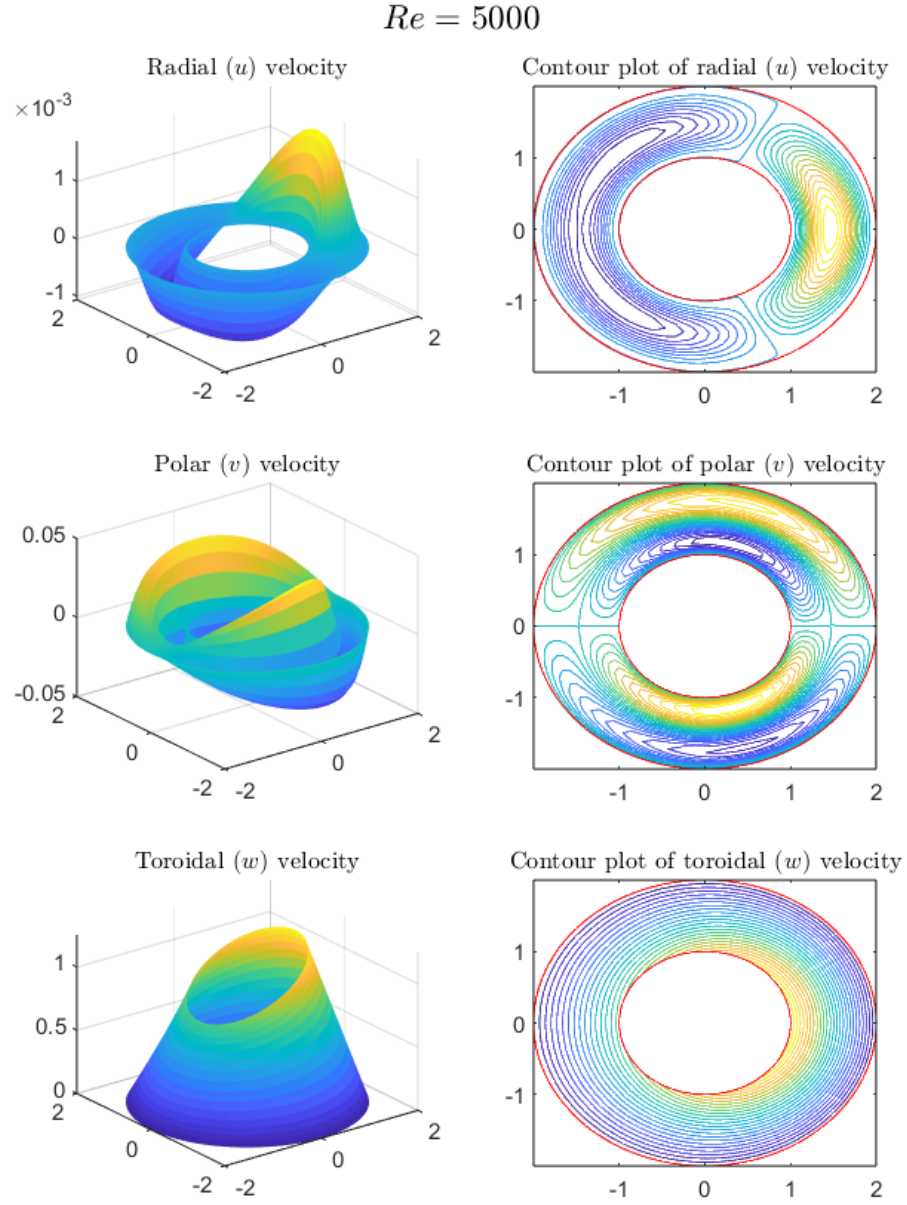


Figure 6.1: Velocity components at 100s for $r_a = 0.25$, $r_b = 0.28$, $Re = 5000$

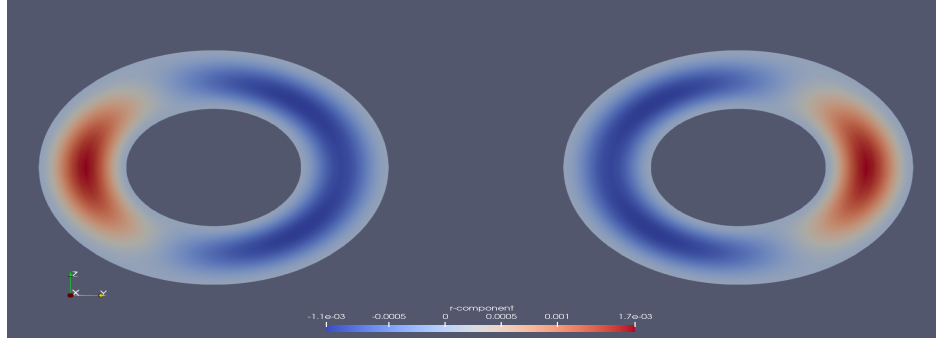


Figure 6.2: r -component of velocity on $\phi = \frac{3\pi}{2}$ (left) and $\phi = \frac{\pi}{2}$ (right) at 100s for $r_a = 0.25$, $r_b = 0.28$, $Re = 5000$

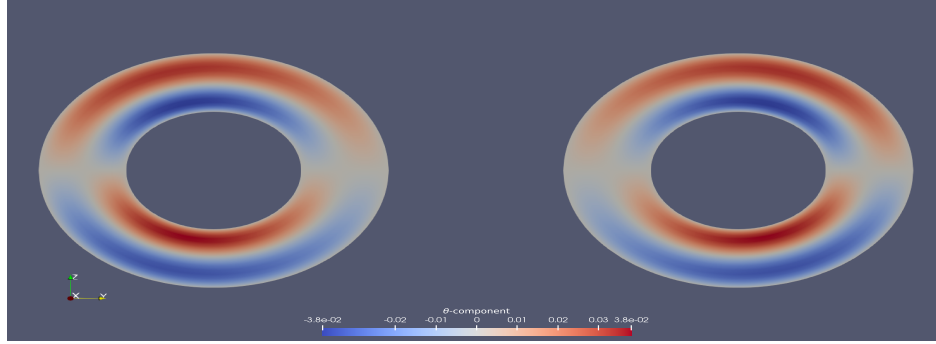


Figure 6.3: θ -component of velocity on $\phi = \frac{3\pi}{2}$ (left) and $\phi = \frac{\pi}{2}$ (right) at 100s for $r_a = 0.25$, $r_b = 0.28$, $Re = 5000$

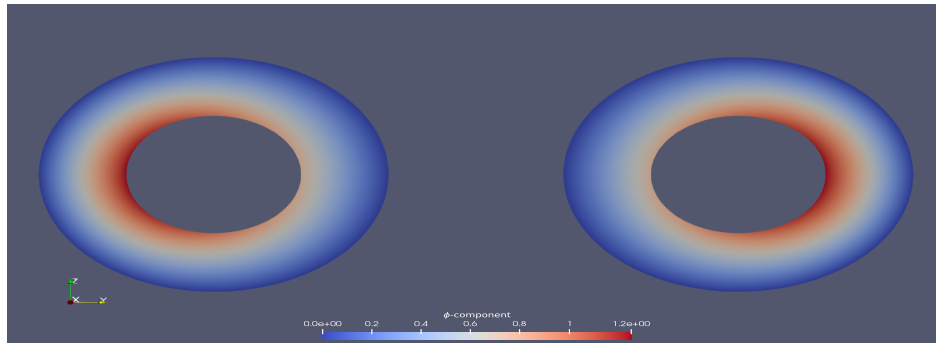


Figure 6.4: ϕ -component of velocity on $\phi = \frac{3\pi}{2}$ (left) and $\phi = \frac{\pi}{2}$ (right) at 100s for $r_a = 0.25$, $r_b = 0.28$, $Re = 5000$

At $Re = 5000$, we have the first kind of flow that can be described as intuitive or as Couette flow. The ϕ -component is the principal component of the velocity; there are negligible contributions from the r - and θ - components. The ϕ -component of velocity gradually decreases from the source of the rotation in the ϕ direction at the inner torus to the stationary outer torus as shown in Figure 6.4.

While negligible, the r - and θ - components of velocity exhibit properties that recur in many of the following cases and it is worth describing them here. While the r -component appears to be divided into two parts, the parity of the speeds indicates that the flow is directed towards the region of the torus that experiences higher speeds, see Figure 6.2. On the other hand, the θ -component is divided into two parts seemingly symmetric about $\theta = 0$ and compartmentalised in the regions where $0 < \theta < \pi$ and $\pi < \theta < 2\pi$, see Figure 6.3. The red or positive regions represent a counter-clockwise motion while the blue or negative regions represent a clockwise motion. We next examine the flow when the Reynolds number is increased to 8000.

6.1.2 Case 2, $r_a = 0.25$, $r_b = 0.28$, $Re = 8000$

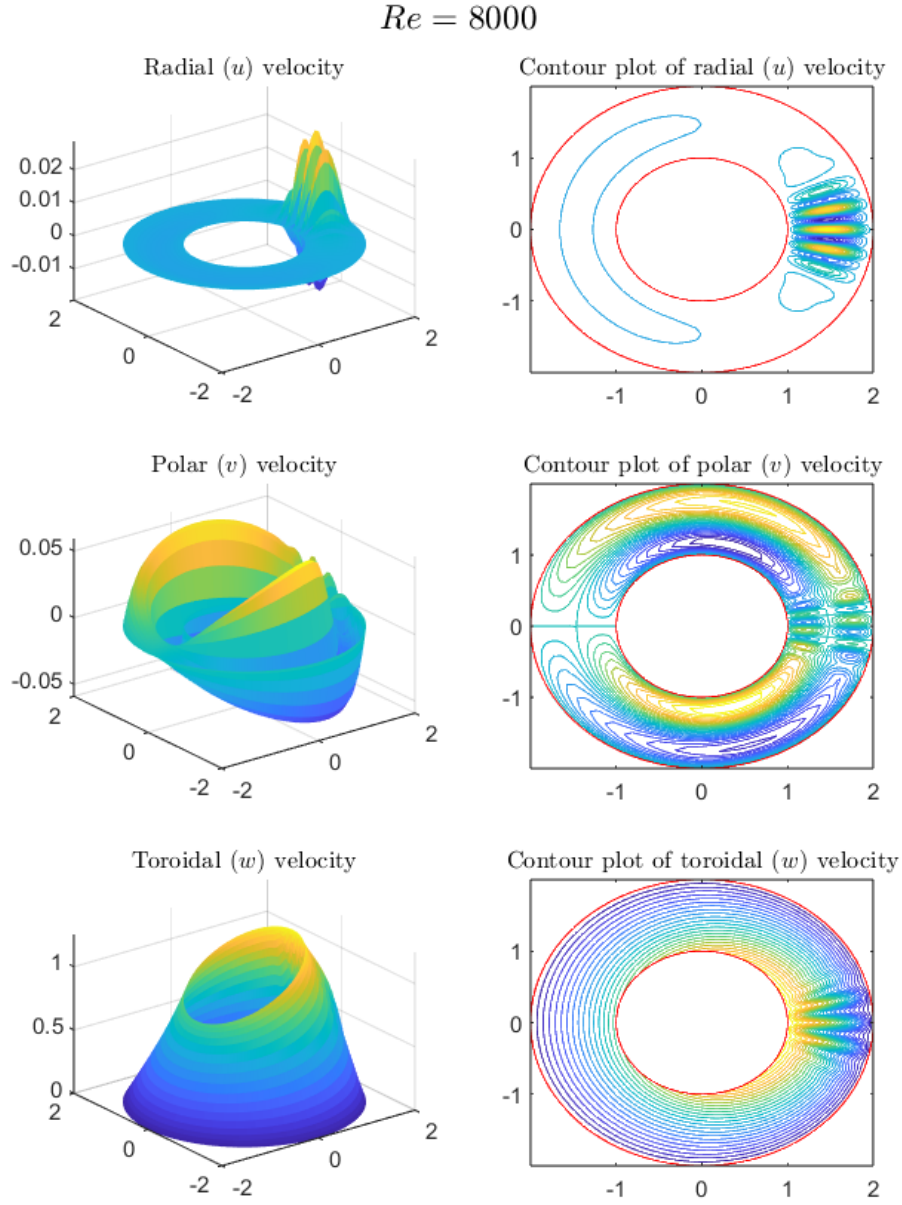


Figure 6.5: Velocity components at 100s for $r_a = 0.25$, $r_b = 0.28$, $Re = 8000$

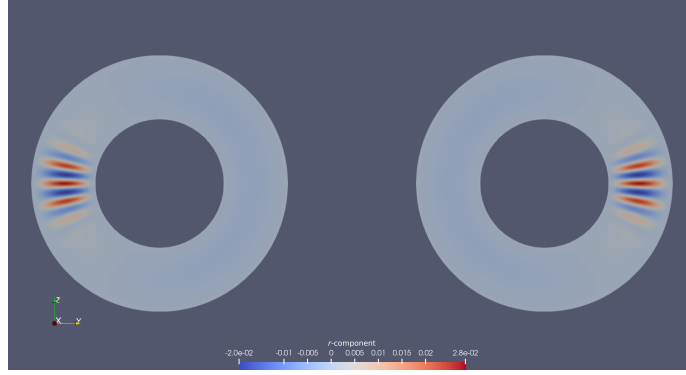


Figure 6.6: r -component of velocity on $\phi = \frac{3\pi}{2}$ (left) and $\phi = \frac{\pi}{2}$ (right) at 100s for $r_a = 0.25$, $r_b = 0.28$, $Re = 8000$

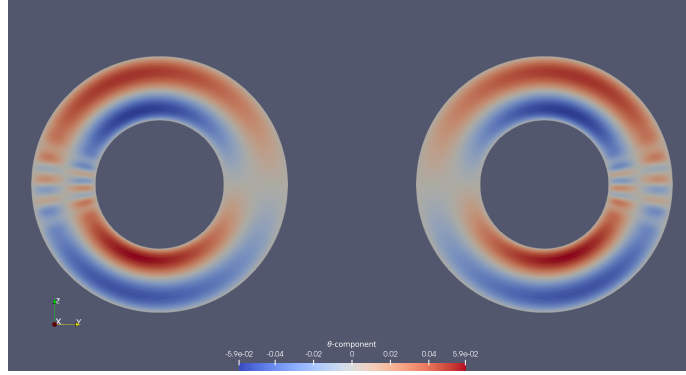


Figure 6.7: θ -component of velocity on $\phi = \frac{3\pi}{2}$ (left) and $\phi = \frac{\pi}{2}$ (right) at 100s for $r_a = 0.25$, $r_b = 0.28$, $Re = 8000$

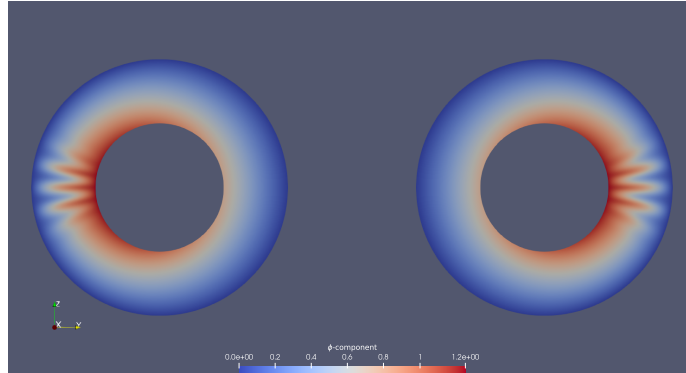


Figure 6.8: ϕ -component of velocity on $\phi = \frac{3\pi}{2}$ (left) and $\phi = \frac{\pi}{2}$ (right) at 100s for $r_a = 0.25$, $r_b = 0.28$, $Re = 8000$

Increasing the Reynolds number to 8000 reveals surprising behaviour in the flow and is illustrated in Figure 6.5. It is not clear if the flow naturally transitions from laminar flow at $Re = 5000$ to banded flow at $Re = 8000$. However, from the cylindrical and spherical counterparts, we expect a threshold Reynolds number for which the flow bifurcates. Distinct bands of speeds (alternatively called fingers or stripes) appear in all three velocity components in the regions of the torus where the speed of the fluid is highest. We examine each component of the flow individually.

The r -component has completely transformed from its state when $Re = 5000$. The speed is constant and acting towards the polar centre everywhere except in this new region which displays a novel flow pattern. In this region, the flow moves considerably faster as indicated by the intensity of the colour shown in Figure 6.6. The most remarkable feature is the alternating striped red and blue pattern that spans almost the entire gap width. The blue stripes represent flow towards the polar centre and the red stripes represent flow away from the polar centre. Presumably, the flow in the r -direction follows a sinusoid in the high-speed region and then smoothly transitions to a slower evenly distributed flow directed at the polar centre. Finally, we note that the r -component of flow is about an order of magnitude larger when compared with its counterpart at $Re = 5000$.

The θ -component has not changed as drastically as the r -component but still has notable features. It retains the features observed at $Re = 5000$ except in the high-speed region where the flow appears to be confined to several small compartments. Figure 6.7 reveals a red (counter-clockwise) and blue (clockwise) pattern unique to the θ -component. The compartments of flow are separated by what appears to be lines of zero speed. One line of zero speed appears approximately halfway between r_a and r_b and the other lines of zero speed are perpendicular and located in the high-speed region. Another strange observation is that the flow is not fastest in the high-speed region as again indicated by the colour intensity. We also note that the magnitude of the θ -component is roughly the same as it was when $Re = 5000$.

The ϕ -component, and the main component of the flow, also has remarkable behaviour as seen in Figure 6.8. The high-speed region contains bands of both high and low speed in the ϕ -direction that span roughly half the gap width. This feature persists in the overall velocity since the contributions from the other components are still much smaller than that present in the ϕ -component.

With such striking observations from the flow at $Re = 8000$, we are excited to see what happens when the Reynolds number is increased further at $Re = 15000$.

6.1.3 Case 3, $r_a = 0.25$, $r_b = 0.28$, $Re = 15000$

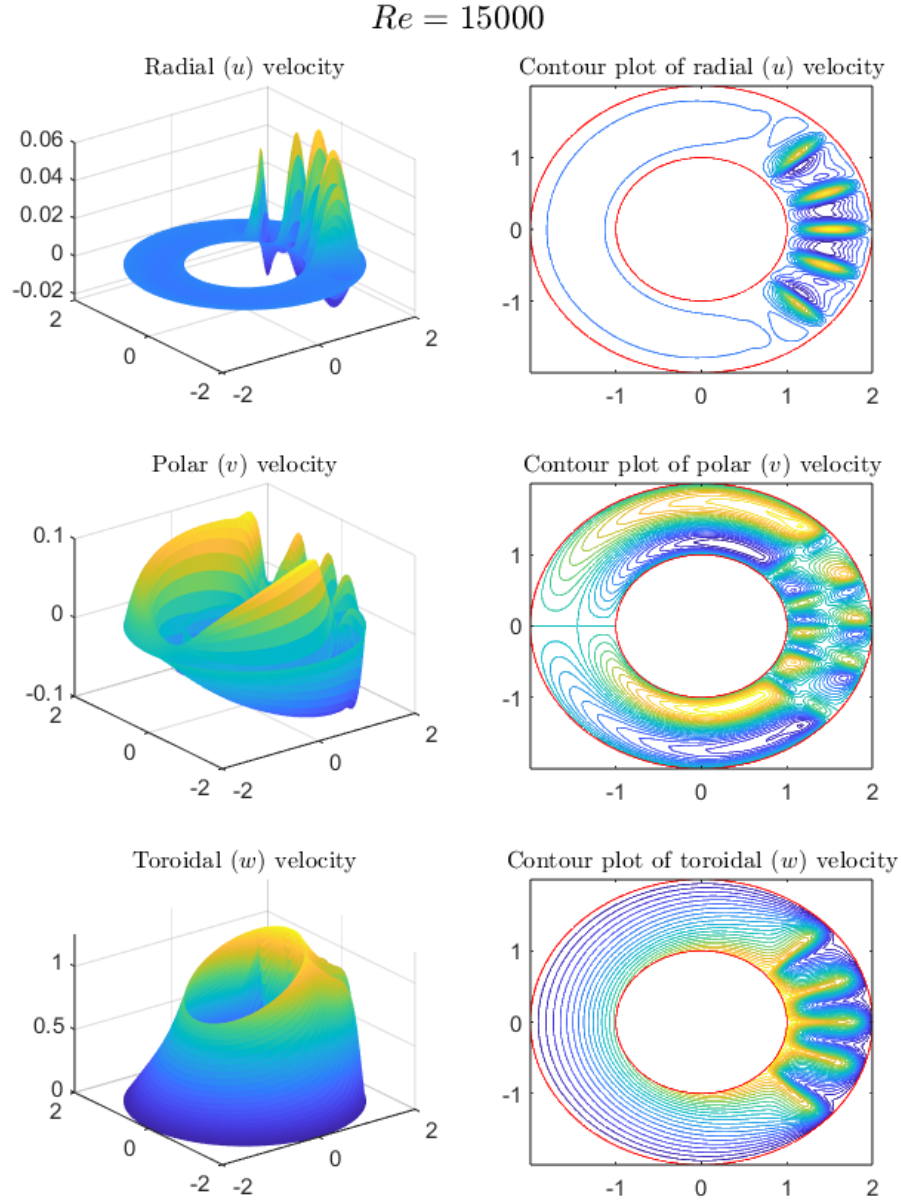


Figure 6.9: Velocity components at 100s for $r_a = 0.25$, $r_b = 0.28$, $Re = 15000$

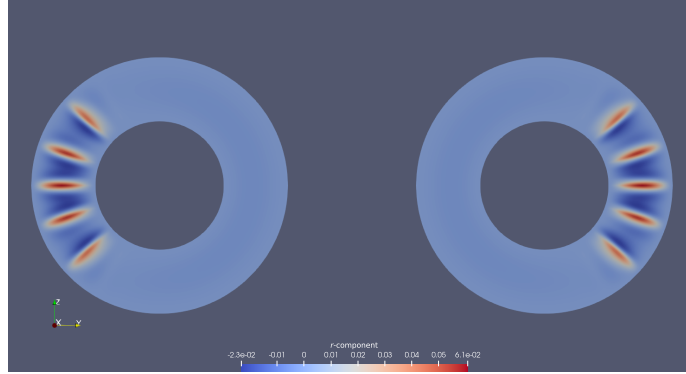


Figure 6.10: r -component of velocity on $\phi = \frac{3\pi}{2}$ (left) and $\phi = \frac{\pi}{2}$ (right) at 100s for $r_a = 0.25$, $r_b = 0.28$, $Re = 15000$

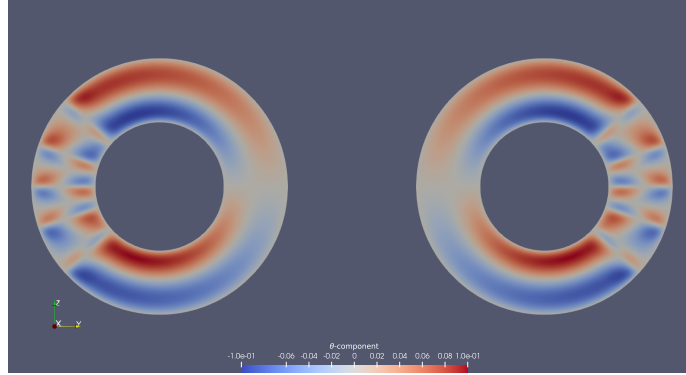


Figure 6.11: θ -component of velocity on $\phi = \frac{3\pi}{2}$ (left) and $\phi = \frac{\pi}{2}$ (right) at 100s for $r_a = 0.25$, $r_b = 0.28$, $Re = 15000$

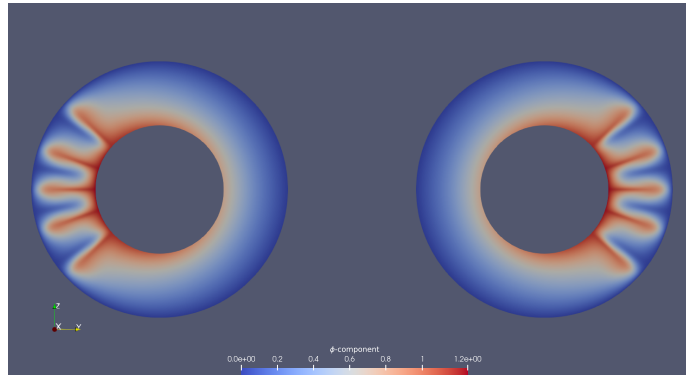


Figure 6.12: ϕ -component of velocity on $\phi = \frac{3\pi}{2}$ (left) and $\phi = \frac{\pi}{2}$ (right) at 100s for $r_a = 0.25$, $r_b = 0.28$, $Re = 15000$

At $Re = 15000$, the features observed at $Re = 8000$ become more prominent, widespread and numerous, see Figure 6.9. The alternating pattern now occupies a larger section of the gap and the overall velocity is distinguished with five fingers of high speed that span almost the entire gap width. There is a sharper velocity gradient near the boundary in the ϕ -component in the high-speed region because the fingers span almost the entire gap width which can be seen in Figure 6.10 and Figure 6.12.

6.1.4 Case 4, $r_a = 0.25$, $r_b = 0.28$, $Re = 20000$

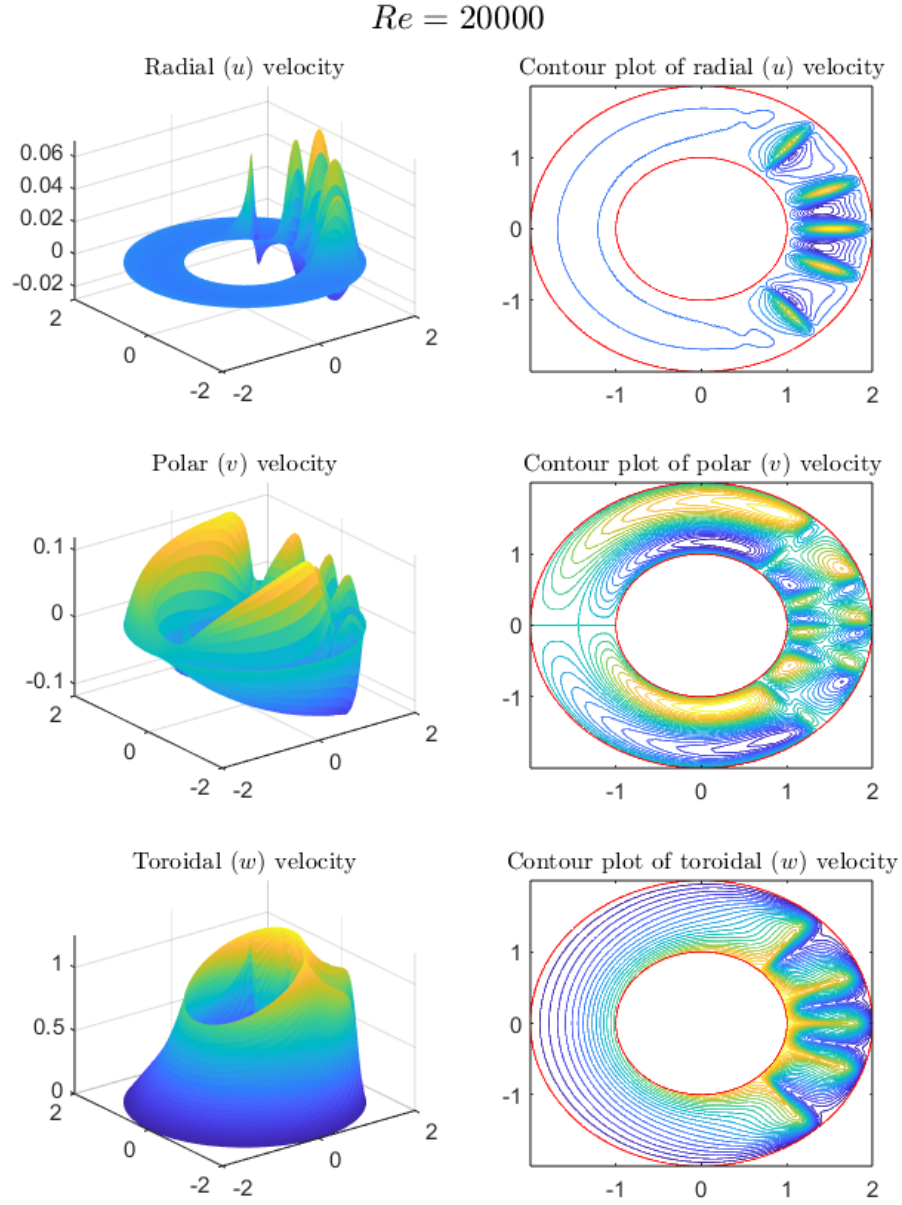


Figure 6.13: Velocity components at 100s for $r_a = 0.25$, $r_b = 0.28$, $Re = 20000$, $N_r = 30$

$Re = 20000$

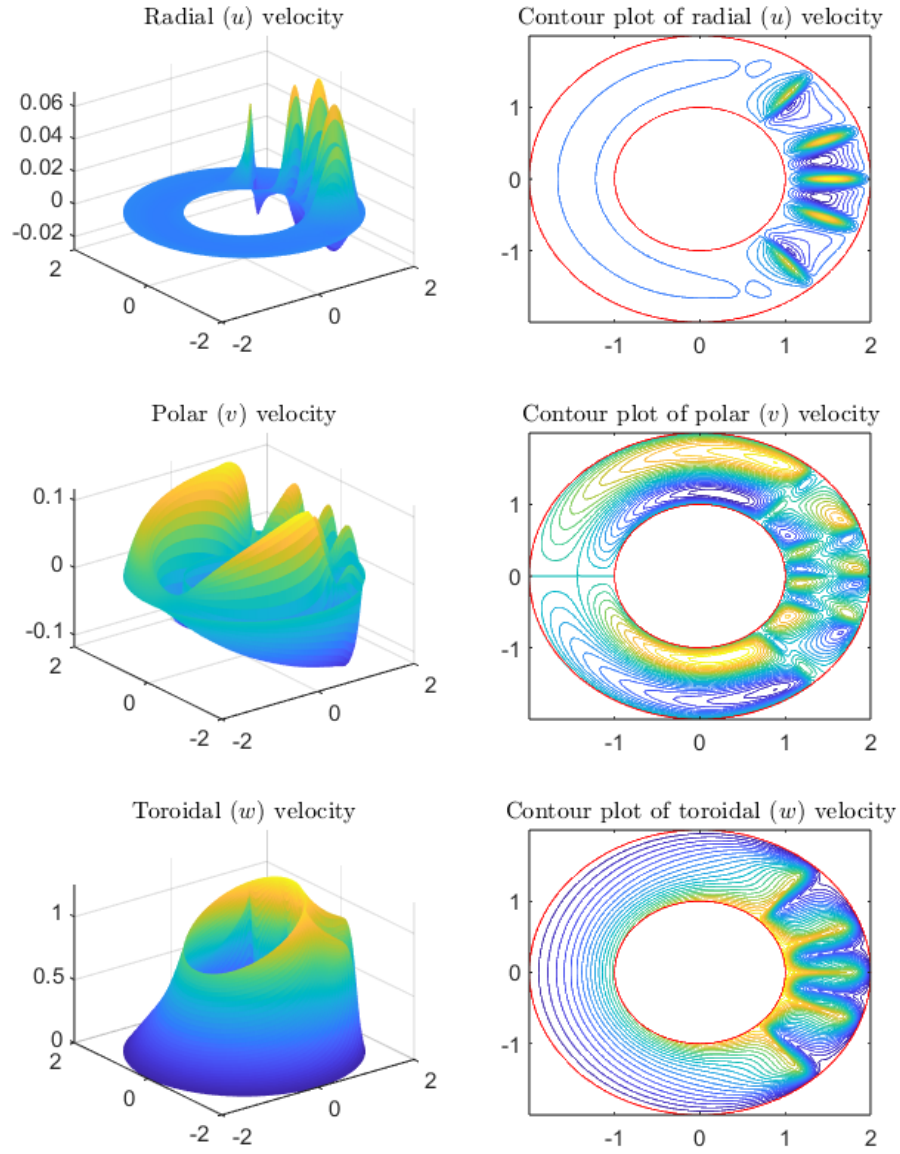


Figure 6.14: Velocity components at 100s for $r_a = 0.25$, $r_b = 0.28$, $Re = 20000$, $N_r = 40$

6.1.5 Case 5, $r_a = 0.25$, $r_b = 0.28$, $Re = 30000$

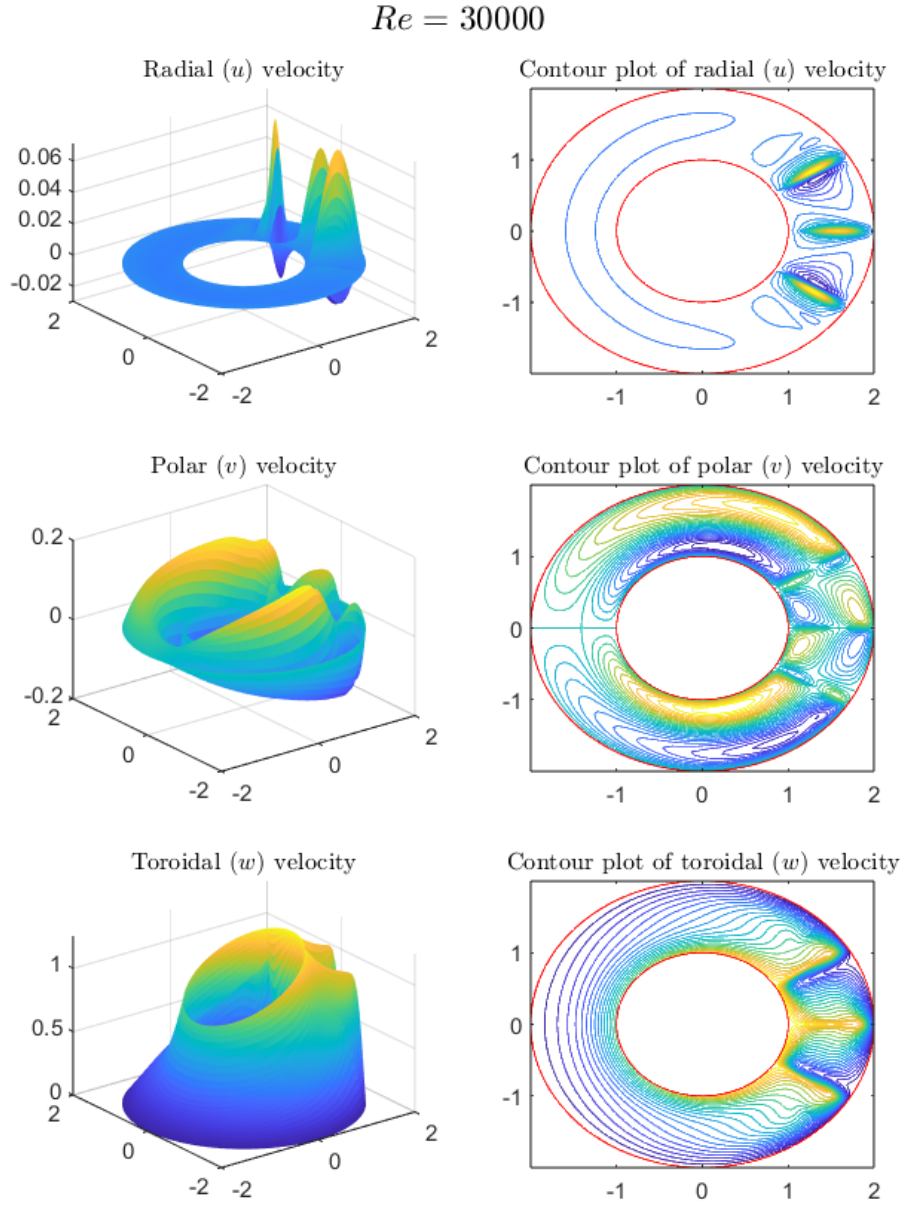


Figure 6.15: Velocity components at 100s for $r_a = 0.25$, $r_b = 0.28$, $Re = 30000$, $Nr = 30$

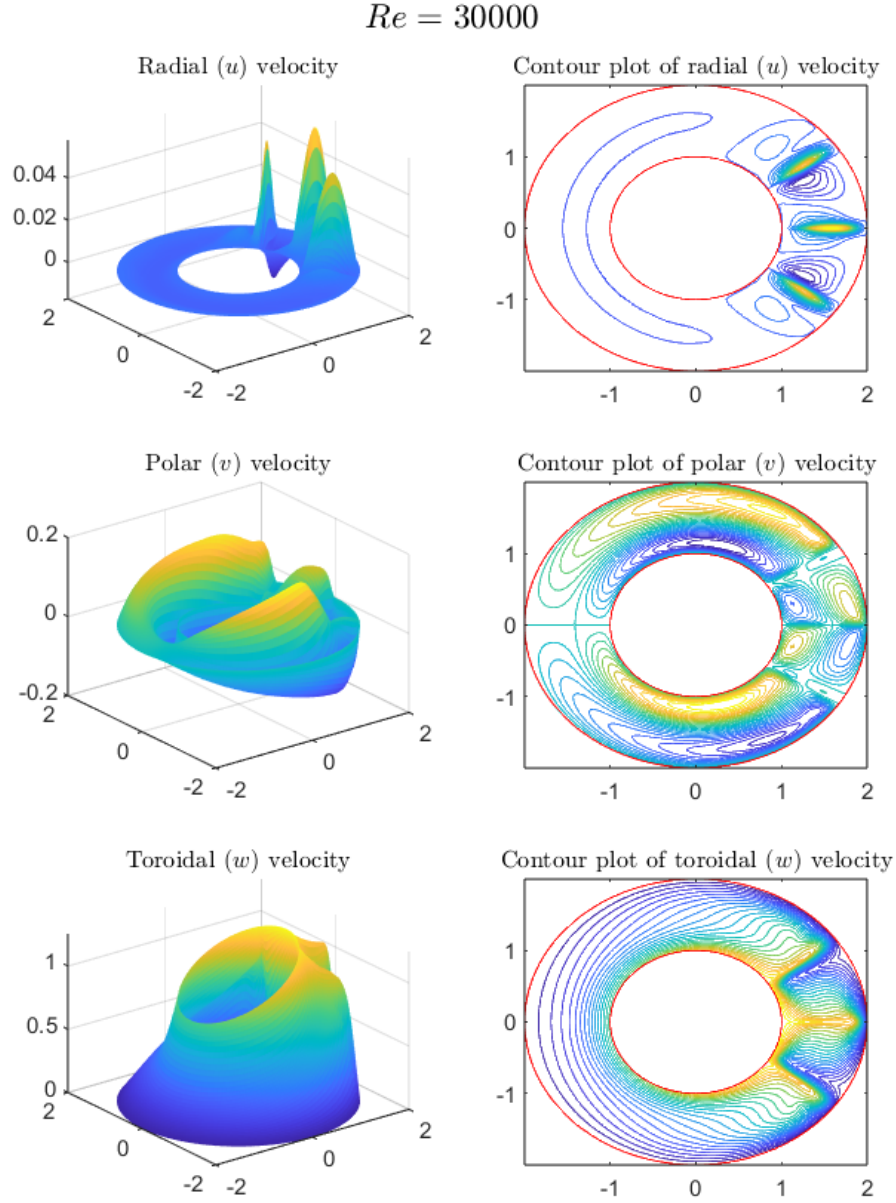


Figure 6.16: Velocity components at 100s for $r_a = 0.25$, $r_b = 0.28$, $Re = 30000$, $Nr = 40$

We examined two other higher Reynolds numbers, $Re = 20000$ and $Re = 30000$, but there is no significant change to the general flow features already observed. The number of fingers does not increase with the Reynolds number; at $Re = 20000$, we observe the same five fingers

but at $Re = 30000$, we observe three fingers, see Figure 6.13 and Figure 6.15.

Finally, we illustrate the flow generated with two different radial grid sizes: $Nr = 30$ (as shown in Table 6.1) and $Nr = 40$ for $Re = 20000$, see Figure 6.14, and for $Re = 30000$, see 6.16. These examples demonstrate that the flow pattern has converged properly since the results for both radial grids are the same.

6.1.6 Summary of results

The most obvious observation is that the flow changes significantly beyond a particular Reynolds number. The cylindrical and spherical counterparts both display a threshold Reynolds number and we expect the same in our toroidal geometry. Though we are unable to pin down the threshold Reynolds number, our simulations suggest it lies between $Re = 5000$ and $Re = 8000$. We expect Couette flow below this threshold, similar to what is observed at $Re = 5000$, and the first form of Taylor-Couette flow above this threshold.

However, the exact nature of the Taylor-Couette instabilities vary for the Reynolds numbers simulated. The most discernible difference is the number of fingers of high speed that appear in the overall velocity profiles. The number of fingers that appear at the simulated Reynolds numbers is summarised in Figure 6.17.

We stopped our numerical exploration at $Re = 30000$ because the numerical grids needed for larger Reynolds numbers required further refinement. Table 6.1 shows that Reynolds numbers at and beyond 15000 required ten more radial points than the cases for $Re = 5000$ and $Re = 8000$. Finer grids translate to longer run times which was untenable for the completion of a thesis with the computational resources available. Regardless, our simulations suggest that there is a range of Reynolds numbers for which the Taylor-Couette instabilities are most prominent.

Another observation is that the sharpness of the gradient on the boundary of the high-speed region of the ϕ -component increases with the Reynolds number. This is made clear in Figure 6.13 (for $Re = 20000$) and in Figure 6.15 (for $Re = 30000$) and is an expected result. The

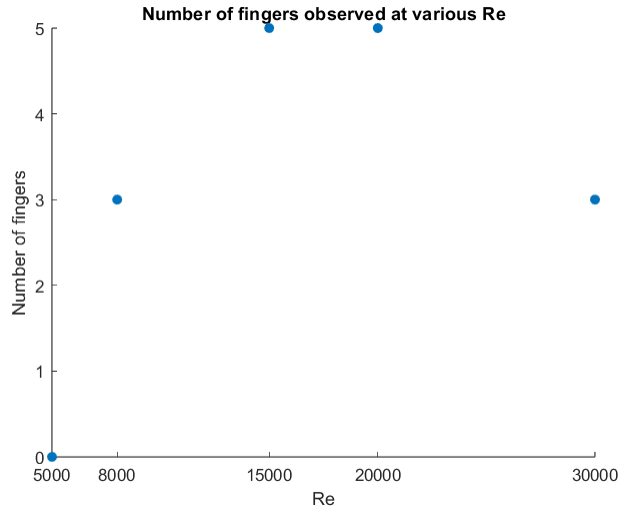


Figure 6.17: Number of fingers observed at various Reynolds numbers

r -component and θ -component are about 5% and 10% the magnitude of the ϕ -component respectively in Taylor-Couette flow.

Finally, none of the flows simulated exhibit dependence in the ϕ -direction; the Taylor-Couette instabilities observed are two-dimensional. In a subsequent section, we explore the flows generated by experimenting with different Reynolds numbers, different gap widths and longer times.

6.2 Pressure and divergence

We now consider two quantities of equal importance to the previously examined velocities: pressure and divergence. These quantities for all the cases examined in the first section of this chapter are shown in Figure 6.18, Figure 6.19, Figure 6.20, Figure 6.21 and Figure 6.22 respectively i.e. for $Re = 5000$, $Re = 8000$, $Re = 15000$, $Re = 20000$, $Re = 30000$.

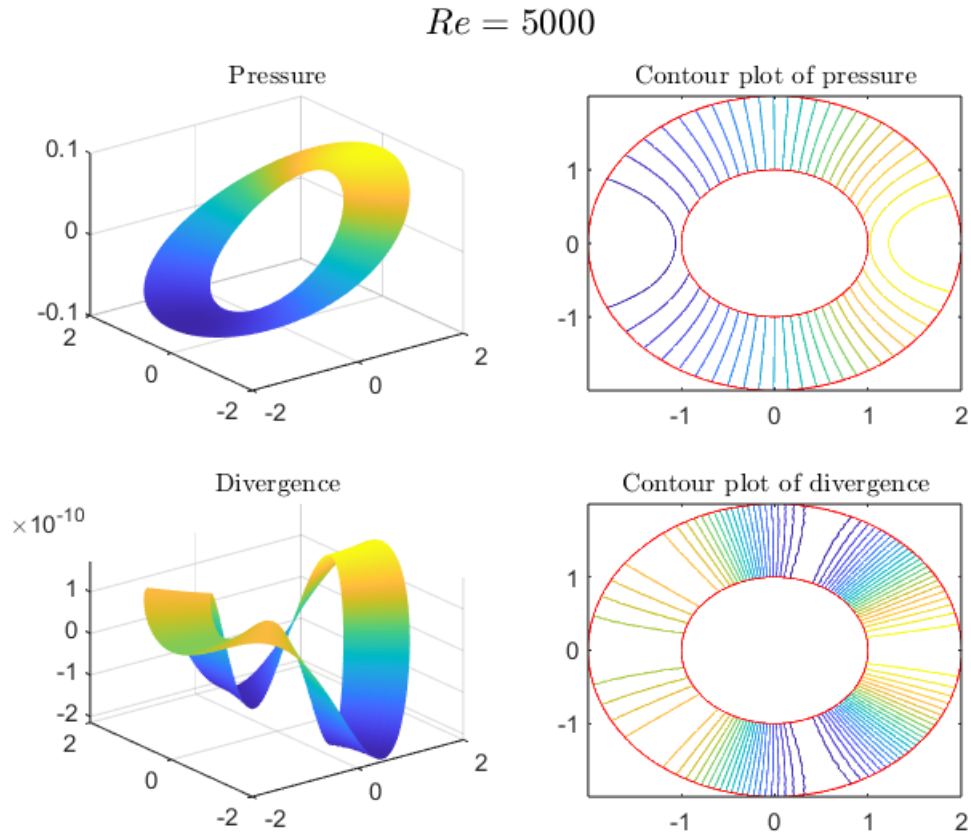


Figure 6.18: Pressure and divergence at 100s for $r_a = 0.25$, $r_b = 0.28$, $Re = 5000$ at $\phi = 0$

$Re = 8000$

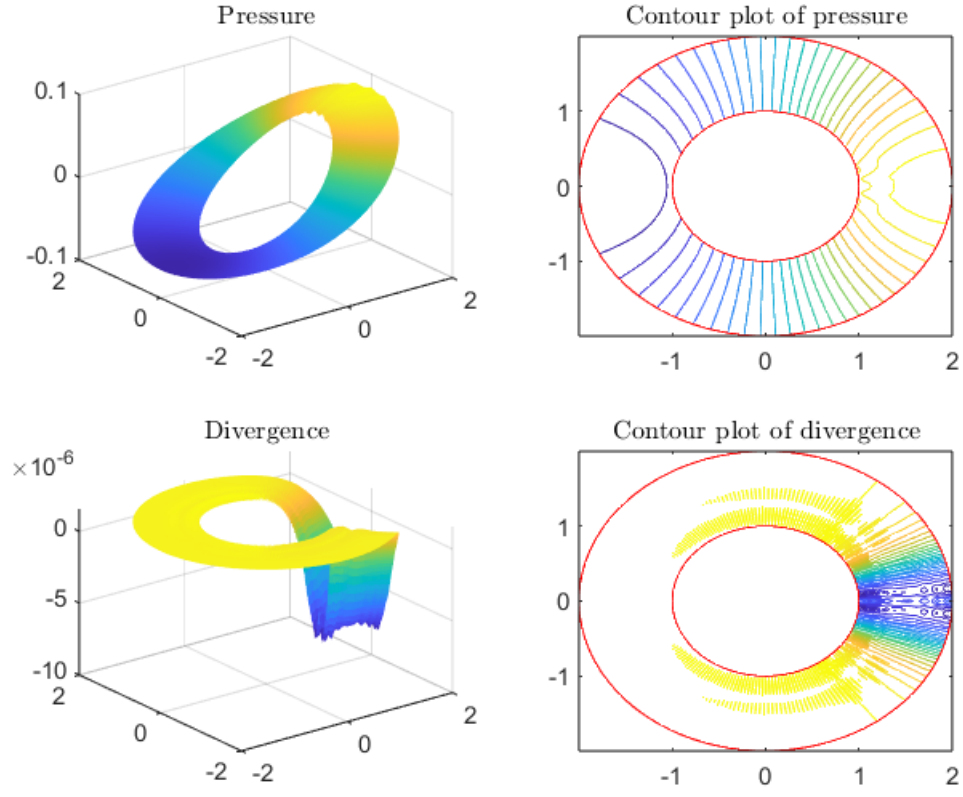


Figure 6.19: Pressure and divergence at 100s for $r_a = 0.25$, $r_b = 0.28$, $Re = 8000$ at $\phi = 0$

$Re = 15000$

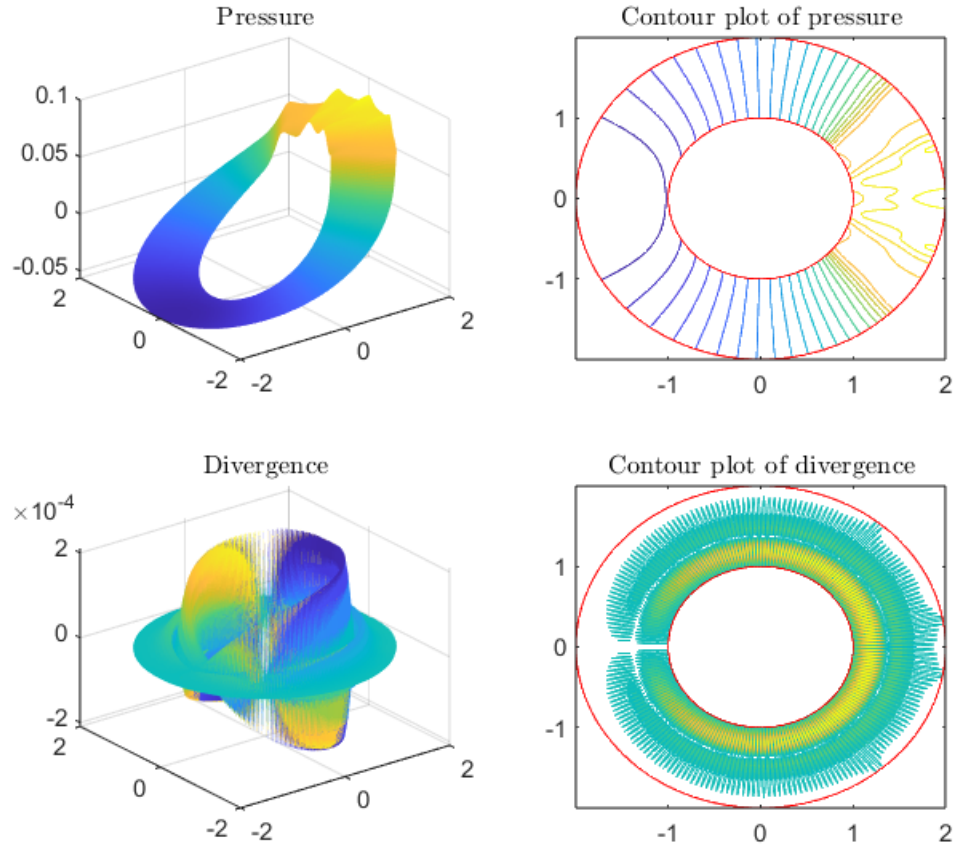


Figure 6.20: Pressure and divergence at 100s for $r_a = 0.25$, $r_b = 0.28$, $Re = 15000$ at $\phi = 0$

$Re = 20000$

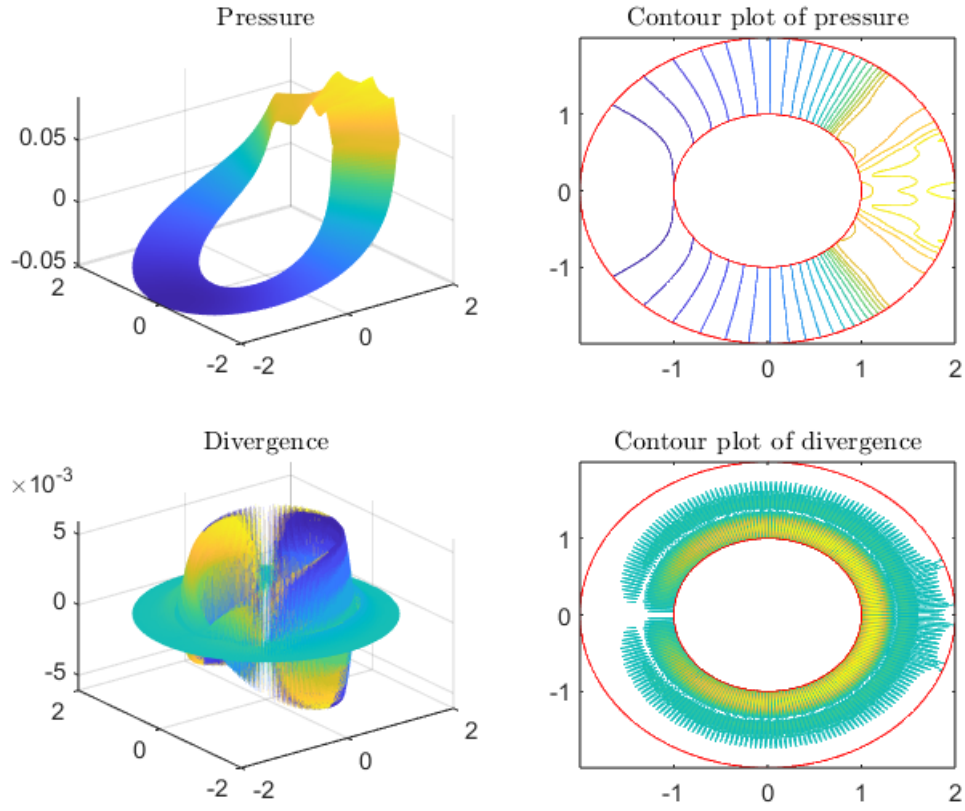


Figure 6.21: Pressure and divergence at 100s for $r_a = 0.25$, $r_b = 0.28$, $Re = 20000$ at $\phi = 0$

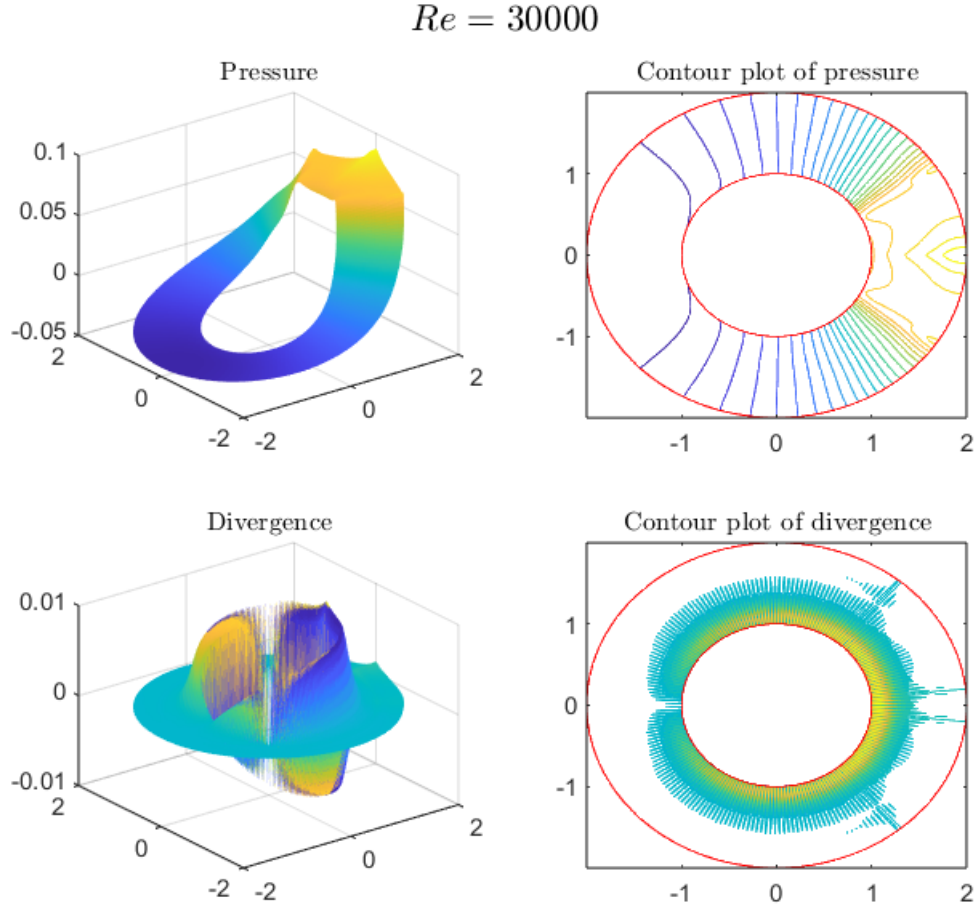


Figure 6.22: Pressure and divergence at 100s for $r_a = 0.25$, $r_b = 0.28$, $Re = 30000$ at $\phi = 0$

We observe that there appears to be negative pressure in all of the cases studied, an example of which can be found in Figure 6.18. However, this is a mathematical artifact of the Poisson equation and does not necessarily represent or is close to the true pressure. Recall that the imposed zero mean condition on the Poisson solver forces the solution to be such that the pressure, p , assumes negative values to uphold the zero mean condition. Additionally, the pressure, p , is not strictly necessary for the numerical solvers to work. Instead, it is the gradient of the pressure, ∇p , which is needed to update the velocity and the constant present in the true solution of the pressure Poisson equation vanishes when its gradient is calculated.

In spite of the potential absence of the true pressure, we can still use the numerically calculated

pressure to analyse our flows. At this point, we clarify what is meant by pressure in the context of the Navier-Stokes equations. Recall from a more abstract form of the Navier-Stokes equations that the pressure, p , is derived from the trace of the Cauchy stress tensor and refers to the volumetric stress experienced by fluid particles i.e. the forces experienced during deformation that typically change the volume of the fluid particle. This is not to be confused with other references of pressures (none of which appear in this thesis) such as gauge pressure or hydrostatic pressure.

As expected from rotating flows [93], we observe that the pressure is highest in the region furthest from the axis of rotation and lowest in the region closest to the axis of rotation. Upon rotation, a centripetal acceleration is generated that keeps the fluid moving in a circular path. In other words, there must exist a radial pressure gradient that balances the centrifugal force [94]. Additionally, Figure 6.20, Figure 6.21 and Figure 6.22 illustrate ripples in the pressure corresponding to the fingers observed in their respective velocity plots. These ripples are further described as alternating bands of high and low pressure variation in the θ -direction while still maintaining the radial pressure gradient. At lower Reynolds numbers, there are no fully formed fingers so the pressure is without these ripples and, therefore, smoother.

Recall that zero divergence throughout the domain for all $t \geq 0$ was crucial in establishing equivalence between the Navier-Stokes equations and its pressure Poisson formulation. We note that the divergence is effectively zero everywhere which is not only a useful sanity check but also as a kind of error measure. While the divergence is not exactly zero, as seen in Figure 6.18, because of numerical error which accumulates over each time iteration, it is remarkably small everywhere (almost to machine precision in this instance) and is considered sufficient for our work.

However, from $Re = 15000$ onward, it becomes more difficult to make the argument that the zero divergence requirement is upheld. While this is a serious breach, it can be easily rectified by using finer grids and it does not affect the key features of the flow. For the cases studied in this section, further refining the radial grid reduces the maximum absolute value of the

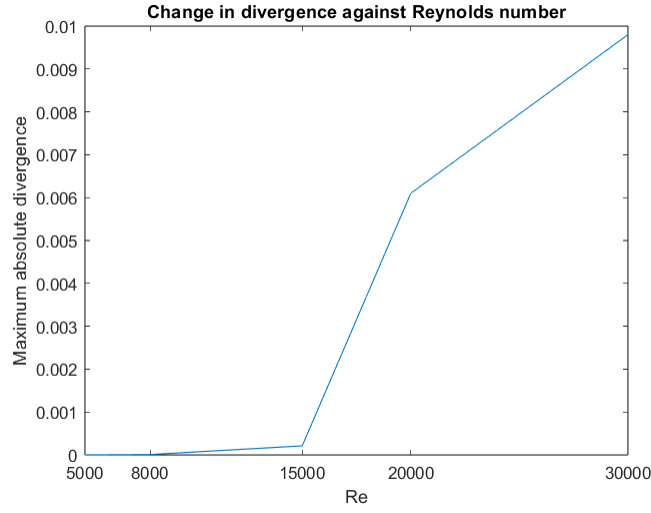


Figure 6.23: Change in divergence against Reynolds number

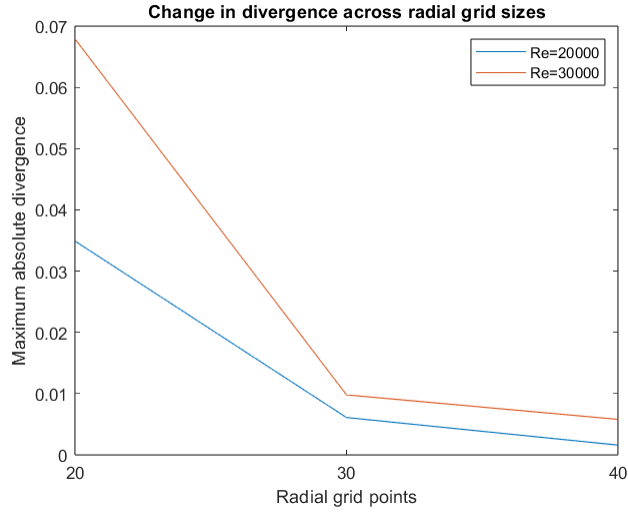


Figure 6.24: Change in divergence with different radial grid points

divergence. In particular, the radial grids for $Re = 15000$, $Re = 20000$ and $Re = 25000$ are finer than those for $Re = 5000$ and $Re = 8000$, see Table 6.1, because the maximum absolute divergence in each of these cases was too large. However, the increase in the number of radial grid points is accompanied by a severe computational burden making it tedious to explore its impact on the divergence while providing little to no impact on the overall flow features. We illustrate these ideas in Figure 6.24 for the previously examined cases of $Re = 20000$ and

$Re = 30000$ and recall that the flow was similar for $Nr = 30$ and $Nr = 40$ for each of these Reynolds numbers.

In the subsequent sections, we omit plots for the pressure and divergence to avoid a large collection of figures that are visually similar.

6.3 Longer time simulations and wider gaps

Longer time simulations are necessary to determine the stability of the various flows that were observed in the previous section. In the following simulations, the spin-up time was increased from 50s to 500s. We begin by observing the development of the flow through the spin-up time and beyond while keeping the other parameters fixed so that we may observe the various stages of evolution of the flow. We took snapshots of the velocity and pressure at every 100s for the first 600s and then at 1000s. For each snapshot in time, we have the following types of figures though not all of them are presented for brevity of presentation and to avoid needless repetition.

- Profile of each velocity component, u , v and w , and their corresponding contour plots generated using MATLAB
- Cross-sections of the tori which illustrate the speed of the flow at each point between the two tori generated using Paraview
- Profile of the pressure, p , and divergence, $\nabla \cdot \mathbf{u}$, within the domain and their corresponding contour plots generated using MATLAB

Note that we have magnified the gap between the tori in the subsequent plots purely for visual effect; magnification does not change the fundamental features of the flow. We first show the flow only after spin-up at 500s and after the flow has (almost) fully developed at 1000s for a fixed Reynolds number and then discuss the three cases after the figures. Finally, we summarise the impact of widening the gap on the flow for all Reynolds numbers.

6.3.1 Case 1, $r_a = 0.25$, $r_b = 0.28$, $Re = 15000$

We begin with the following parameters in Table 6.2 which explore the effect of widening the gap width for $Re = 15000$.

N_r	N_θ	N_ϕ	Re	r_a	$\mathbf{r_b}$	R_0	Spin-up	Sub-section	Figures
25	125	40	15000	0.25	0.28	1.0	500s	Case 1	6.25, 6.26, 6.27, 6.28, 6.29, 6.30
25	125	40	15000	0.25	0.30	1.0	500s	Case 2	6.31, 6.32, 6.33, 6.34, 6.35, 6.36
30	125	40	15000	0.25	0.35	1.0	500s	Case 3	6.37, 6.38, 6.39, 6.40, 6.41, 6.42

Table 6.2: Parameters used to study the effect of increasing gap width at $Re = 15000$

At 500s

$Re = 15000$

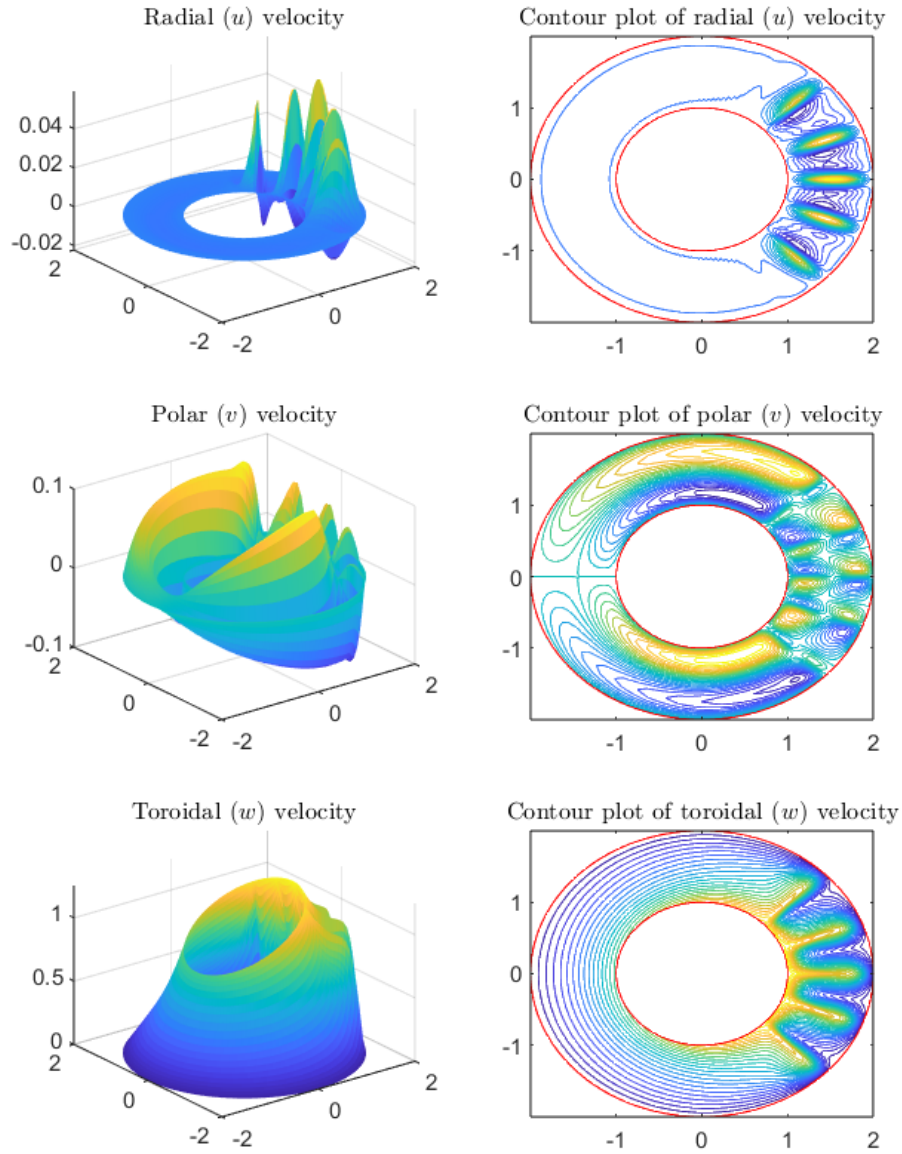


Figure 6.25: Velocity components at 500s for $r_a = 0.25$, $r_b = 0.28$, $Re = 15000$

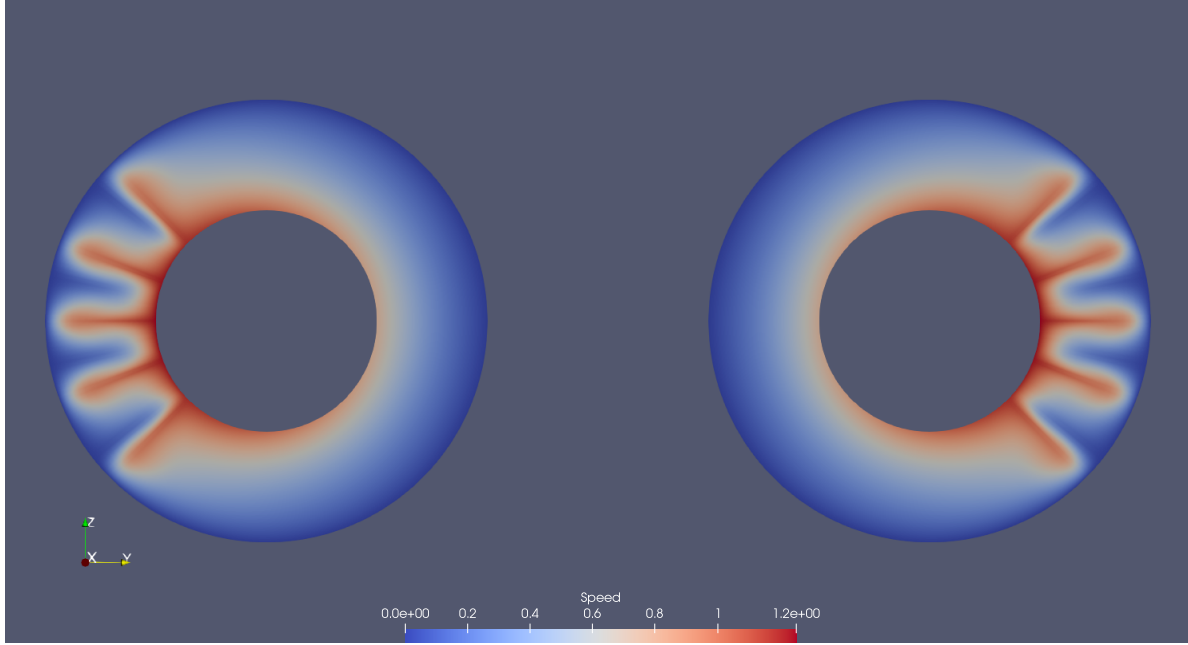


Figure 6.26: Speed at 500s on $\phi = \frac{3\pi}{2}$ (left) and $\phi = \frac{\pi}{2}$ (right) for $r_a = 0.25$, $r_b = 0.28$, $Re = 15000$

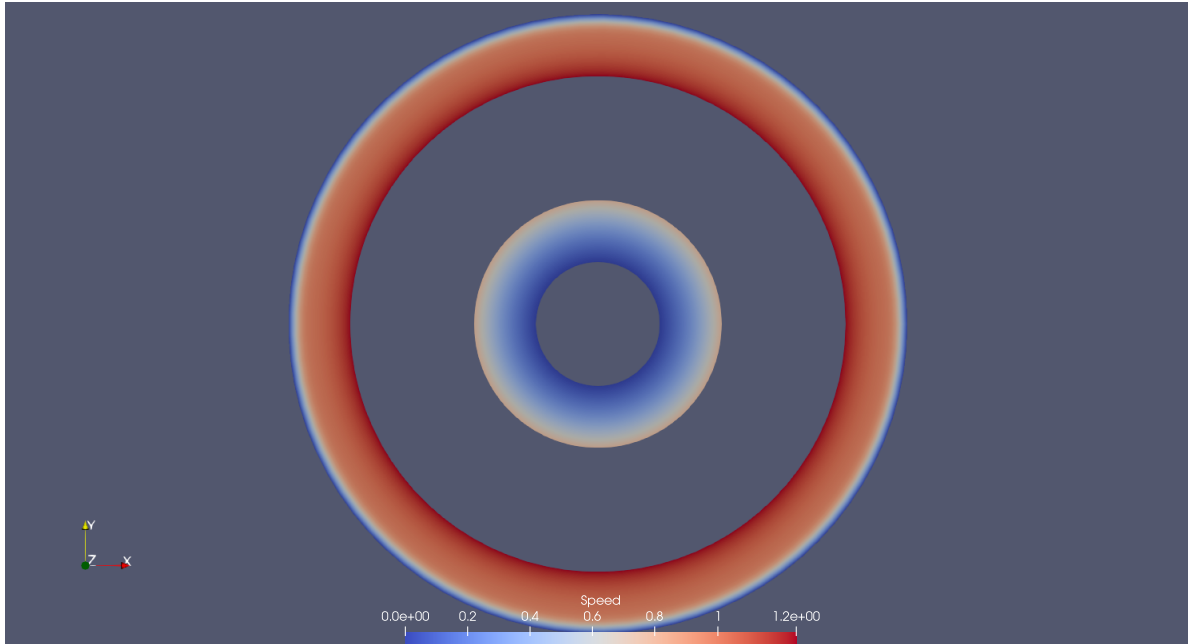


Figure 6.27: Speed at 500s on the plane $\theta = 0$ for $r_a = 0.25$, $r_b = 0.28$, $Re = 15000$

At 1000s

$Re = 15000$

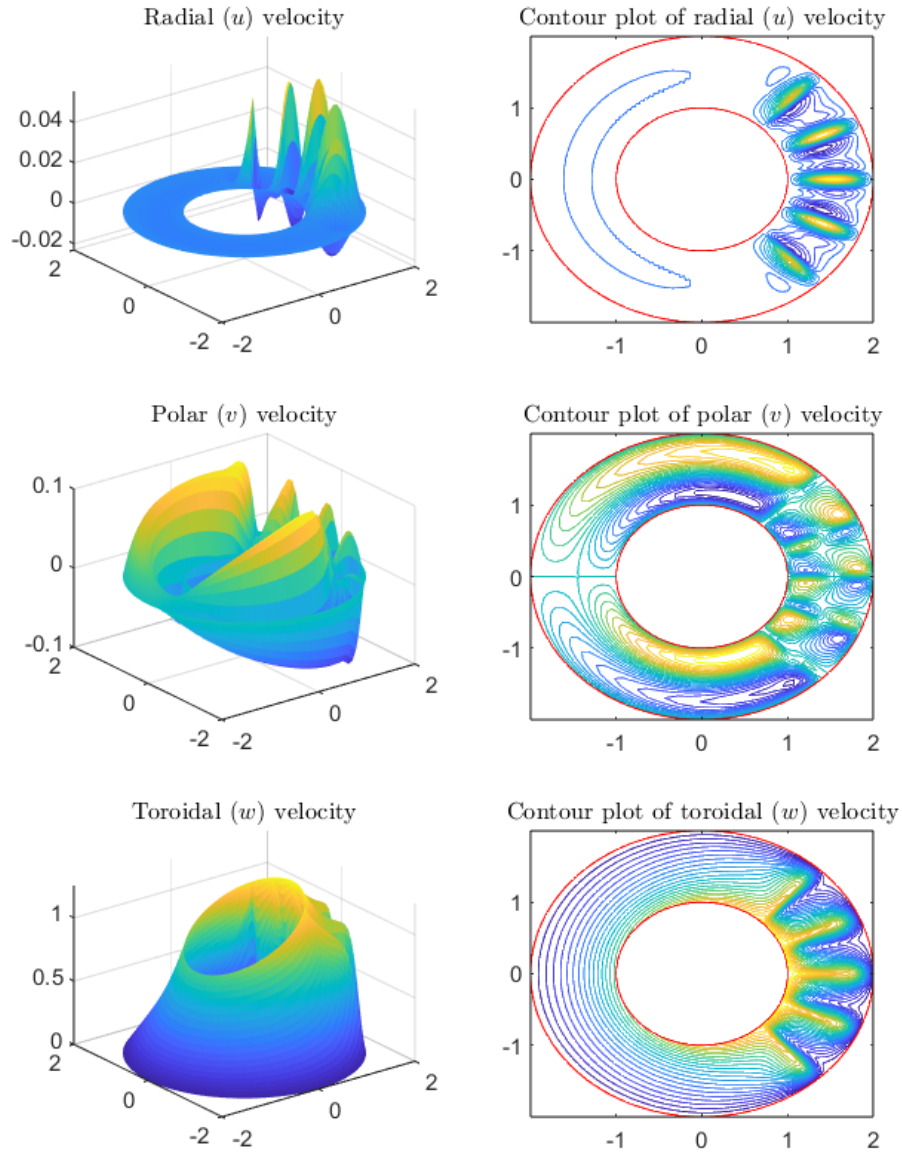


Figure 6.28: Velocity components at 1000s for $r_a = 0.25$, $r_b = 0.28$, $Re = 15000$

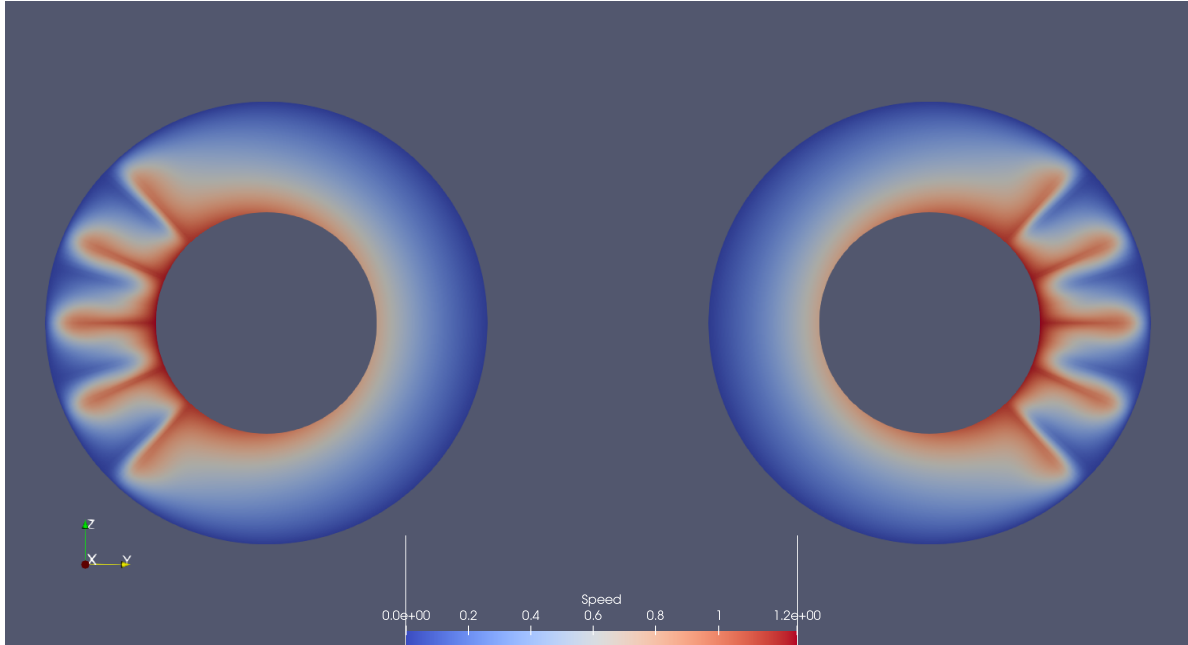


Figure 6.29: Speed at 1000s on $\phi = \frac{3\pi}{2}$ (left) and $\phi = \frac{\pi}{2}$ (right) for $r_a = 0.25$, $r_b = 0.28$, $Re = 15000$

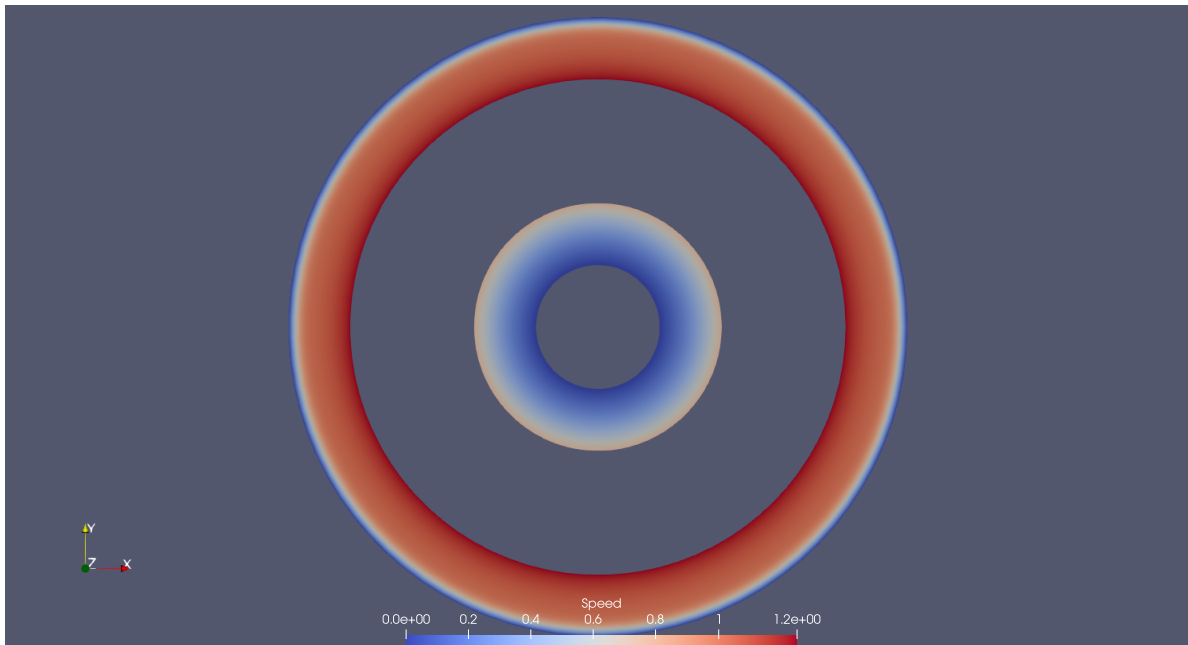


Figure 6.30: Speed at 1000s on the plane where $\theta = 0$ for $r_a = 0.25$, $r_b = 0.28$, $Re = 15000$

6.3.2 Case 2, $r_a = 0.25$, $r_b = 0.30$, $Re = 15000$

At 500s

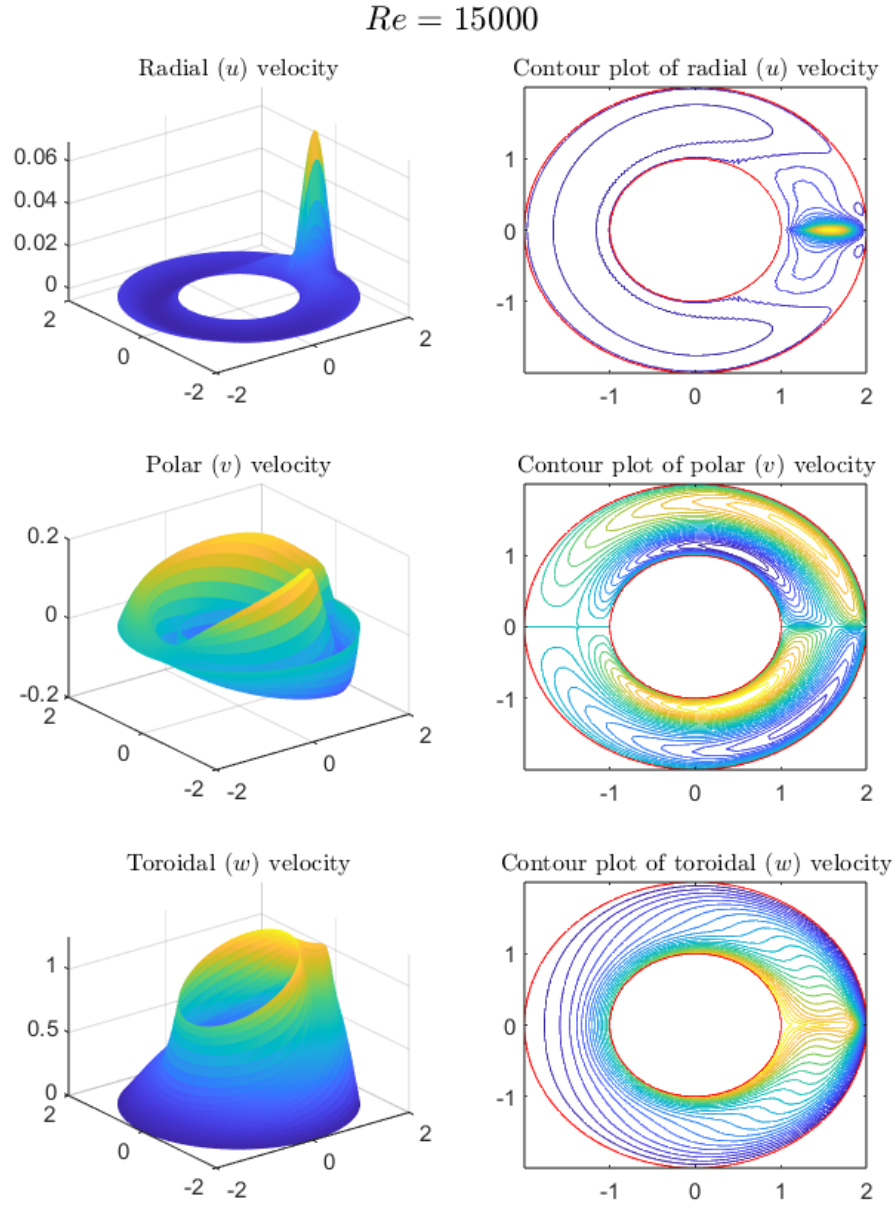


Figure 6.31: Velocity components at 500s for $r_a = 0.25$, $r_b = 0.30$, $Re = 15000$

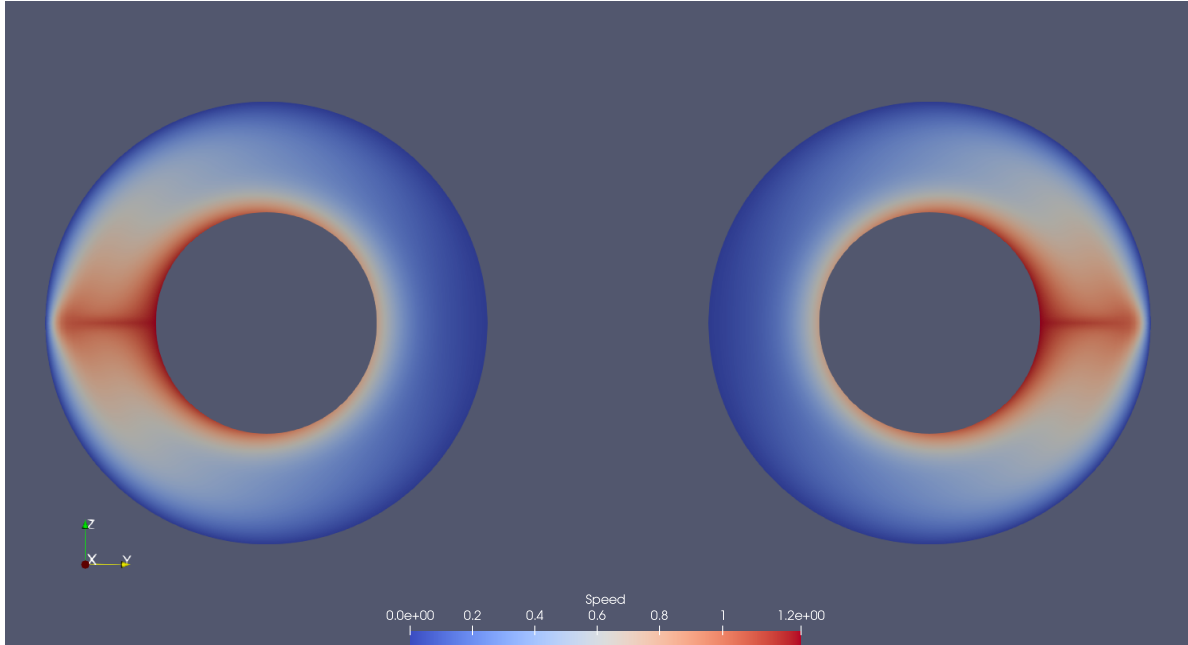


Figure 6.32: Speed at 500s on $\phi = \frac{3\pi}{2}$ (left) and $\phi = \frac{\pi}{2}$ (right) for $r_a = 0.25$, $r_b = 0.30$, $Re = 15000$

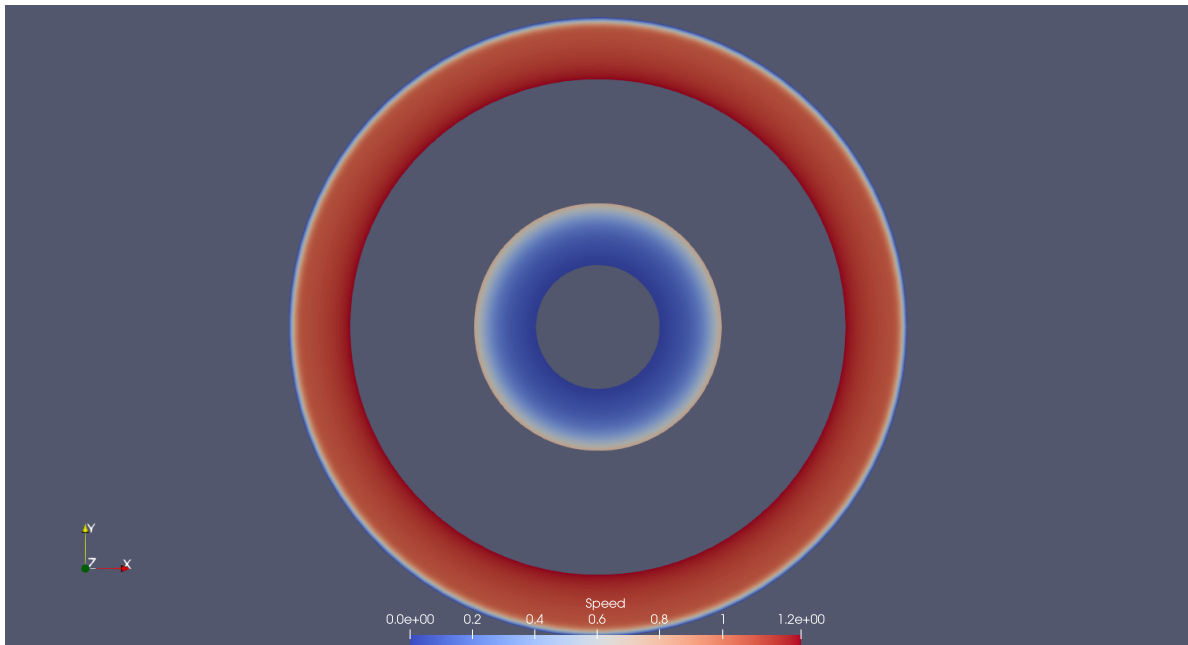


Figure 6.33: Speed at 500s on the plane $\theta = 0$ for $r_a = 0.25$, $r_b = 0.30$, $Re = 15000$

At 1000s

$Re = 15000$

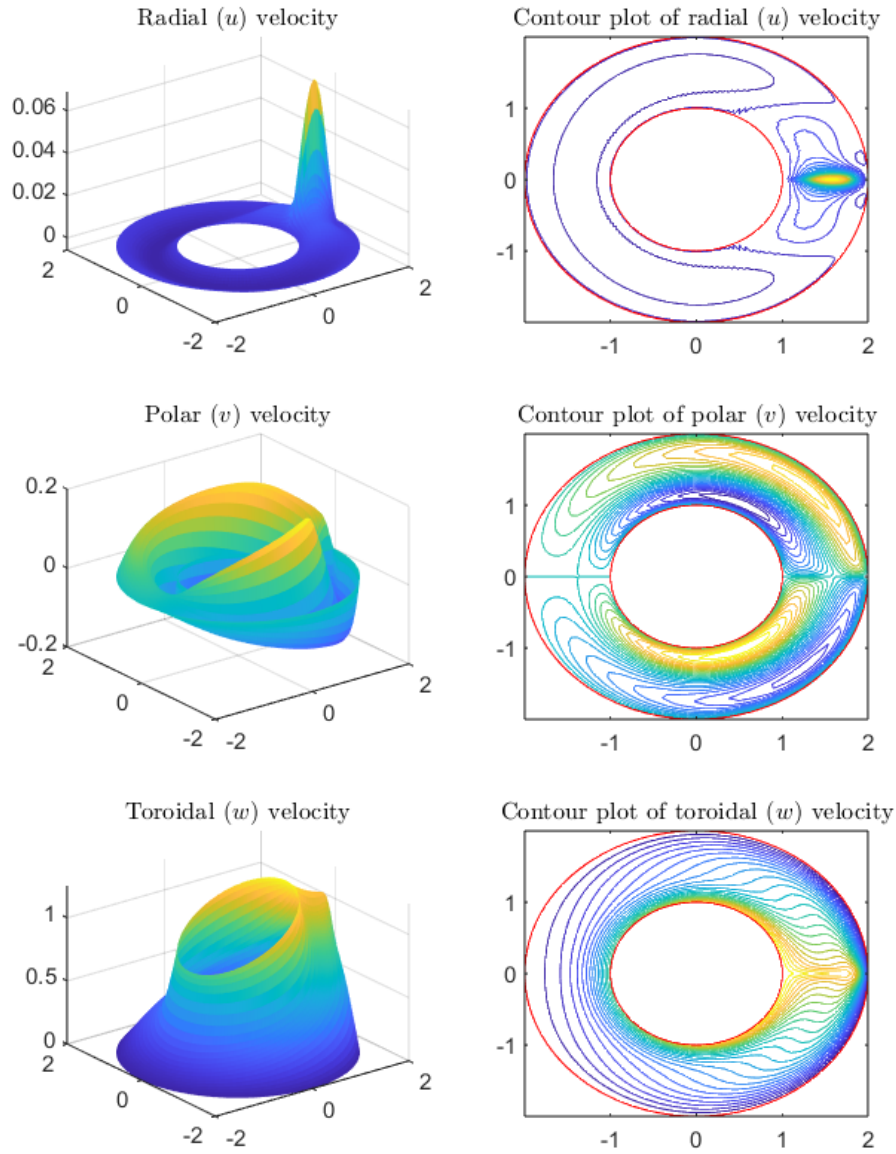


Figure 6.34: Velocity components at 1000s for $r_a = 0.25$, $r_b = 0.30$, $Re = 15000$

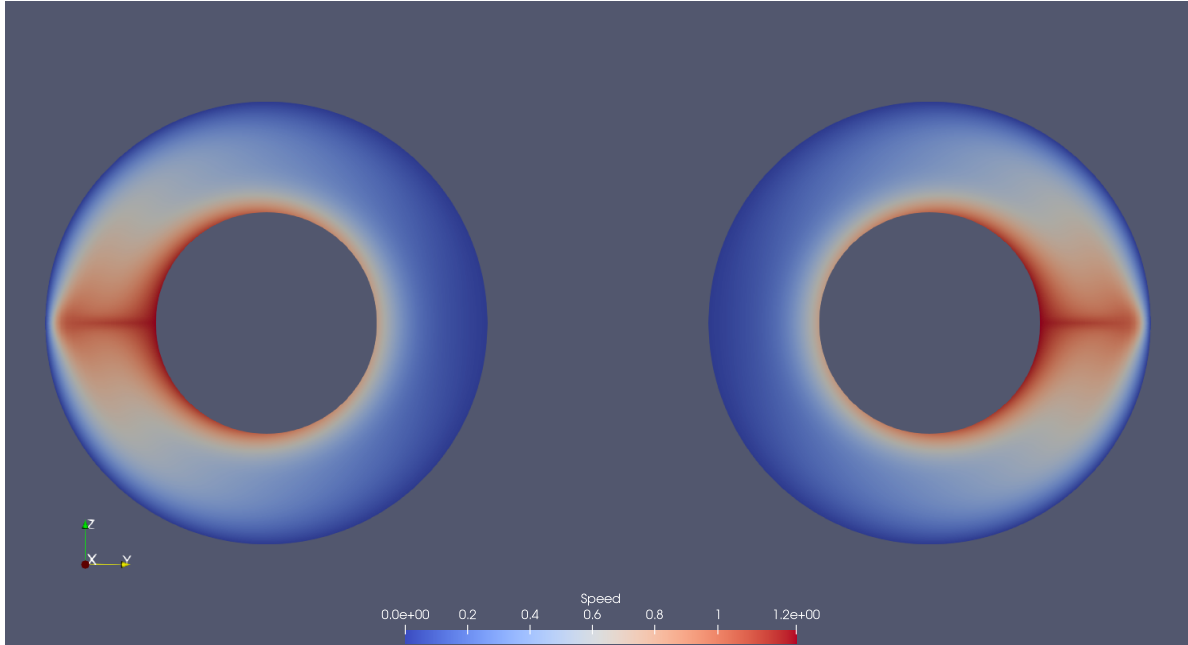


Figure 6.35: Speed at 1000s on $\phi = \frac{3\pi}{2}$ (left) and $\phi = \frac{\pi}{2}$ (right) for $r_a = 0.25$, $r_b = 0.30$, $Re = 15000$

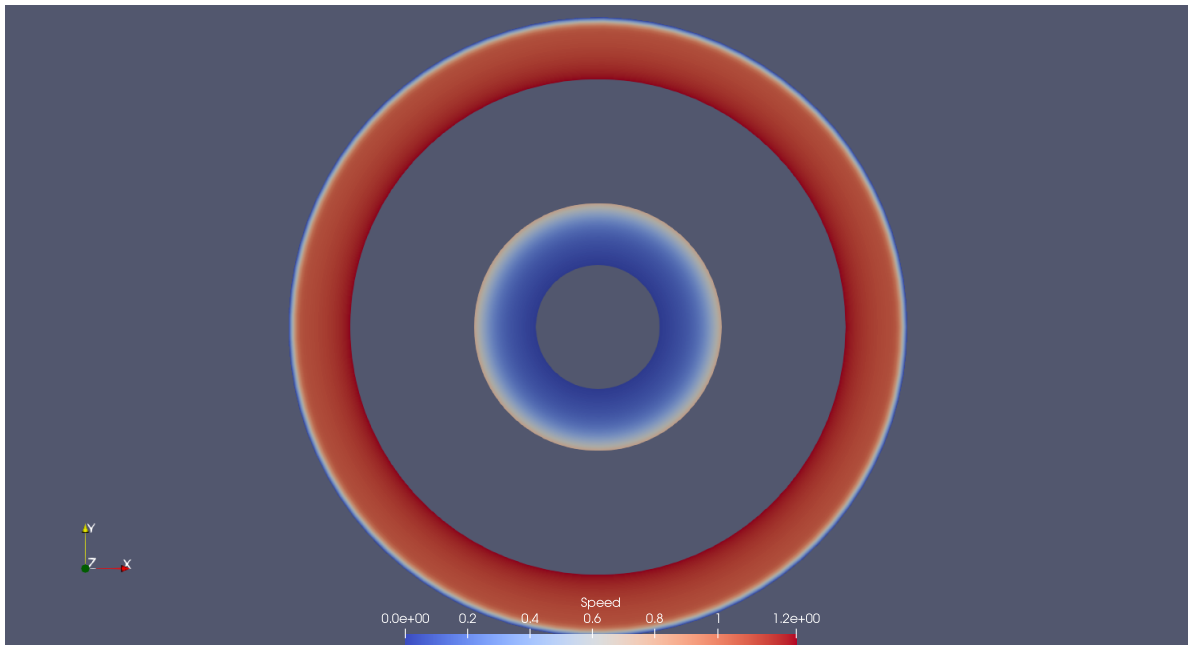


Figure 6.36: Speed at 1000s on the plane $\theta = 0$ for $r_a = 0.25$, $r_b = 0.30$, $Re = 15000$

6.3.3 Case 3, $r_a = 0.25$, $r_b = 0.35$, $Re = 15000$

At 500s

At 500s

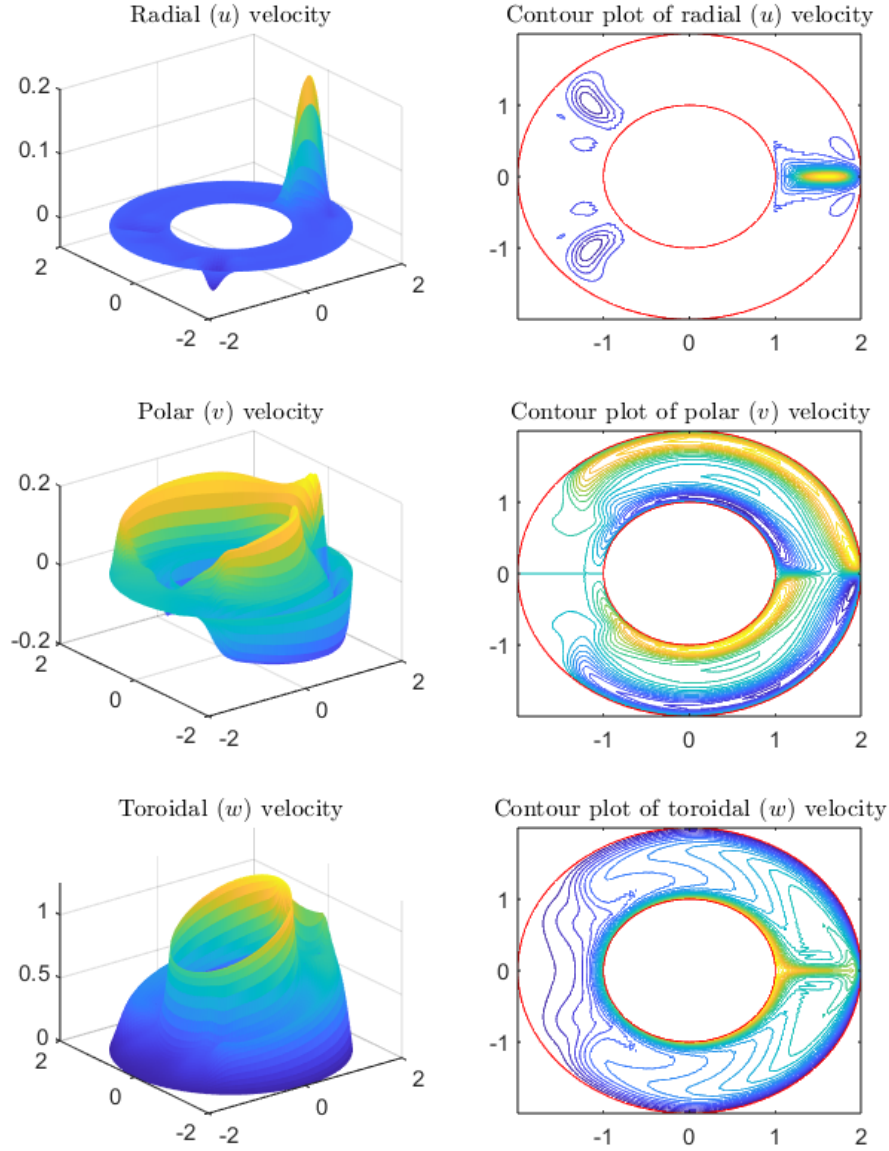


Figure 6.37: Velocity components at 500s for $r_a = 0.25$, $r_b = 0.35$, $Re = 15000$

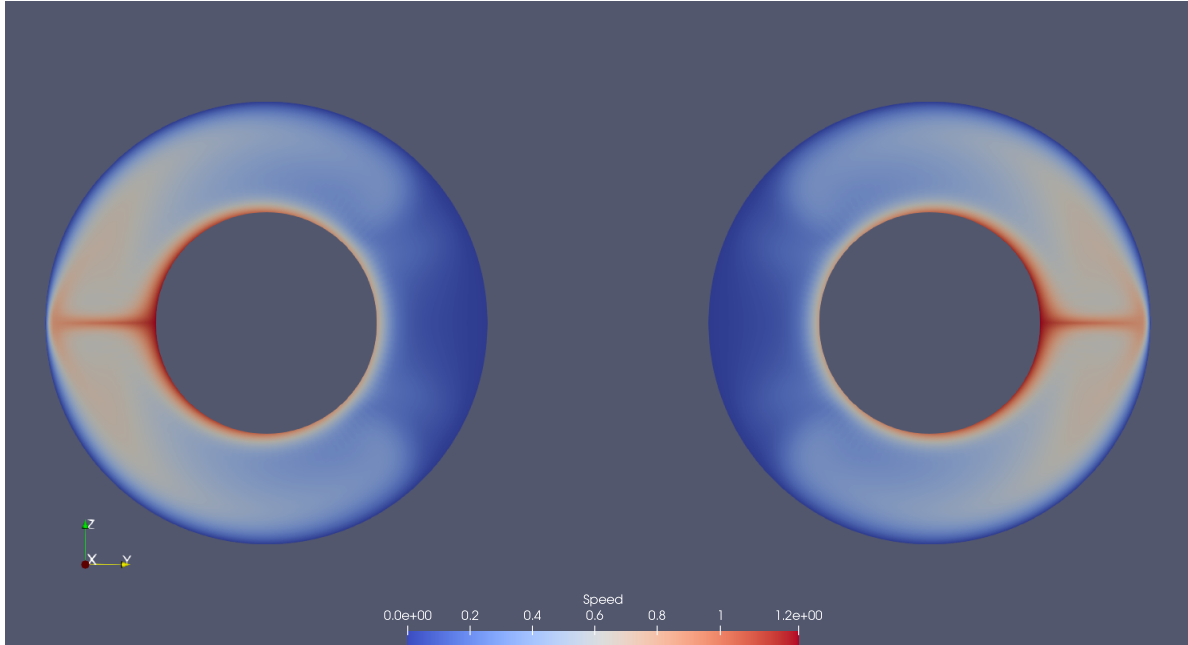


Figure 6.38: Speed at 500s on $\phi = \frac{3\pi}{2}$ (left) and $\phi = \frac{\pi}{2}$ (right) for $r_a = 0.25$, $r_b = 0.35$, $Re = 15000$

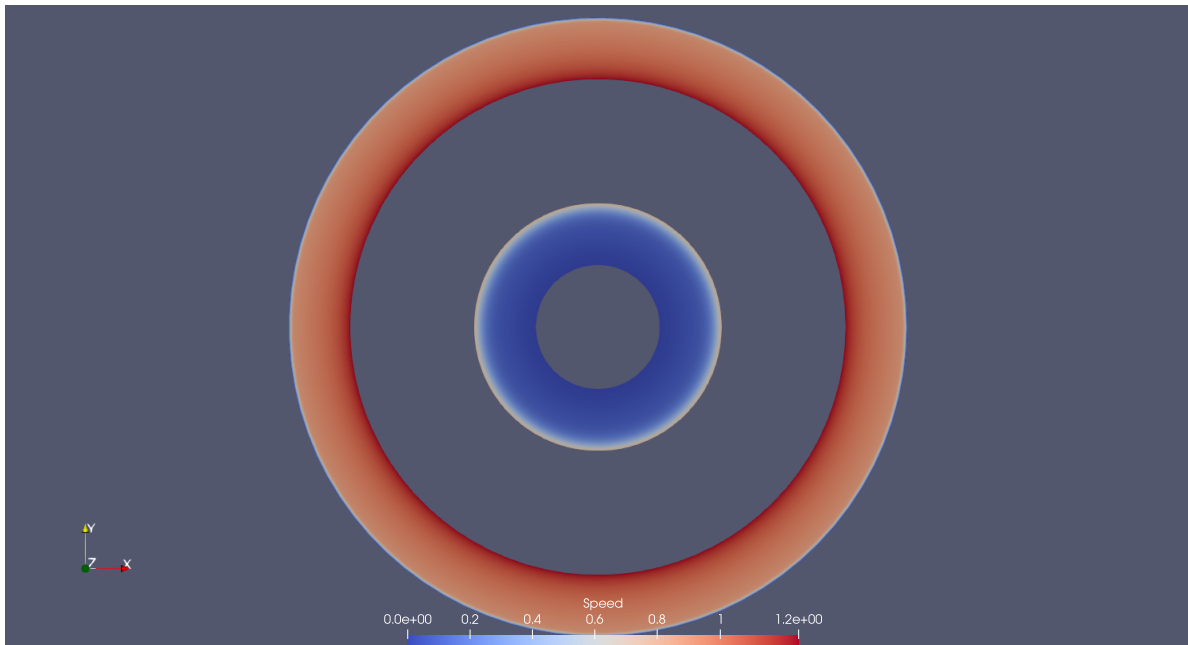


Figure 6.39: Speed at 500s on the plane $\theta = 0$ for $r_a = 0.25$, $r_b = 0.35$, $Re = 15000$

At 1000s

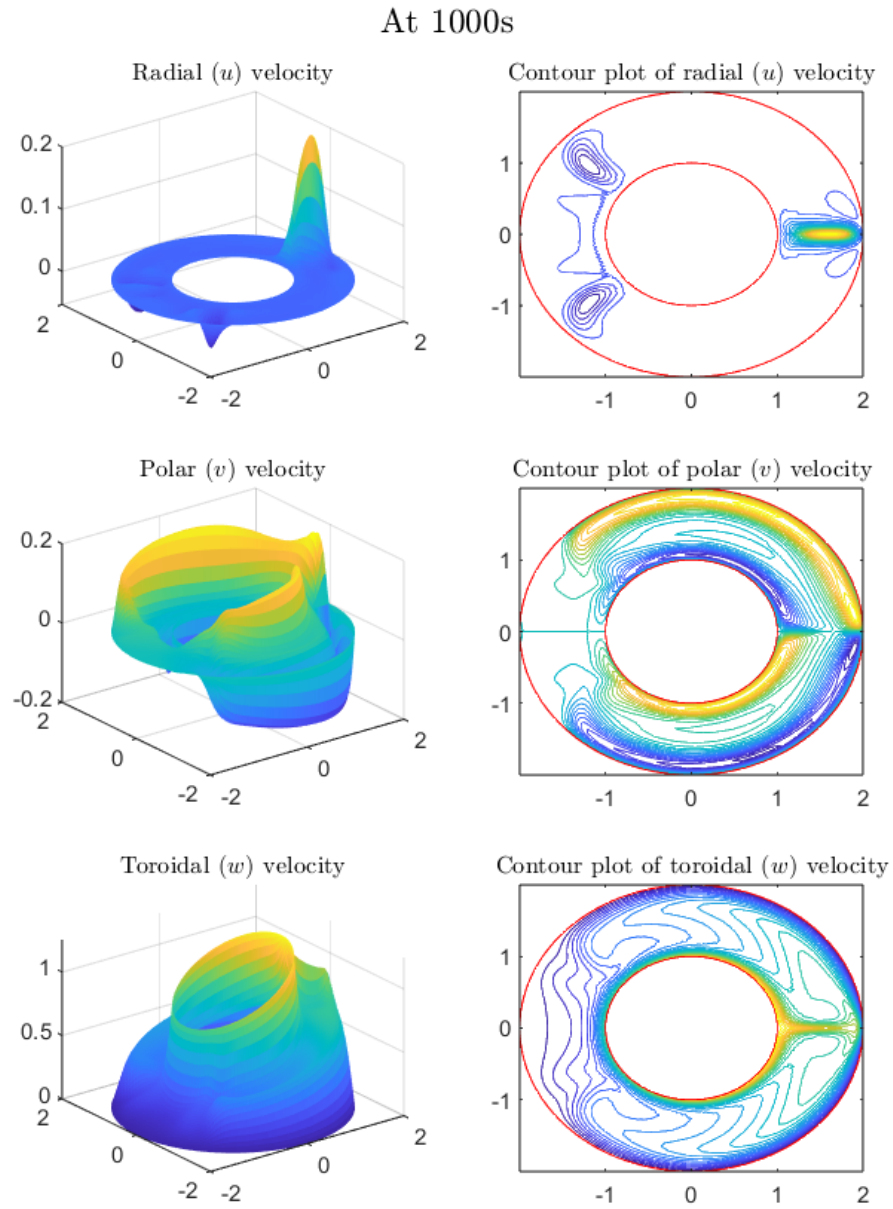


Figure 6.40: Velocity components at 1000s for $r_a = 0.25$, $r_b = 0.35$, $Re = 15000$

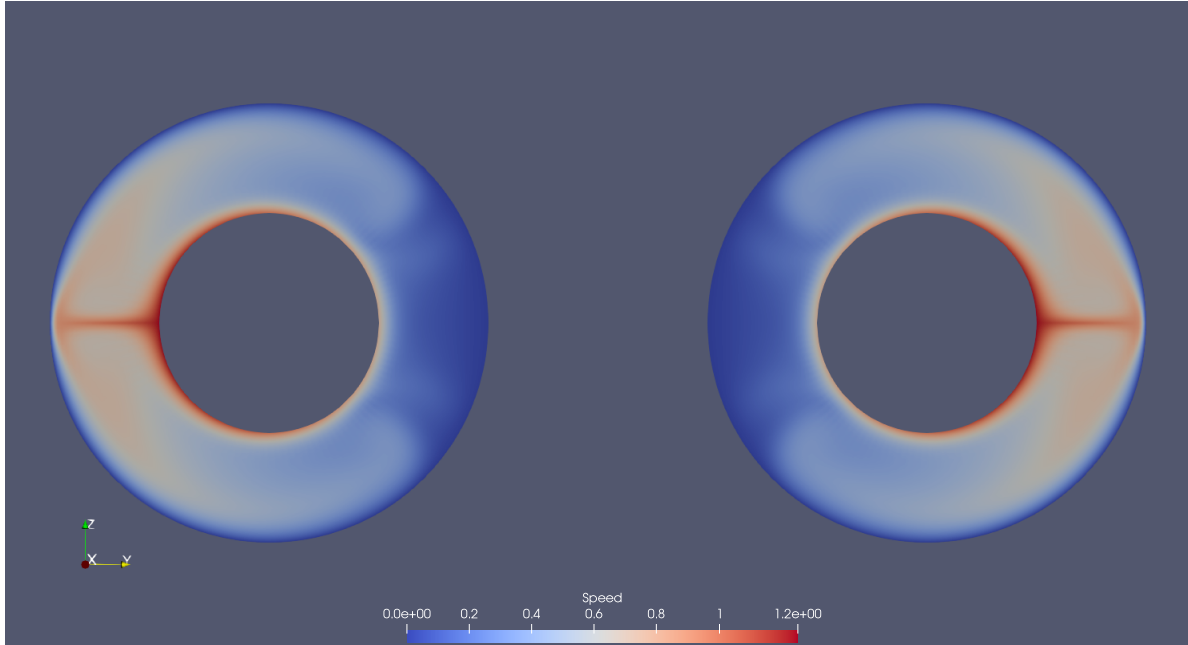


Figure 6.41: Speed at 1000s on $\phi = \frac{3\pi}{2}$ (left) and $\phi = \frac{\pi}{2}$ (right) for $r_a = 0.25$, $r_b = 0.35$, $Re = 15000$

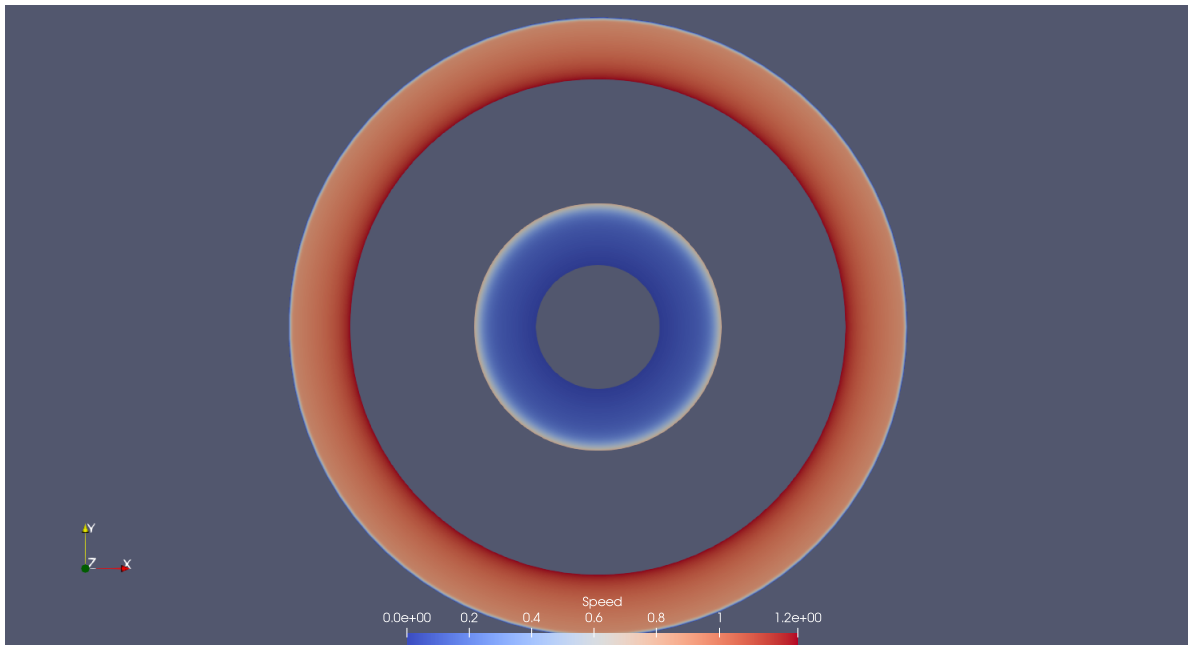


Figure 6.42: Speed at 1000s on the plane $\theta = 0$ for $r_a = 0.25$, $r_b = 0.35$, $Re = 15000$

Discussion

For Case 1, the most notable feature of the flow at 500s is the five distinct, equispaced fingers of approximately equal thickness that span almost the entire gap width illustrated in Figures 6.25, 6.26 and 6.27. At 1000s, most of the features are retained from the 500s case save for the space between the fingers which have been reduced slightly and is illustrated in Figures 6.28, 6.29 and 6.30. At both times, there is no variation in ϕ .

Case 2 demonstrates that the increase in gap width has a significant effect on the number of fingers that appear after the full spin-up time of 500s. There is only one finger when the gap width is 0.05 as opposed to when the gap width is 0.03 shown in Figures 6.31, 6.32 and 6.33. The reduction in the number of fingers is accompanied by the absence of the pockets of circulating flow in the θ -component found in Case 1. The gradient at the boundary for the toroidal velocity, w , is sharper in Case 2 and there is no ϕ -dependence. Finally, there is no significant change to these features at 1000s, see Figures 6.34, 6.35 and 6.36. These components combine to produce a different flow pattern characterised by a thin band of high speed at $\theta = 0$ and $\theta = \pi$ which seemingly diffuses into the gap along the boundary of the outer torus.

Case 3 describes the widest gap studied which is between $r_a = 0.25$ and $r_b = 0.35$ and provides us with an additional interesting observation. We are referring to the appearance of symmetrical regions of negative radial velocity, u , outside the typical region where instabilities occur at both 500s and 1000s, see Figures 6.37 and 6.40. However, the magnitude of these pockets of radial velocity appear to be too small to change the overall velocity profile, see Figures 6.38 and 6.41. Additionally, the sharpest toroidal velocity gradient on the boundary is observed with this gap width. Finally, there is no ϕ -dependence in this flow pattern, see Figures 6.39 and 6.42, which results in a flow pattern similar to Case 2 despite the novel feature in the r -component.

We summarise the effect of widening the gap width on the Taylor-Couette instabilities at $Re = 15000$ in Table 6.3 and repeat this presentation and discussion on the effect of gap

width on the flow for higher Reynolds numbers, $Re = 20000$ and $Re = 25000$.

Re	r_a	r_b	Fingers observed
15000	0.25	0.28	5
15000	0.25	0.30	1
15000	0.25	0.35	1

Table 6.3: Effect of gap width on Taylor-Couette instabilities at $Re = 15000$

6.3.4 Case 4, $r_a = 0.25$, $r_b = 0.28$, $Re = 20000$

The parameters for cases 4 through 6 are summarised in Table 6.4.

N_r	N_θ	N_ϕ	Re	r_a	$\mathbf{r_b}$	R_0	Spin-up	Sub-section	Figures
25	165	40	20000	0.25	0.28	1.0	500s	Case 4	6.43, 6.44, 6.45, 6.46, 6.47, 6.48
25	165	40	20000	0.25	0.30	1.0	500s	Case 5	6.49, 6.50, 6.51, 6.52, 6.53, 6.54
30	165	40	20000	0.25	0.35	1.0	500s	Case 6	6.55, 6.56, 6.57, 6.58, 6.59, 6.60

Table 6.4: Parameters used to study the effect of increasing gap width at $Re = 20000$

At 500

$Re = 20000$

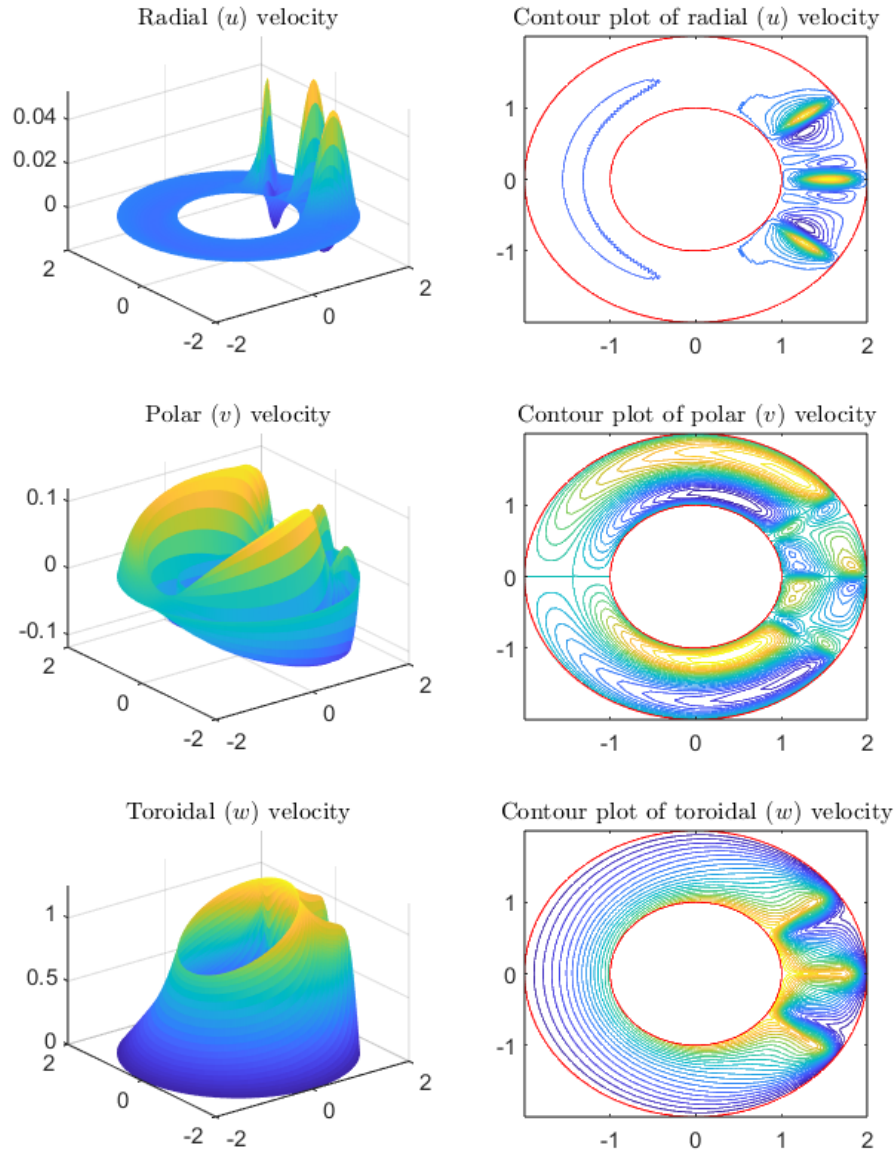


Figure 6.43: Velocity components at 500s for $r_a = 0.25$, $r_b = 0.28$, $Re = 20000$

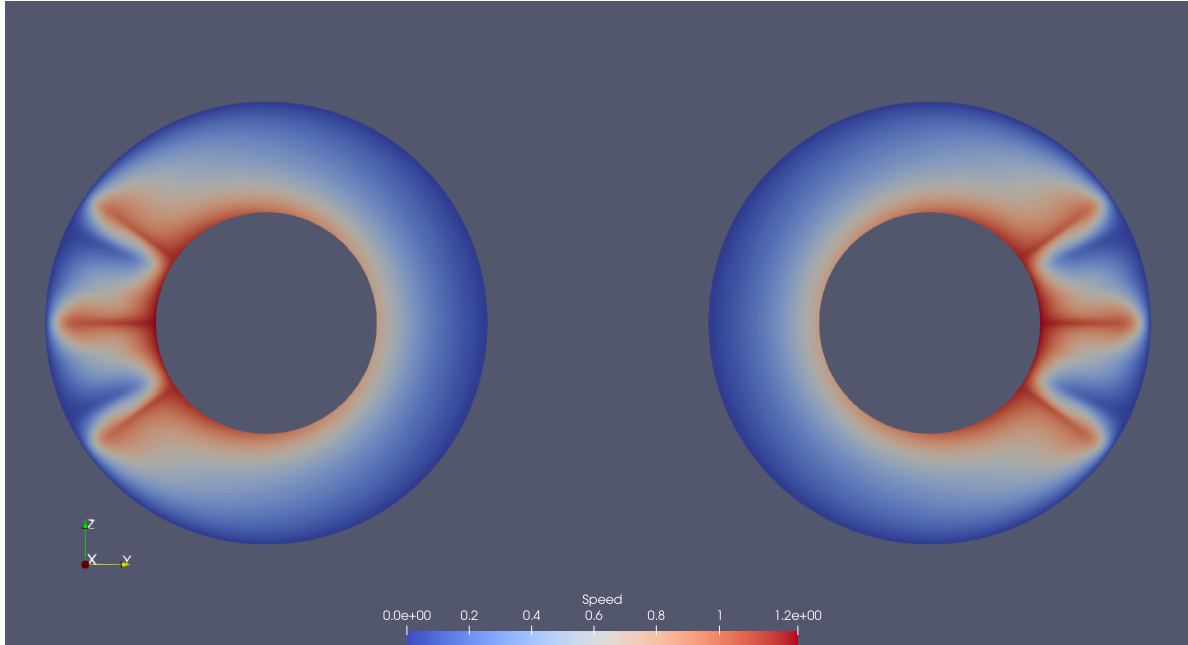


Figure 6.44: Speed at 1000s on $\phi = \frac{3\pi}{2}$ (left) and $\phi = \frac{\pi}{2}$ (right) for $r_a = 0.25$, $r_b = 0.28$, $Re = 20000$

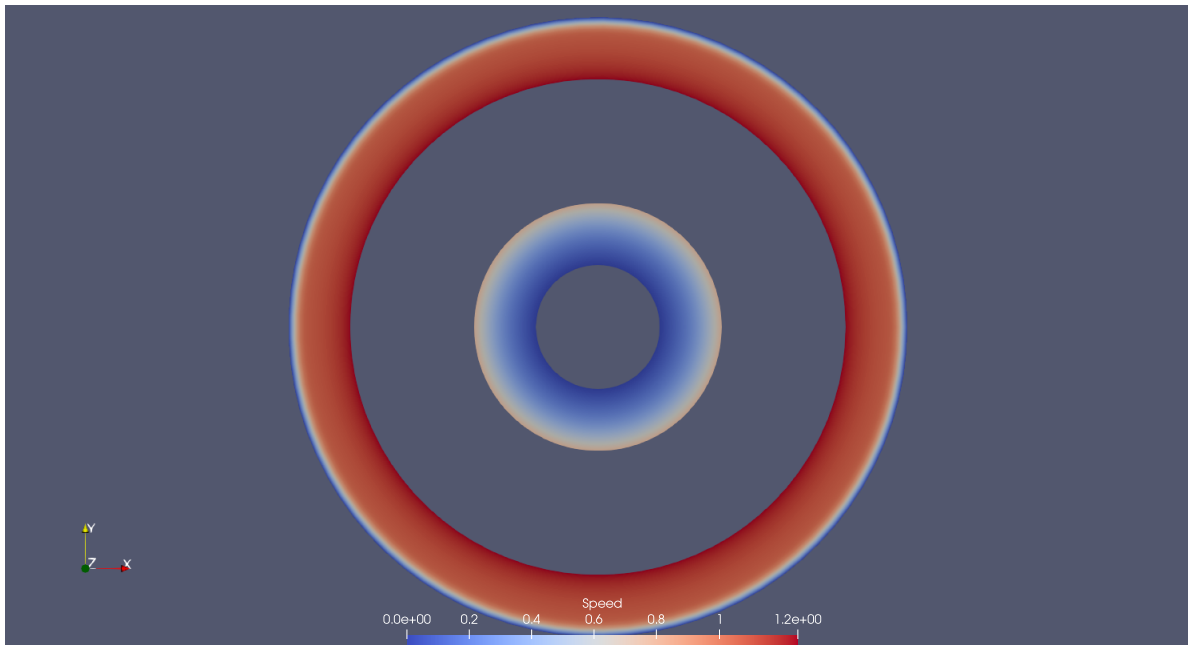


Figure 6.45: Speed at 1000s on the plane $\theta = 0$ for $r_a = 0.25$, $r_b = 0.28$, $Re = 20000$

At 1000s

$Re = 20000$

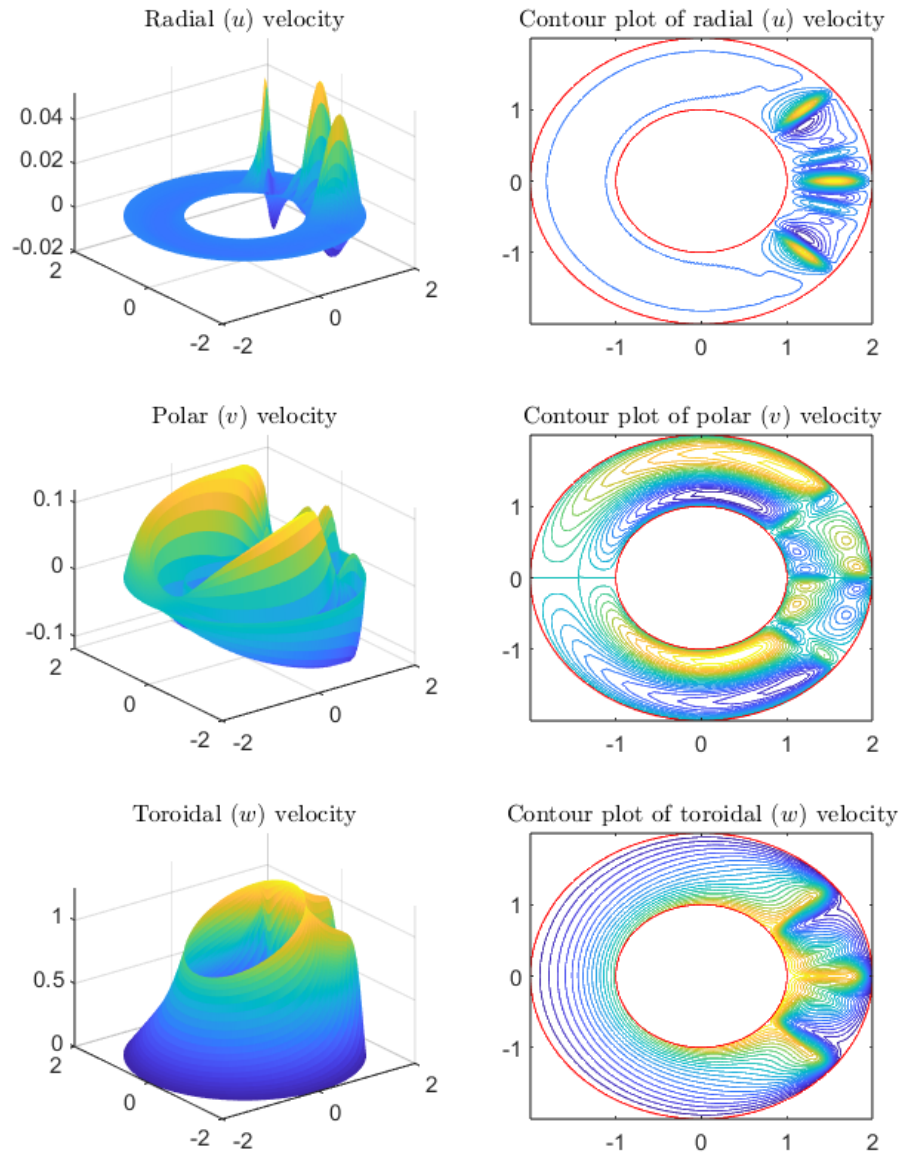


Figure 6.46: Velocity components at 1000s for $r_a = 0.25$, $r_b = 0.28$, $Re = 20000$

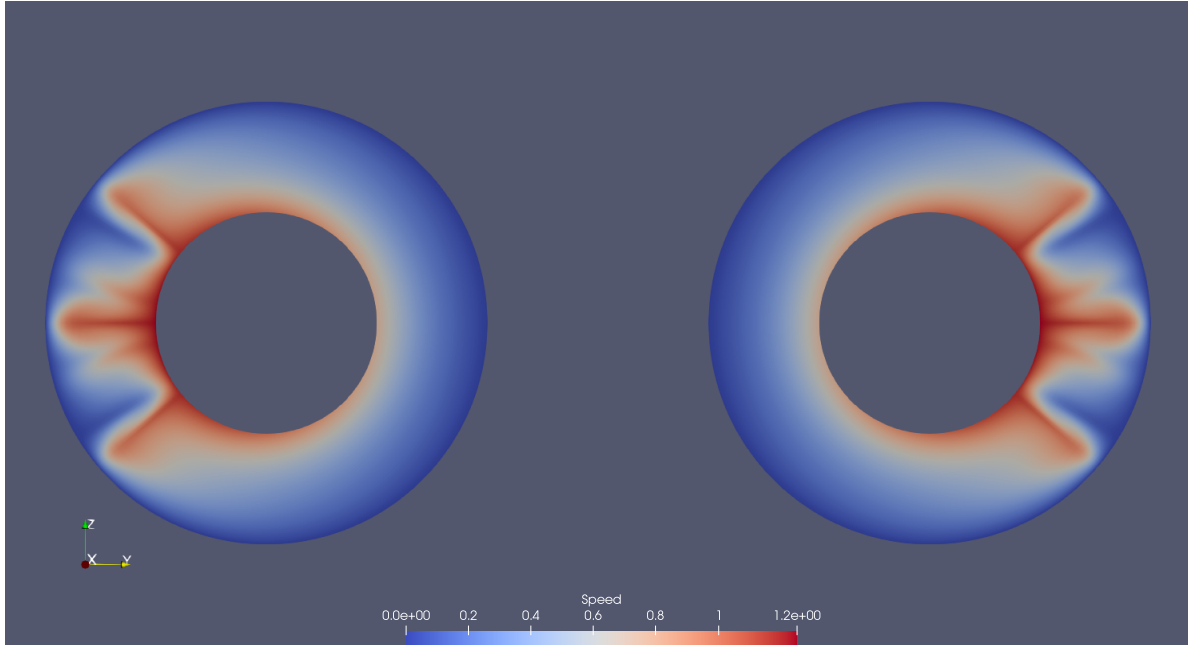


Figure 6.47: Speed at 1000s on $\phi = \frac{3\pi}{2}$ (left) and $\phi = \frac{\pi}{2}$ (right) for $r_a = 0.25$, $r_b = 0.28$, $Re = 20000$

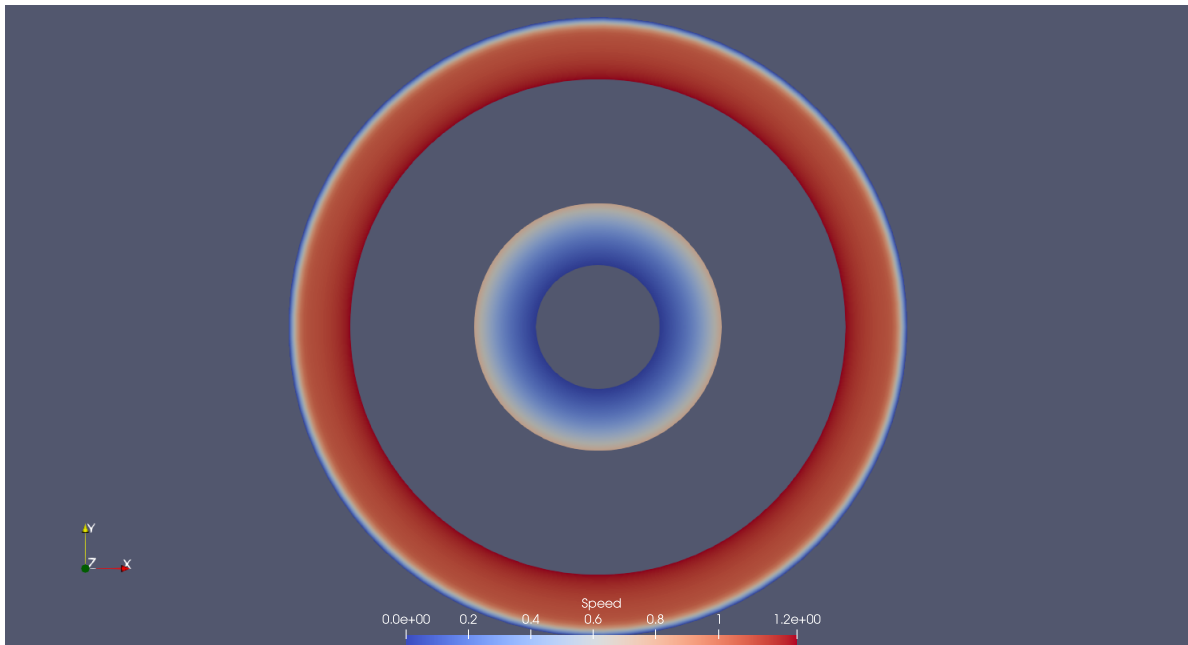


Figure 6.48: Speed at 1000s on the plane $\theta = 0$ for $r_a = 0.25$, $r_b = 0.28$, $Re = 20000$

6.3.5 Case 5, $r_a = 0.25$, $r_b = 0.30$, $Re = 20000$

At 500s

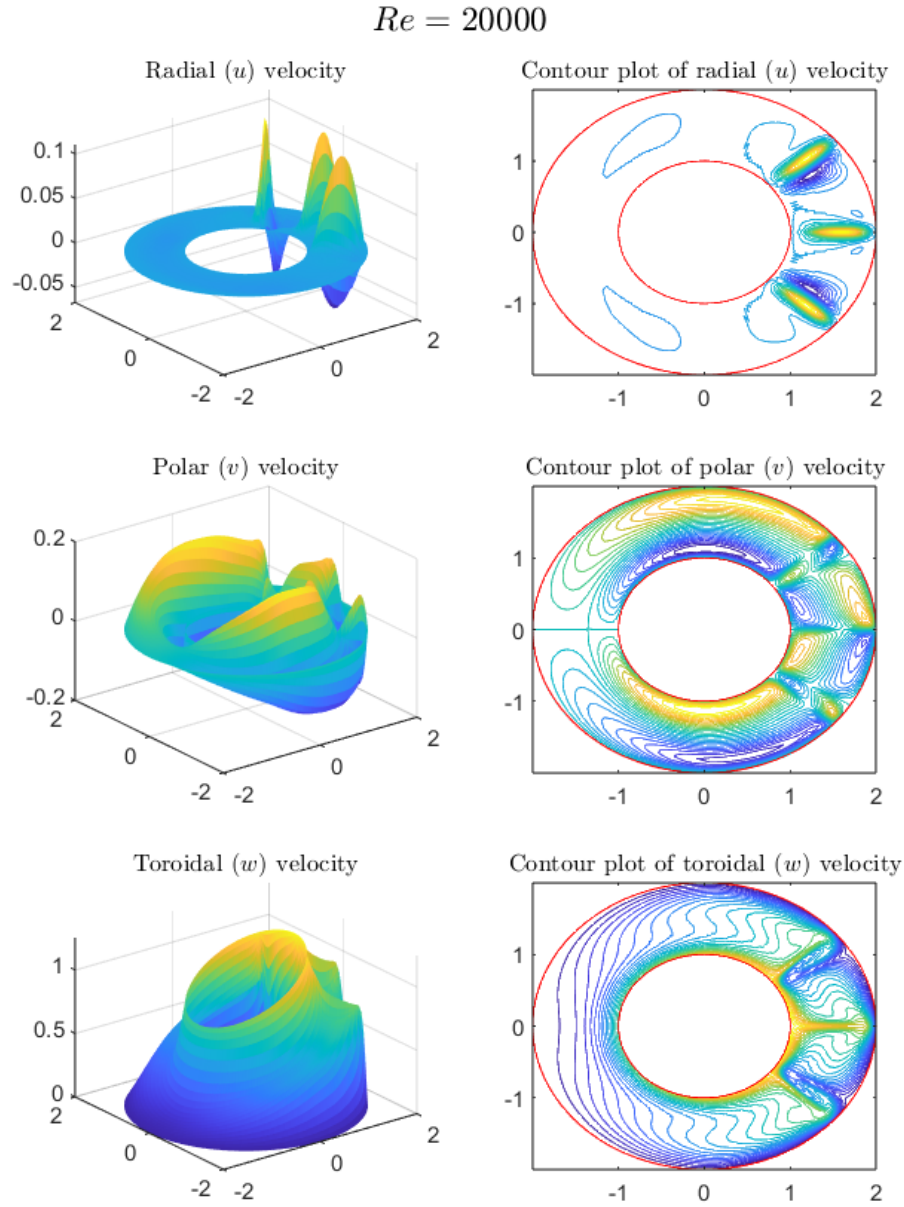


Figure 6.49: Velocity components at 500s for $r_a = 0.25$, $r_b = 0.30$, $Re = 20000$

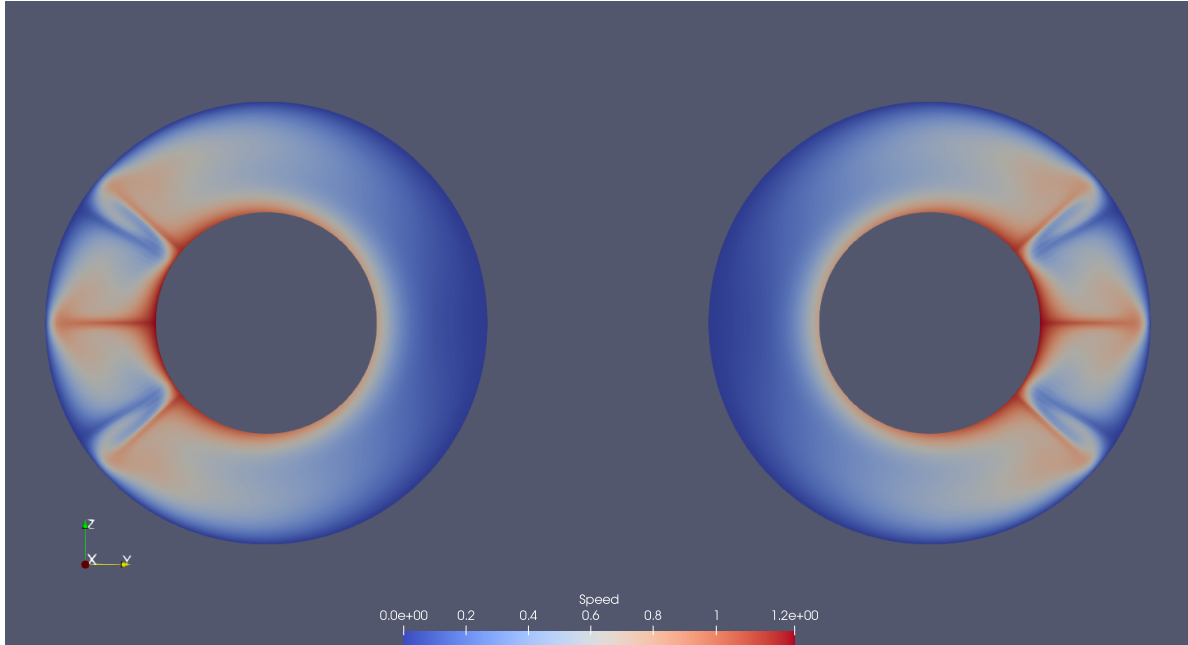


Figure 6.50: Speed at 500s on $\phi = \frac{3\pi}{2}$ (left) and $\phi = \frac{\pi}{2}$ (right) for $r_a = 0.25$, $r_b = 0.30$, $Re = 20000$

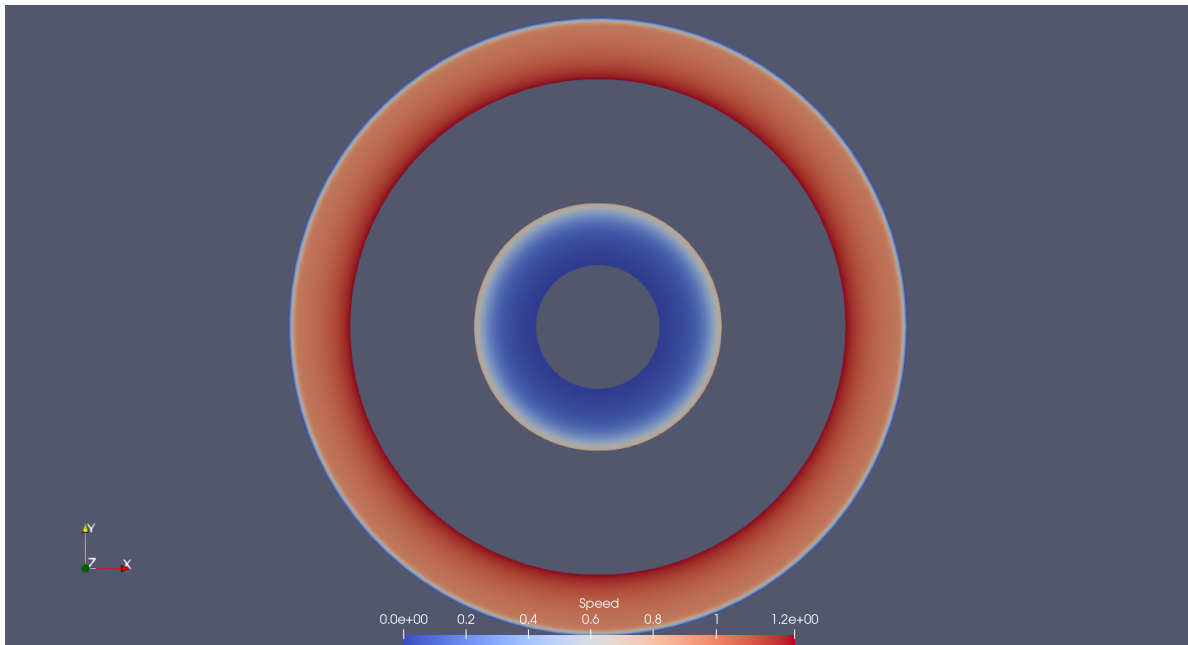


Figure 6.51: Speed at 500s on the plane $\theta = 0$ for $r_a = 0.25$, $r_b = 0.30$, $Re = 20000$

At 1000s

$Re = 20000$

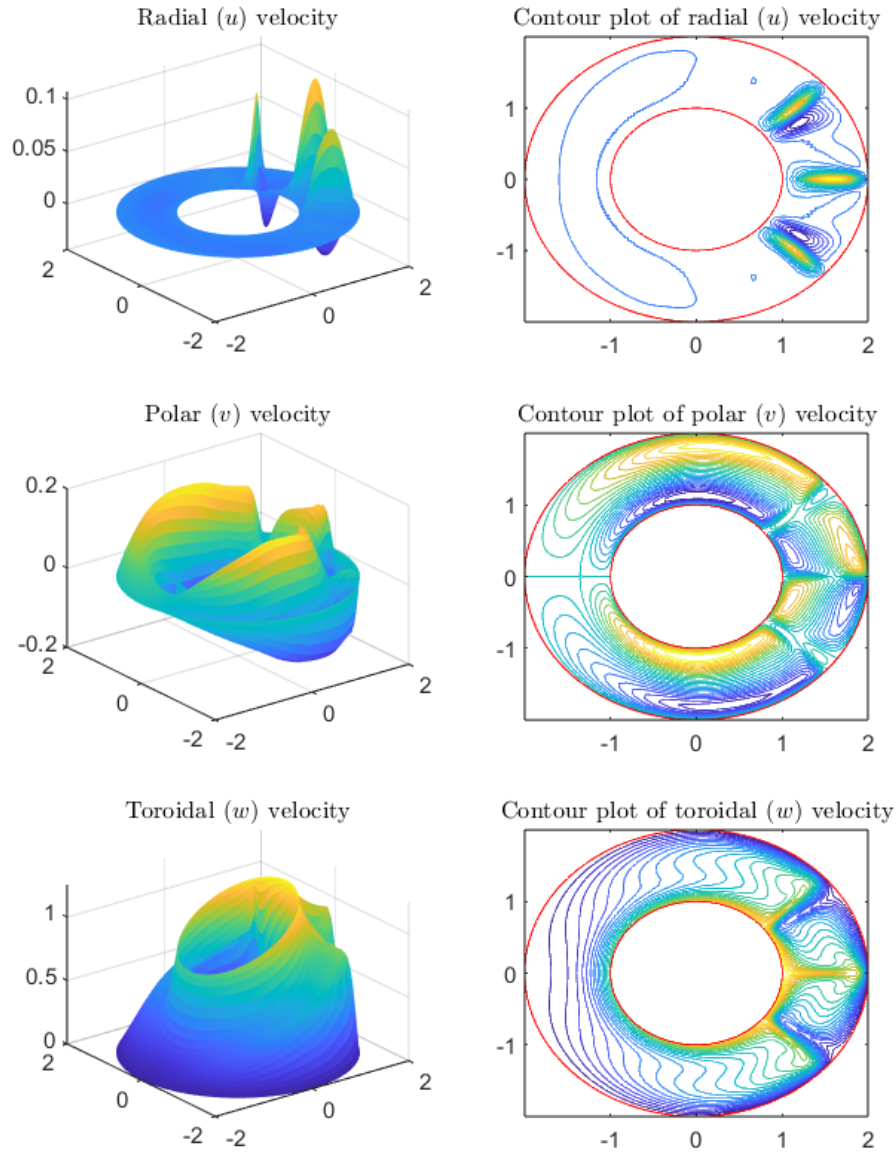


Figure 6.52: Velocity components at 1000s for $r_a = 0.25$, $r_b = 0.30$, $Re = 20000$

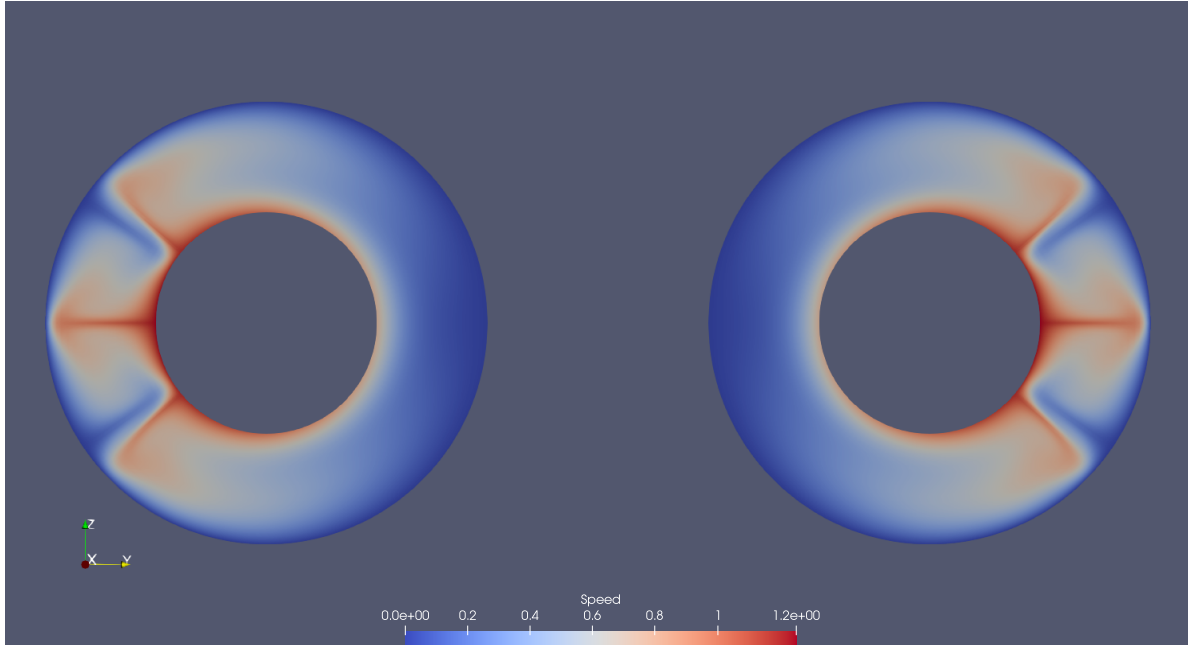


Figure 6.53: Speed at 1000s on $\phi = \frac{3\pi}{2}$ (left) and $\phi = \frac{\pi}{2}$ (right) for $r_a = 0.25$, $r_b = 0.30$, $Re = 20000$

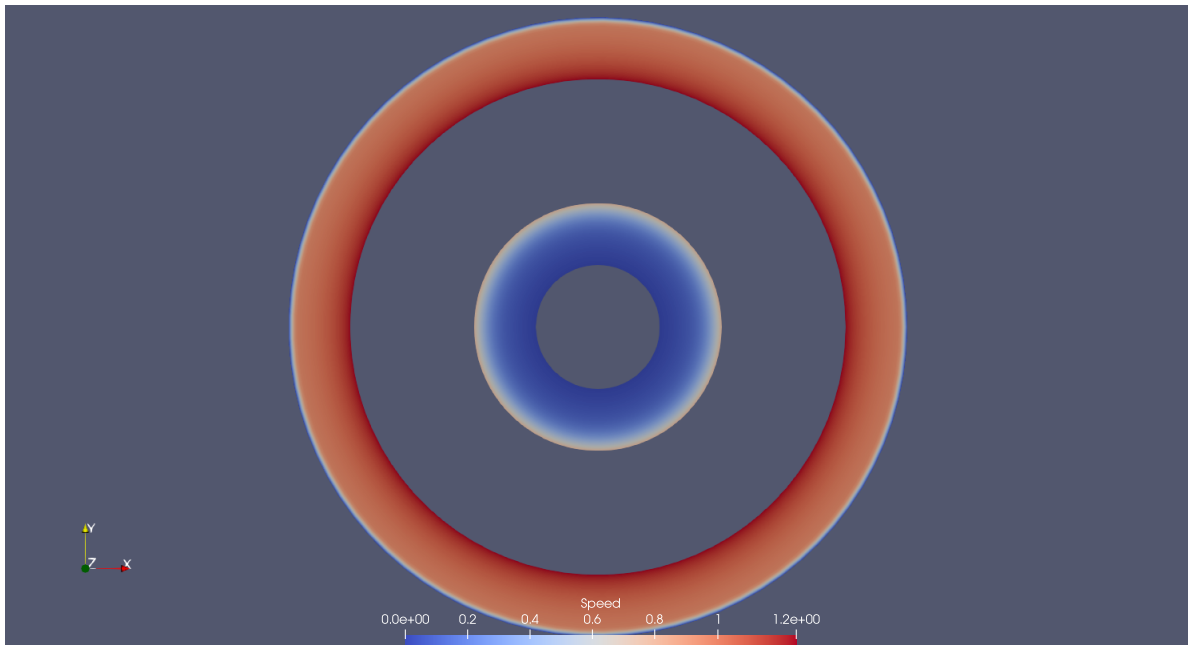


Figure 6.54: Speed at 1000s on the plane $\theta = 0$ for $r_a = 0.25$, $r_b = 0.30$, $Re = 20000$

6.3.6 Case 6, $r_a = 0.25$, $r_b = 0.35$, $Re = 20000$

At 500

At 500s

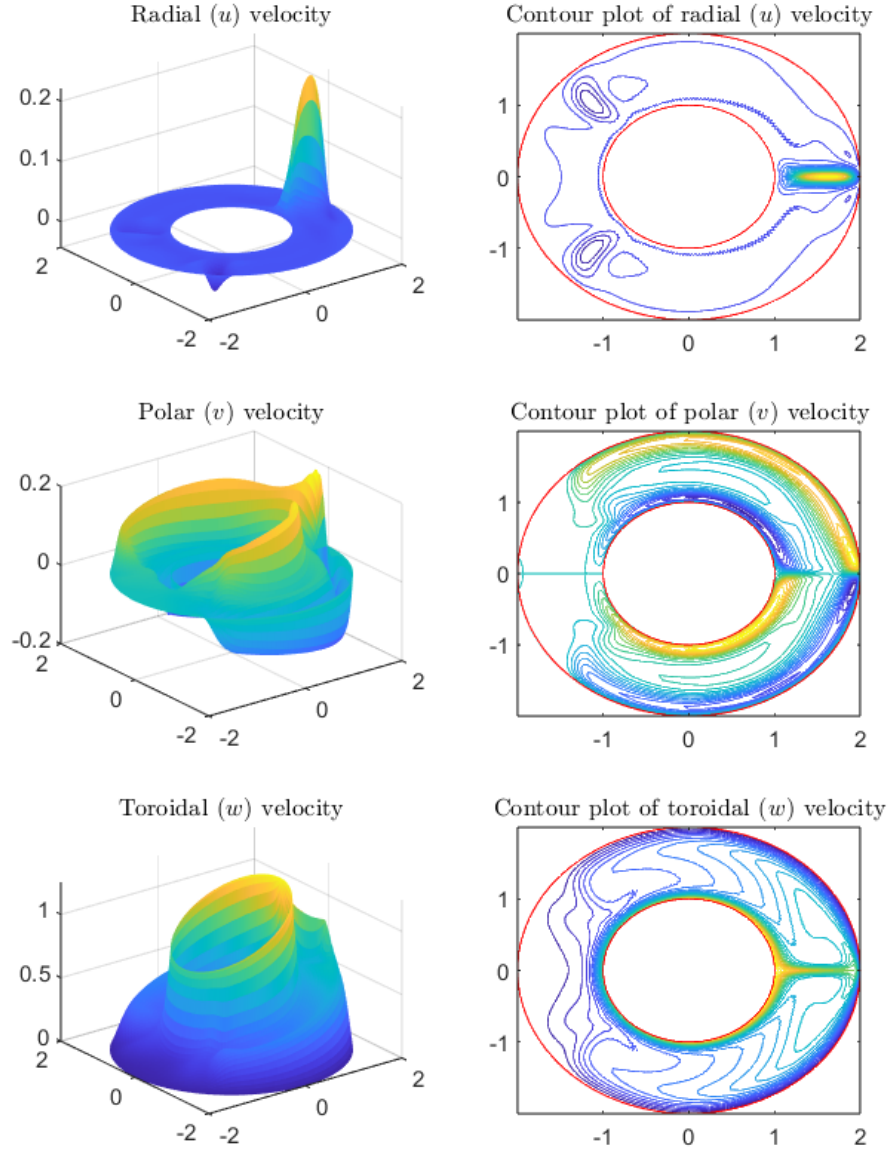


Figure 6.55: Velocity components at 500s for $r_a = 0.25$, $r_b = 0.35$, $Re = 20000$

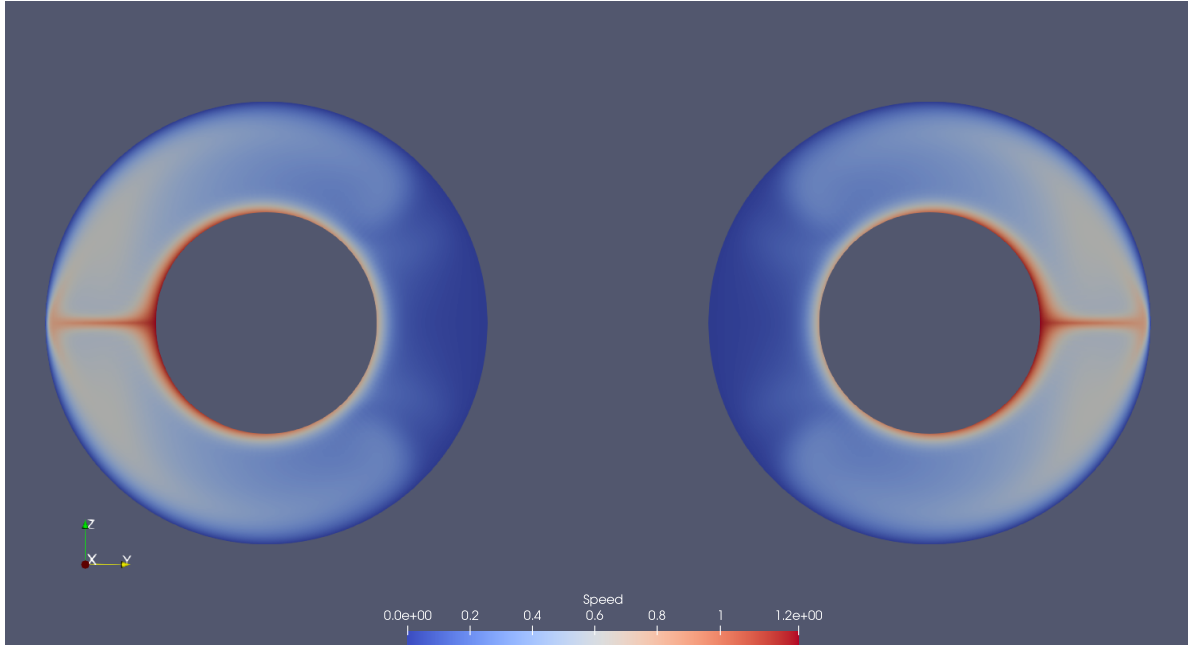


Figure 6.56: Speed at 500s on $\phi = \frac{3\pi}{2}$ (left) and $\phi = \frac{\pi}{2}$ (right) for $r_a = 0.25$, $r_b = 0.35$, $Re = 20000$

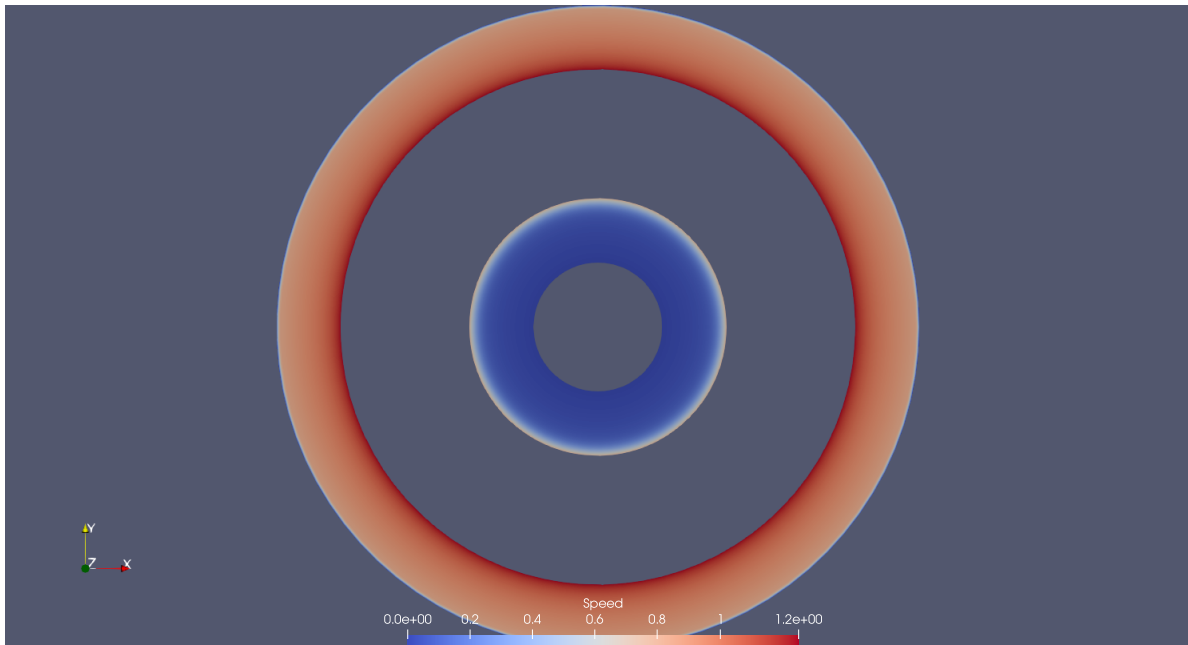


Figure 6.57: Speed at 500s on the plane $\theta = 0$ for $r_a = 0.25$, $r_b = 0.35$, $Re = 20000$

At 1000s

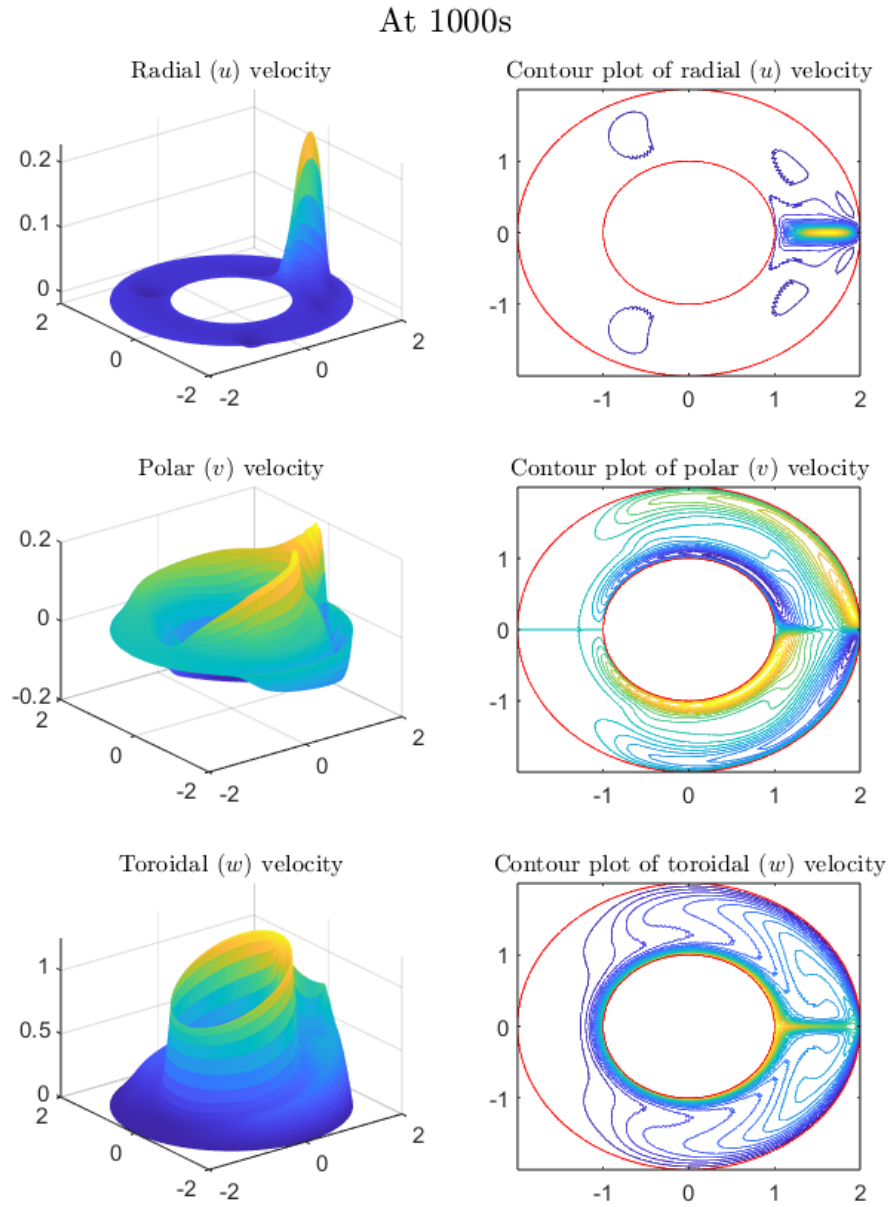


Figure 6.58: Velocity components at 1000s for $r_a = 0.25$, $r_b = 0.35$, $Re = 20000$

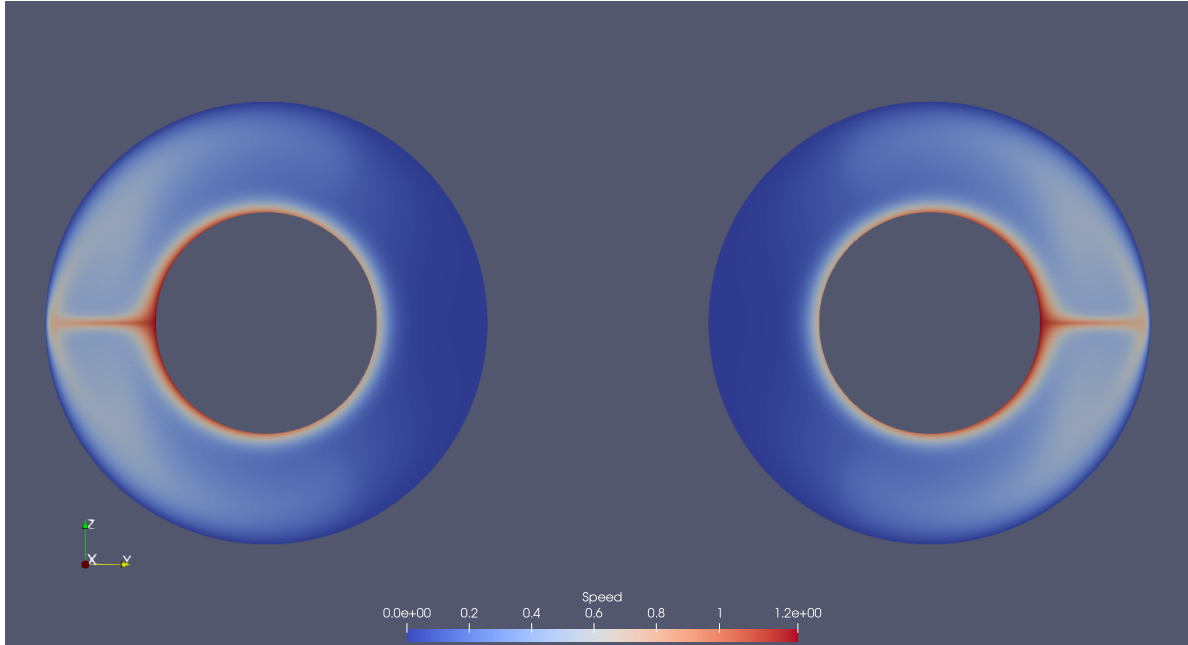


Figure 6.59: Speed at 1000s on $\phi = \frac{3\pi}{2}$ (left) and $\phi = \frac{\pi}{2}$ (right) for $r_a = 0.25$, $r_b = 0.35$, $Re = 20000$

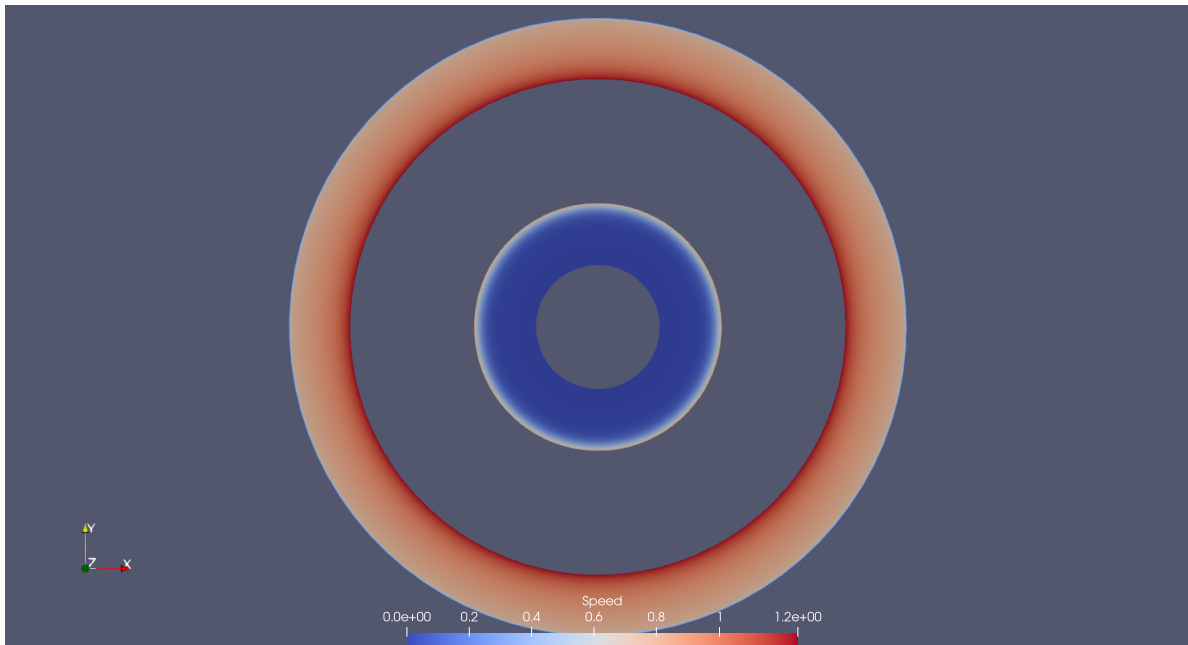


Figure 6.60: Speed at 1000s on the plane $\theta = 0$ for $r_a = 0.25$, $r_b = 0.35$, $Re = 20000$

Discussion

Case 4 shows only three distinct, equispaced fingers of roughly the same thickness at 500s, along with the usual accompanying features in the r - and θ -components as opposed to the five fingers displayed in Case 1, see Figures 6.43, 6.44, 6.45. Unlike Case 1 at 500s, the central finger is surrounded by a region of high speed. There is another difference between Case 1 and Case 4 at 1000s. There are still three main fingers but there appear to be two smaller fingers either extending from or growing alongside the central finger and potentially threatening to break off and create two additional fingers. This peculiar feature is shown in Figures 6.46, 6.47, 6.48.

There are three fingers in Case 5 as well but there is a large gap away from the central finger. Further, the fingers away from the central finger represent a speed lower than that found in the central finger, see Figures 6.49, 6.50, 6.51 whereas previously, we observed that all the fingers represented bands of approximately speed. Again, these features persist at 1000s and are shown in Figures 6.52, 6.53, 6.54.

Similar to its counterpart in Case 3, there are small symmetric pockets of negative radial velocity in Case 6, a single finger representing a slender band of high speed and the sharpest gradient in the toroidal velocity, w , see Figures 6.55, 6.56, 6.57. While the main features persist at 1000s, the region of low speed has widened and appears to display zero speed i.e. no flow occurs in this region.

We again summarise the number of fingers observed in cases 4 through 6 at 1000s in Table 6.5

Re	r_a	r_b	Fingers observed
20000	0.25	0.28	3
20000	0.25	0.30	3
20000	0.25	0.35	1

Table 6.5: Effect of gap width on Taylor-Couette instabilities at $Re = 20000$

6.3.7 Case 7, $r_a = 0.25$, $r_b = 0.28$, $Re = 25000$

Cases 7 through 9 make use of the parameters listed in Table 6.6. We show only the flow at 1000s for these cases since we are only interested in the long-time behaviour.

N_r	N_θ	N_ϕ	Re	r_a	$\mathbf{r_b}$	R_0	Spin-up	Sub-section	Figures
25	205	40	25000	0.25	0.28	1.0	500s	Case 7	6.61, 6.62, 6.63
25	205	40	25000	0.25	0.30	1.0	500s	Case 8	6.64, 6.65, 6.66
30	205	40	25000	0.25	0.35	1.0	500s	Case 9	6.67, 6.68, 6.69

Table 6.6: Parameters used to study the effect of increasing gap width at $Re = 25000$

At 1000s

$Re = 25000$

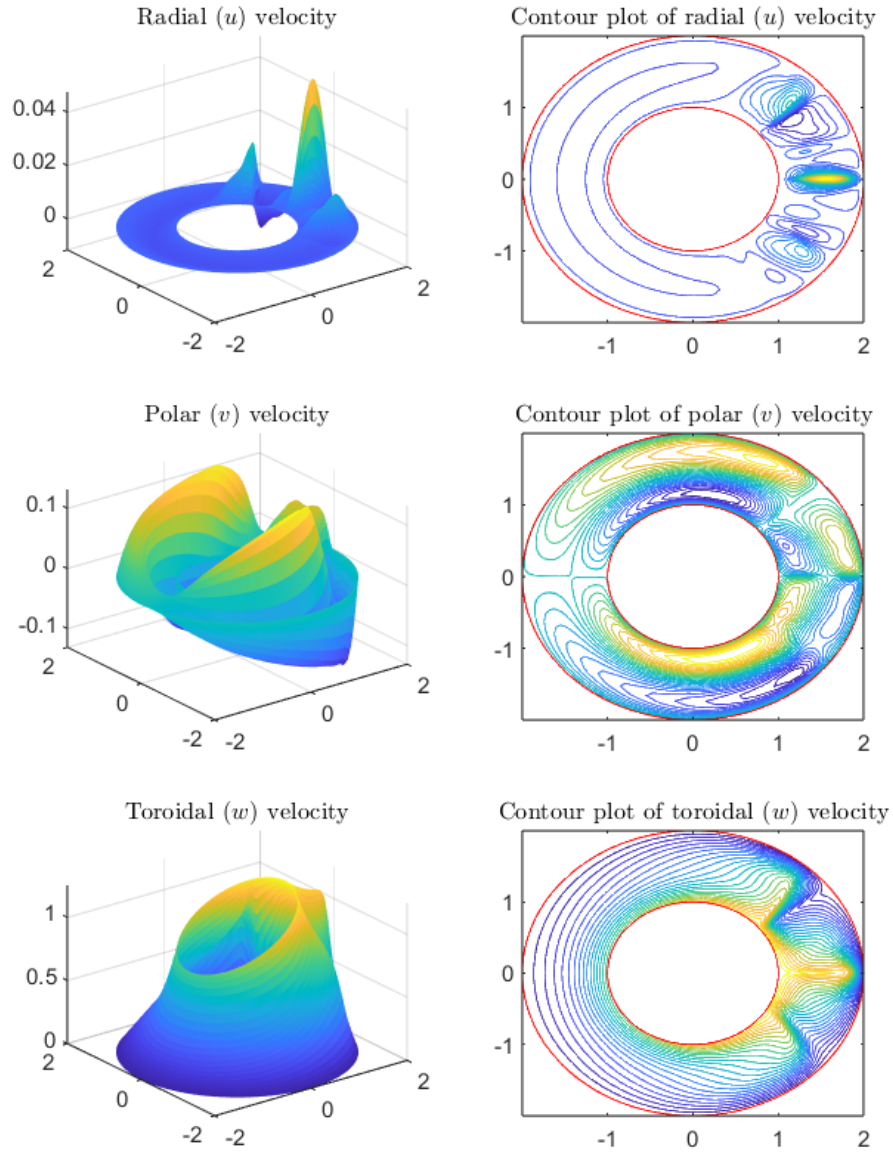


Figure 6.61: Velocity components at 1000s for $r_a = 0.25$, $r_b = 0.28$, $Re = 25000$

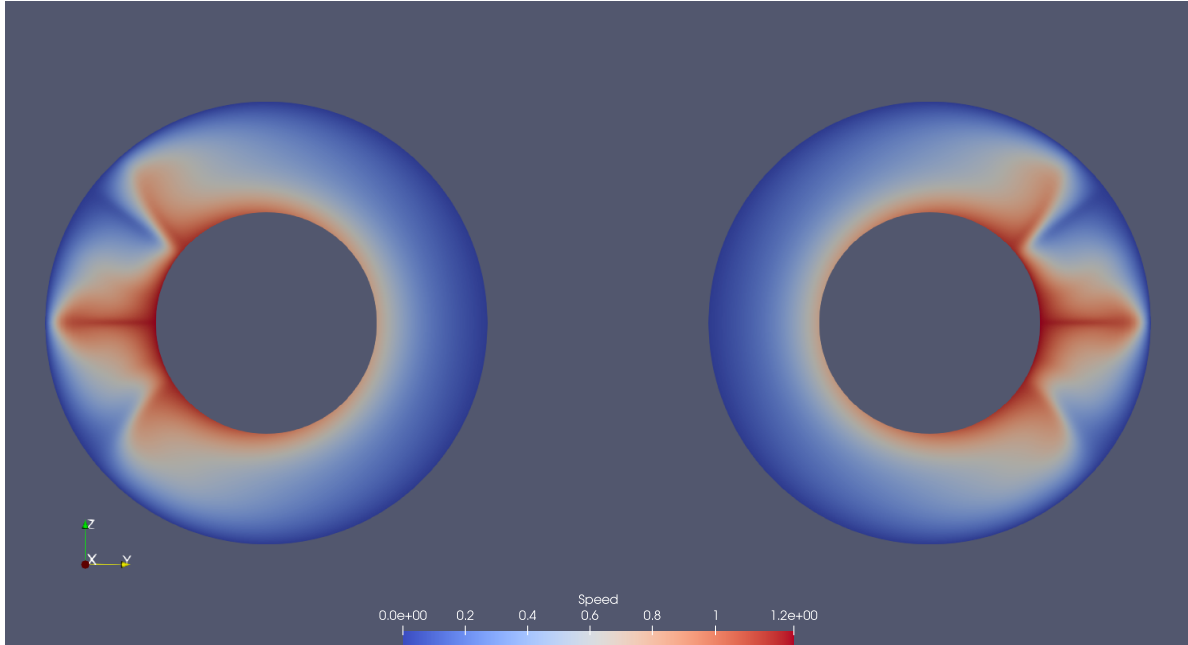


Figure 6.62: Speed at 1000s on $\phi = \frac{3\pi}{2}$ (left) and $\phi = \frac{\pi}{2}$ (right) for $r_a = 0.25$, $r_b = 0.28$, $Re = 25000$

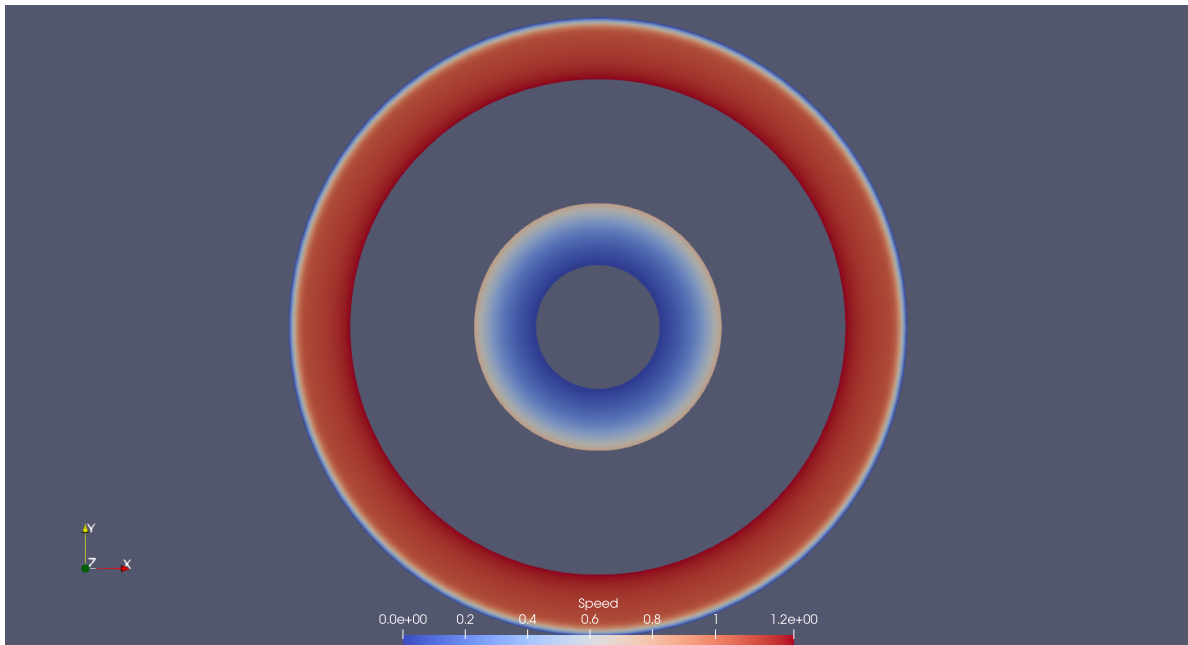


Figure 6.63: Speed at 1000s on the plane $\theta = 0$ for $r_a = 0.25$, $r_b = 0.28$, $Re = 25000$

6.3.8 Case 8, $r_a = 0.25$, $r_b = 0.30$, $Re = 25000$

At 1000s

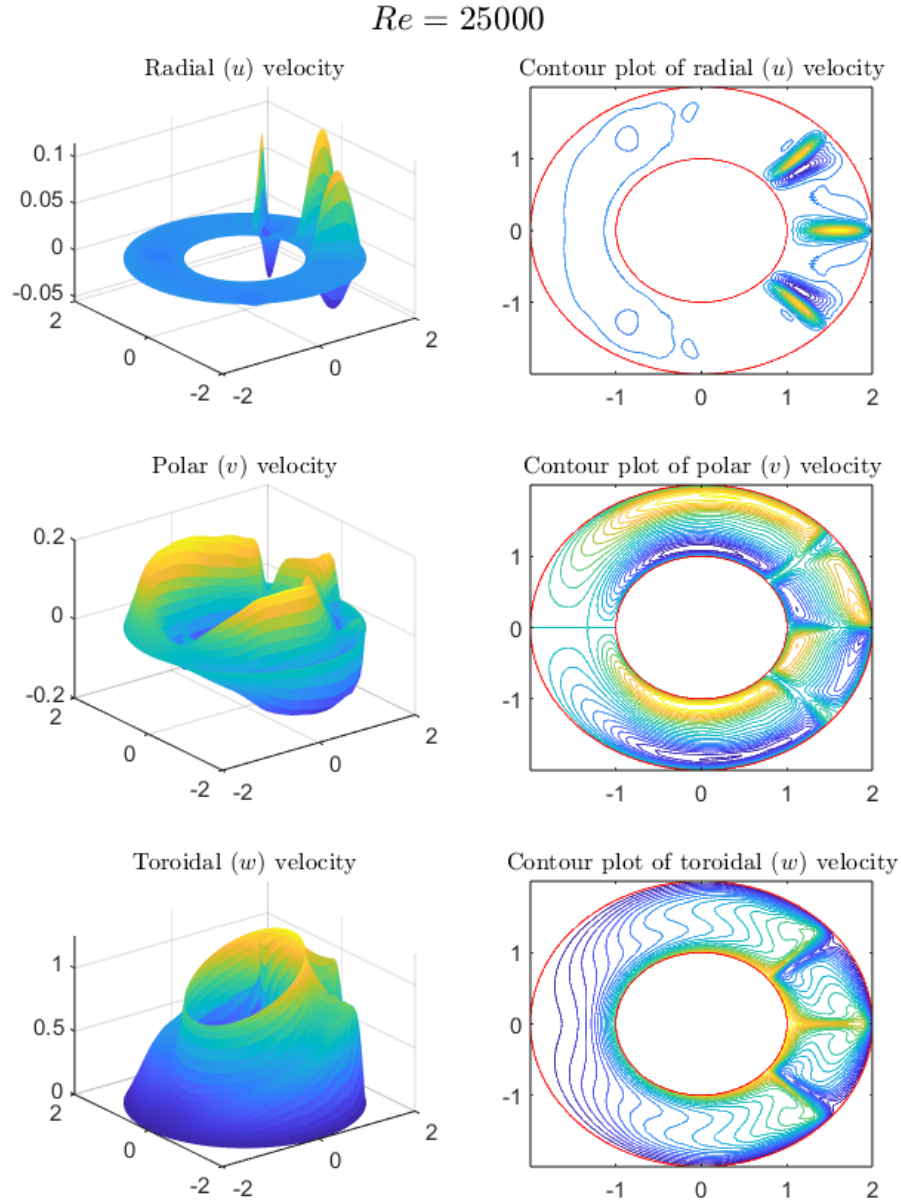


Figure 6.64: Velocity components at 1000s for $r_a = 0.25$, $r_b = 0.30$, $Re = 25000$

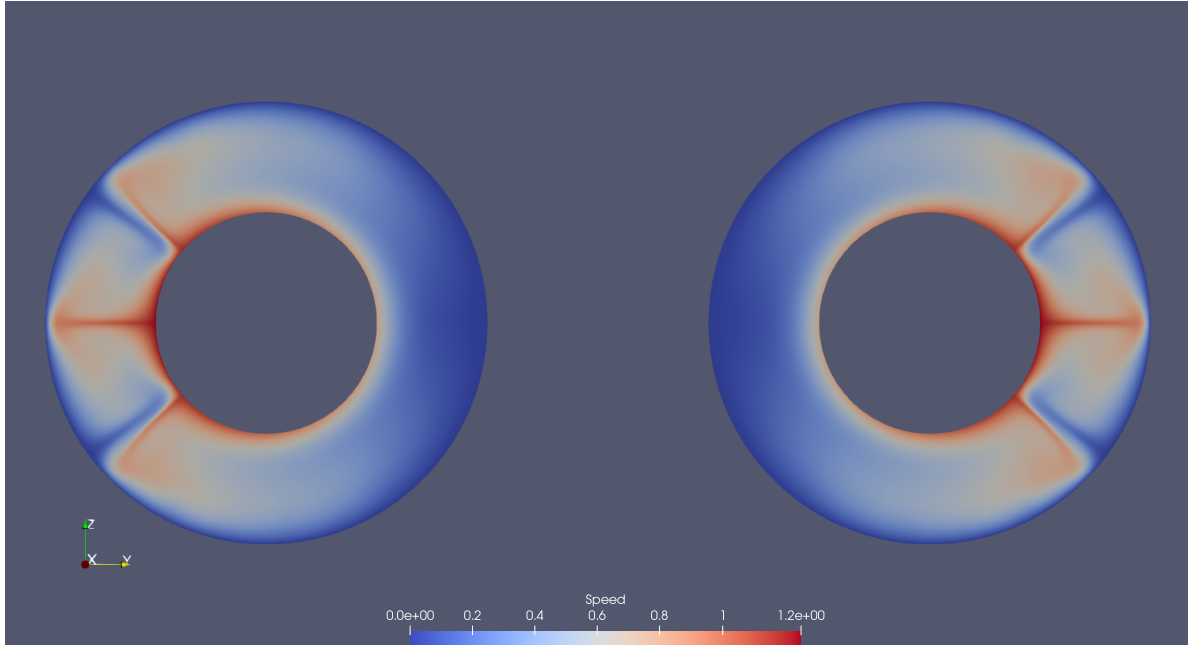


Figure 6.65: Speed at 1000s on $\phi = \frac{3\pi}{2}$ (left) and $\phi = \frac{\pi}{2}$ (right) for $r_a = 0.25$, $r_b = 0.30$, $Re = 25000$

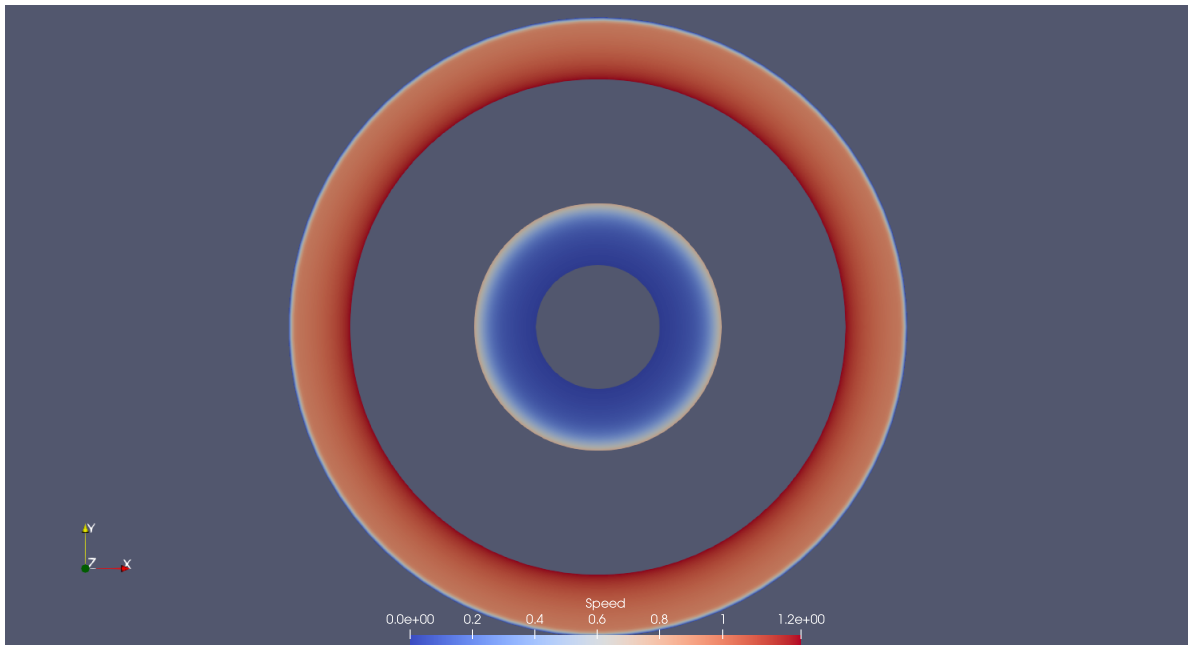


Figure 6.66: Speed at 1000s on the plane $\theta = 0$ for $r_a = 0.25$, $r_b = 0.30$, $Re = 25000$

6.3.9 Case 9, $r_a = 0.25$, $r_b = 0.35$, $Re = 25000$

At 1000s

At 1000s

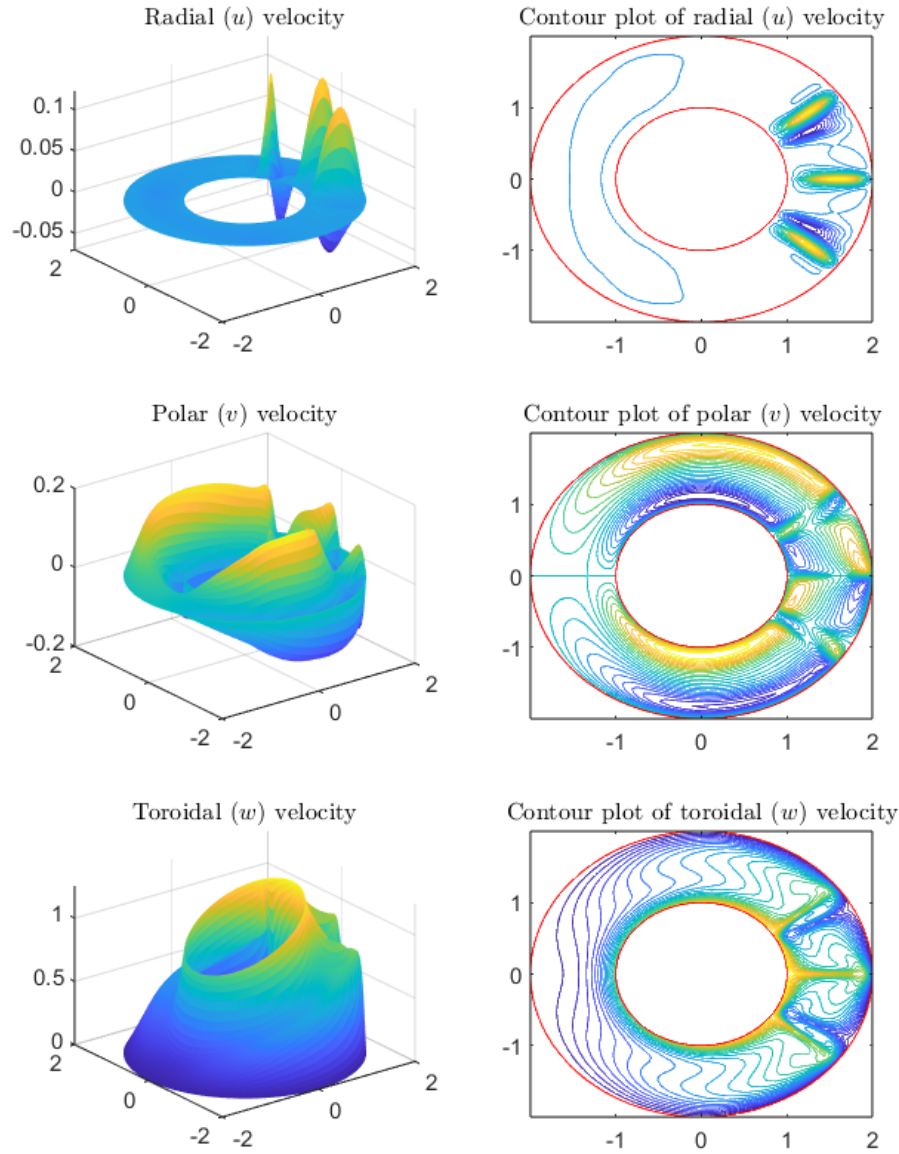


Figure 6.67: Velocity components at 1000s for $r_a = 0.25$, $r_b = 0.35$, $Re = 25000$

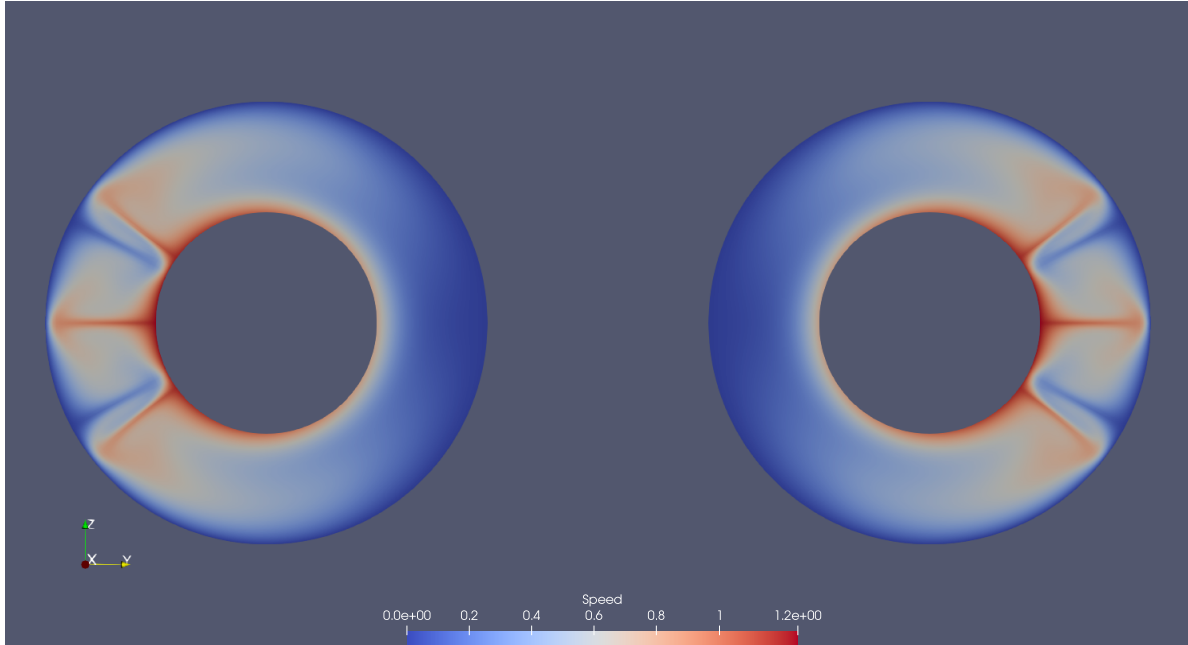


Figure 6.68: Speed at 1000s on $\phi = \frac{3\pi}{2}$ (left) and $\phi = \frac{\pi}{2}$ (right) for $r_a = 0.25$, $r_b = 0.35$, $Re = 25000$

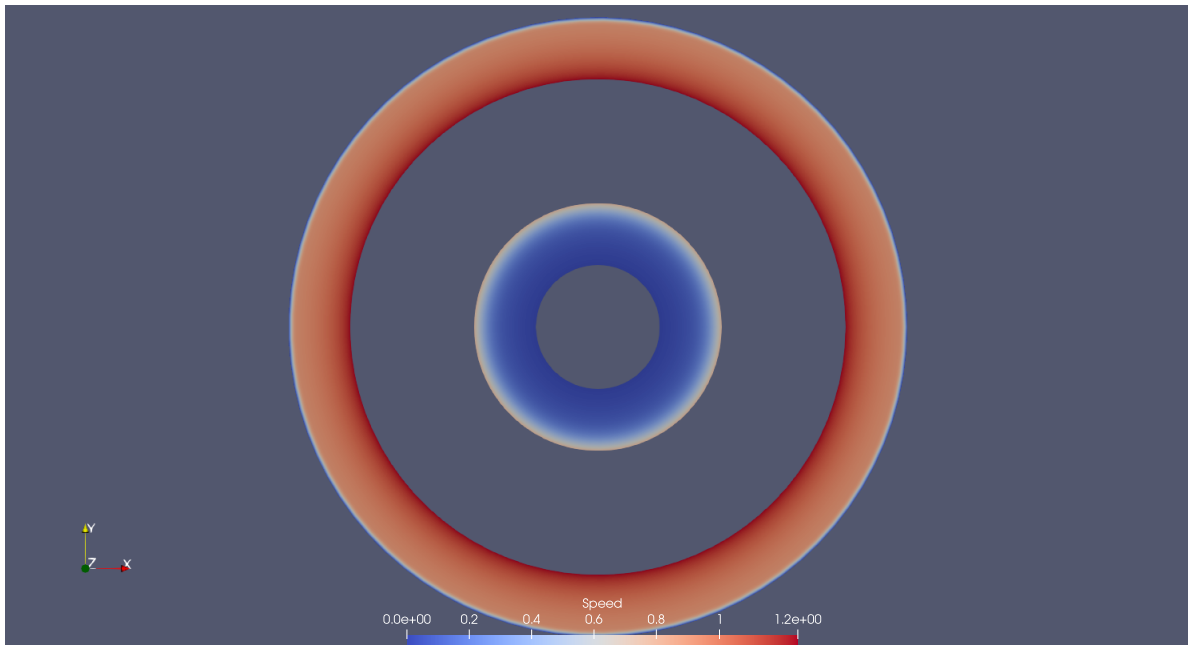


Figure 6.69: Speed at 1000s on the plane $\theta = 0$ for $r_a = 0.25$, $r_b = 0.35$, $Re = 25000$

Discussion

At $Re = 25000$, we observe a deviation from the pattern of decreasing number of fingers as the gap width increases. Case 7, Case 8 and Case 9 all display three fingers although there are differences in each of the cases. At $Re = 15000$ and $Re = 20000$, there is only one finger at the largest gap width; however, at $Re = 25000$, there are three fingers.

In Case 7, the fingers are all different, see Figures 6.61, 6.62, 6.63. The central finger is thicker and surrounded by a region of high speed. The fingers on either side are different distances away from the central finger and span different amounts of the gap width. There is also a suggestion of symmetry breaking because of these two different fingers but we refrain from a definitive statement until further experiments have been conducted.

Case 8 and Case 9 are similar to each other. They both display three slender fingers that span almost the entire gap width and are symmetric, see Figures 6.64, 6.65, 6.66 for Case 8 and Figures 6.67, 6.68, 6.69 for Case 9. The main difference is that the distance between the fingers in Case 9 is smaller than that found in Case 8. Additionally, there are bands of high speed at the end of the fingers closer to the outer torus and extend mostly in the θ -direction near its boundary.

6.3.10 Summary of results

To summarise the narrative of the multitude of figures before us, two-dimensional Taylor-Couette flow or Taylor-Couette instabilities develops after rotating the inner torus at a fixed speed while keeping the outer torus stationary. Taylor-Couette flow develops only within a particular range of Reynolds numbers viz. if the Reynolds number is too low, Couette flow is modeled. We have presented simulations that have found Taylor-Couette instabilities for $Re = 15000, 20000, 25000$ but we note that this is not a strict range. We have also observed Taylor-Couette flow for Reynolds numbers on either side of this range in our work.

The number of fingers and their proximity to each other vary depending on the gap width and Reynolds number but the presence of slender bands of higher speed persists through all

of the nine cases presented. We summarise the findings of the Taylor-Couette flow in this section in Table 6.7 below. In general, wider gaps and larger Reynolds numbers produced less fingers than smaller gaps and smaller Reynolds numbers. Finally, the presence of ϕ -dependent behaviour remains elusive and the search for them is ongoing. Presumably at high enough Reynolds numbers, three-dimensional structures of interest will develop before culminating in turbulence.

We use this opportunity to mention observations from the hundreds of simulations explored for this thesis. The absolute maximum value of the divergence decreases as the number of radial grid points is increased. Finer grids in the polar and toroidal variables have little impact on the divergence. Higher Reynolds numbers require a larger amount of points in the theta grid for smooth resolution. Again, increasing the number of grid points in the other two directions have little to no impact on the resolution as the Reynolds number increases. Finally, there appears to be a range for N_ϕ to guarantee the resolution of symmetric solutions. If N_ϕ is too high ($N_\phi = 60$) or too low ($N_\phi = 10$), then asymmetric solutions are resolved. We expect the first kind of Taylor-Couette flow to be two-dimensional and symmetric about $\theta = 0$ similar to the cylindrical and spherical counterparts so the early appearance of asymmetric solutions seemed illogical.

It was relatively easy to explore the effect of increasing the number of θ - and ϕ - grid points on the resolution of the flows because of our construction of the Poisson solver. As expected, the most time-consuming exploration of the parameters occurred while increasing the number of radial grid points. The radial grid size is of particular importance if we are to explore wide gaps and remains an interesting area of future work especially since we have also observed that a coarse radial grid hides important flow features.

6.4 Shifting the gap

In this section, we examine the effect of ‘moving’ the gap but preserving the gap width. This is the final parameter that can be changed to determine its effect on the flow and is unique

	$r_b = 0.28$	$r_b = 0.30$	$r_b = 0.35$
$Re = 15000$	5	1	1
$Re = 20000$	3	3	1
$Re = 25000$	3	3	3

Table 6.7: Number of fingers observed when $r_a = 0.25$

to our geometry.

In the previous sections, $r_a = 0.25$ but r_b varied to generate different gap widths for examination. Instead, we set $r_a = 0.75$ and then choose different values for r_b in this section. Larger values for r_a and r_b means that the gap is now closer to the axis of rotation and that the tori are now closer geometrically to the degenerate case of the horn torus i.e. the torus with no hole.

6.4.1 Case 1, $r_a = 0.75$, $r_b = 0.78$, $Re = 10000$

We begin our study by examining the same initial gap width of 0.03 but with $r_a = 0.75$ and $r_b = 0.78$ while varying the Reynolds number. We maintain a spin-up of 500s and examine the flow at and after spin-up at 1000s with the parameters shown in Table 6.8.

N_r	N_θ	N_ϕ	Re	r_a	r_b	R_0	Spin-up	Sub-section	Figures
15	285	40	10000	0.75	0.78	1.0	500s	Case 1	6.70, 6.71, 6.72, 6.73, 6.74, 6.75
15	385	40	15000	0.75	0.78	1.0	500s	Case 2	6.76, 6.77, 6.78, 6.79, 6.80, 6.81

Table 6.8: Parameters used to study the effect of different Reynolds numbers with $r_a = 0.75$

At 500s

$Re = 10000$

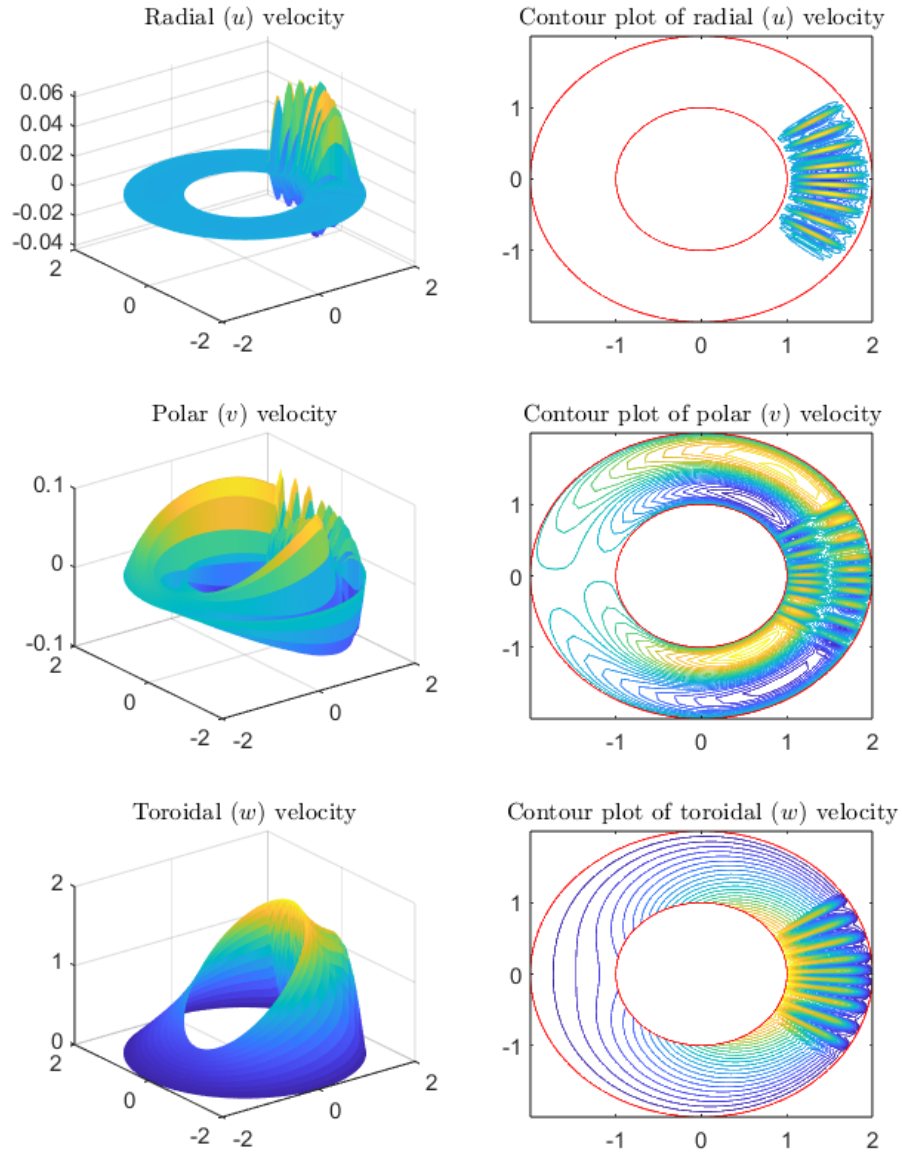


Figure 6.70: Velocity components at 500s for $r_a = 0.75$, $r_b = 0.78$, $Re = 10000$

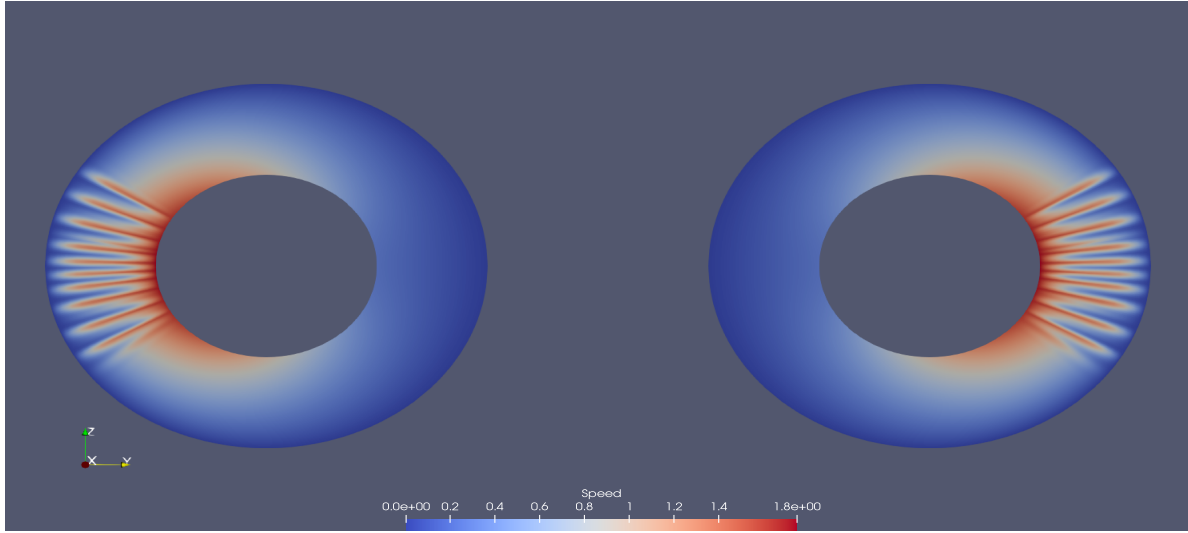


Figure 6.71: Speed at 500s on $\phi = \frac{3\pi}{2}$ (left) and $\phi = \frac{\pi}{2}$ (right) for $r_a = 0.75$, $r_b = 0.78$, $Re = 10000$

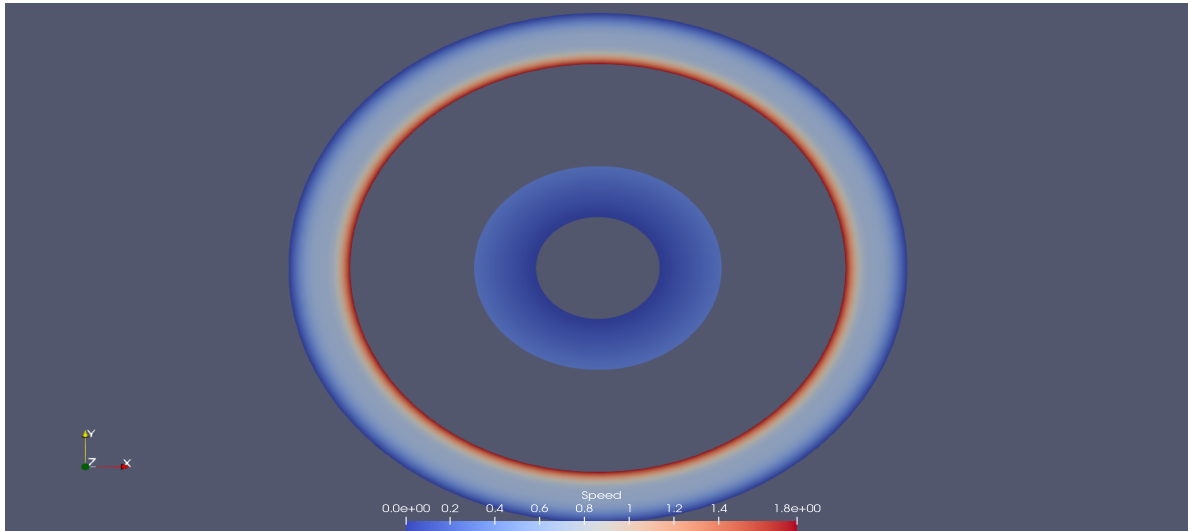


Figure 6.72: Speed at 500s on the plane $\theta = 0$ for $r_a = 0.75$, $r_b = 0.78$, $Re = 10000$

At 1000s

$Re = 10000$

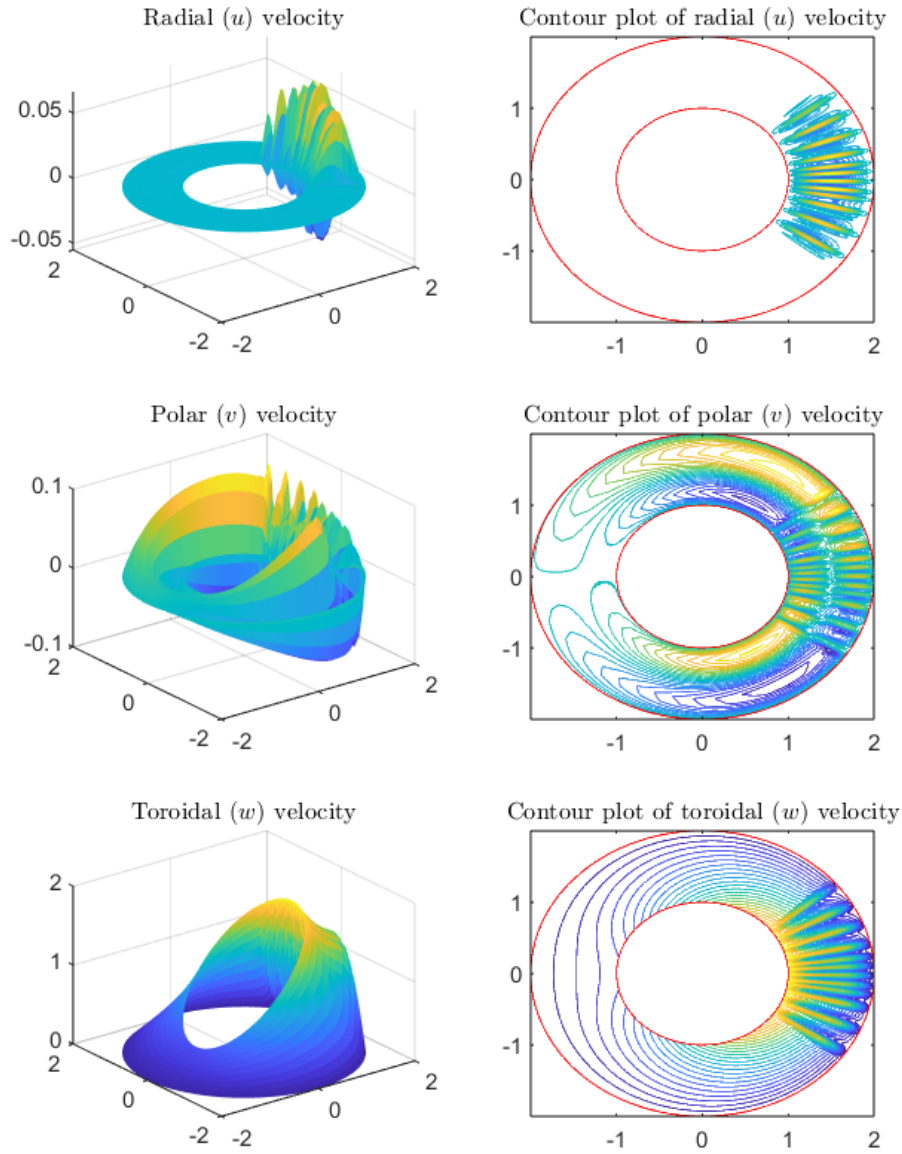


Figure 6.73: Velocity components at 1000s for $r_a = 0.75$, $r_b = 0.78$, $Re = 10000$

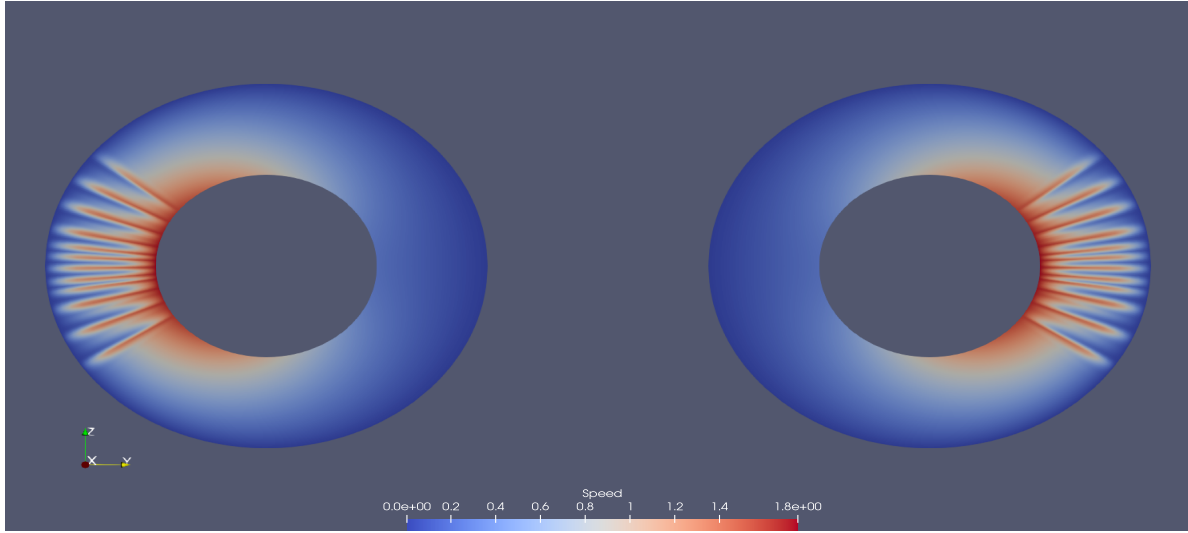


Figure 6.74: Speed at 1000s on $\phi = \frac{3\pi}{2}$ (left) and $\phi = \frac{\pi}{2}$ (right) for $r_a = 0.75$, $r_b = 0.78$, $Re = 10000$

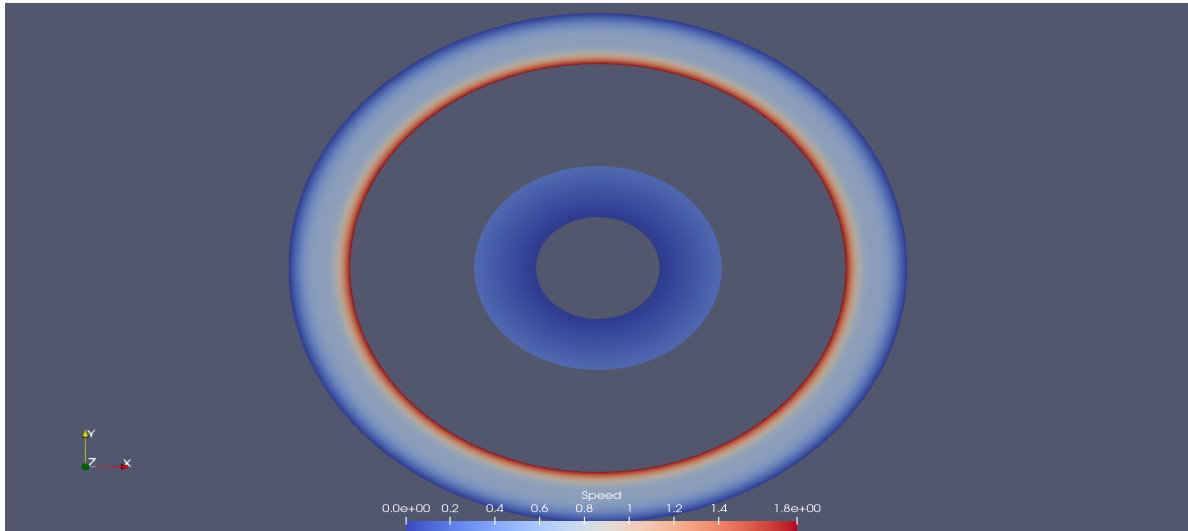


Figure 6.75: Speed at 1000s on the plane $\theta = 0$ for $r_a = 0.75$, $r_b = 0.78$, $Re = 10000$

6.4.2 Case 2, $r_a = 0.75$, $r_b = 0.78$, $Re = 15000$

At 500s

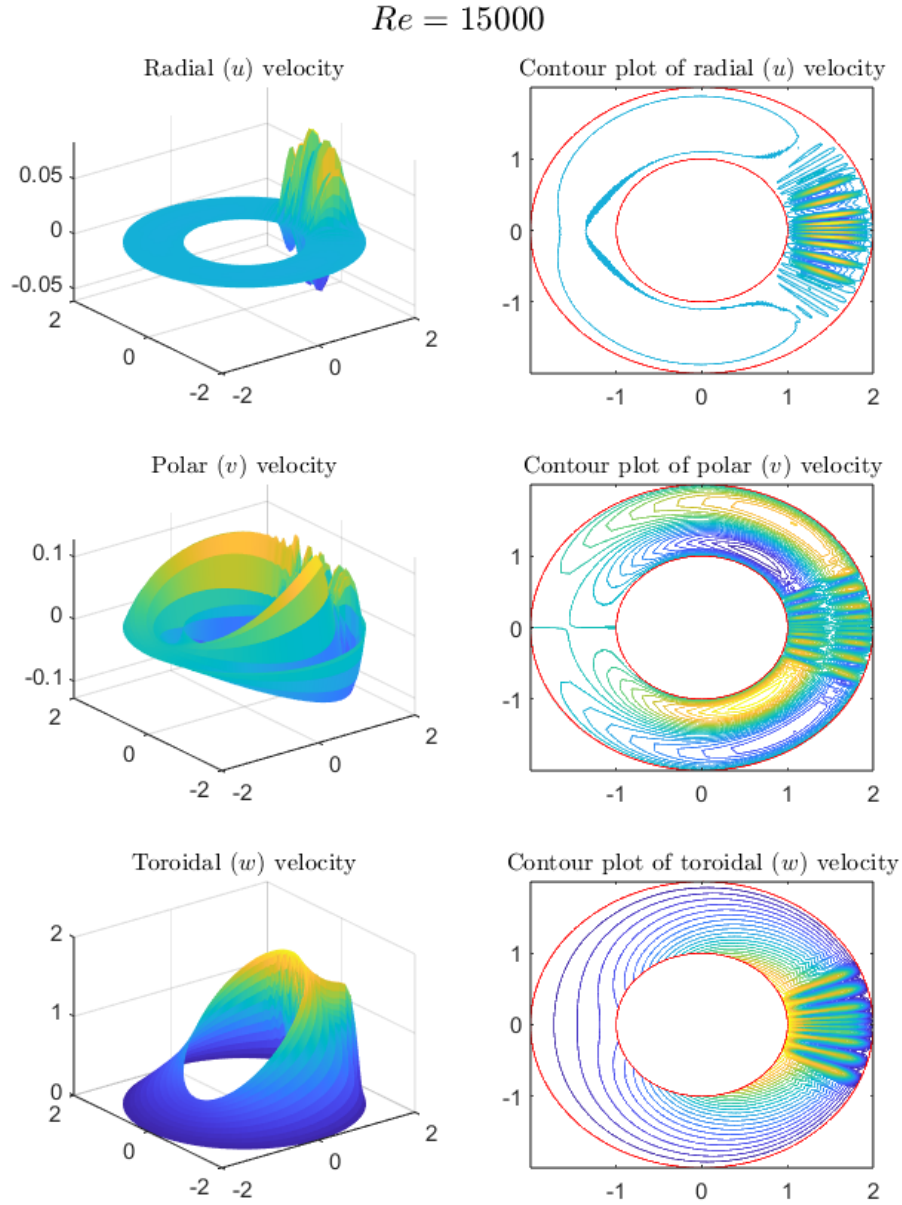


Figure 6.76: Velocity components at 500s for $r_a = 0.75$, $r_b = 0.78$, $Re = 15000$

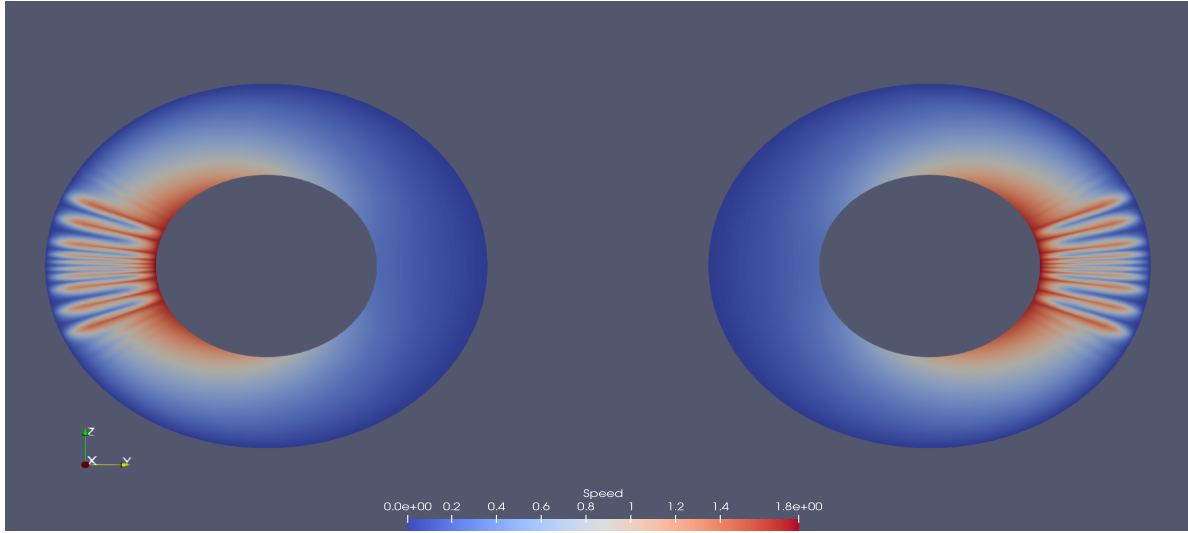


Figure 6.77: Speed at 500s on $\phi = \frac{3\pi}{2}$ (left) and $\phi = \frac{\pi}{2}$ (right) for $r_a = 0.75$, $r_b = 0.78$, $Re = 15000$

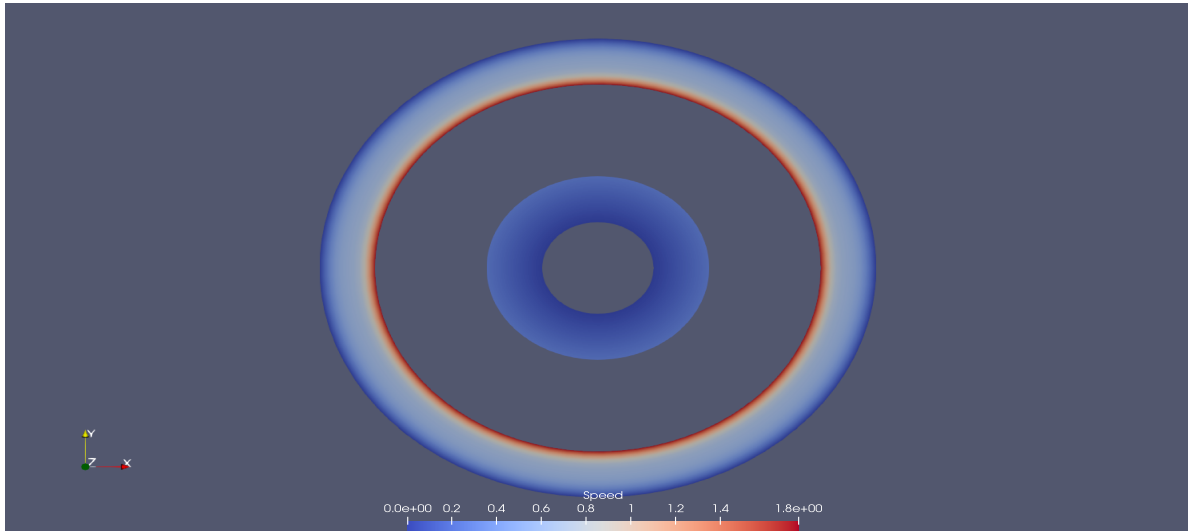


Figure 6.78: Speed at 500s on the plane $\theta = 0$ for $r_a = 0.75$, $r_b = 0.78$, $Re = 15000$

At 1000s

$Re = 15000$

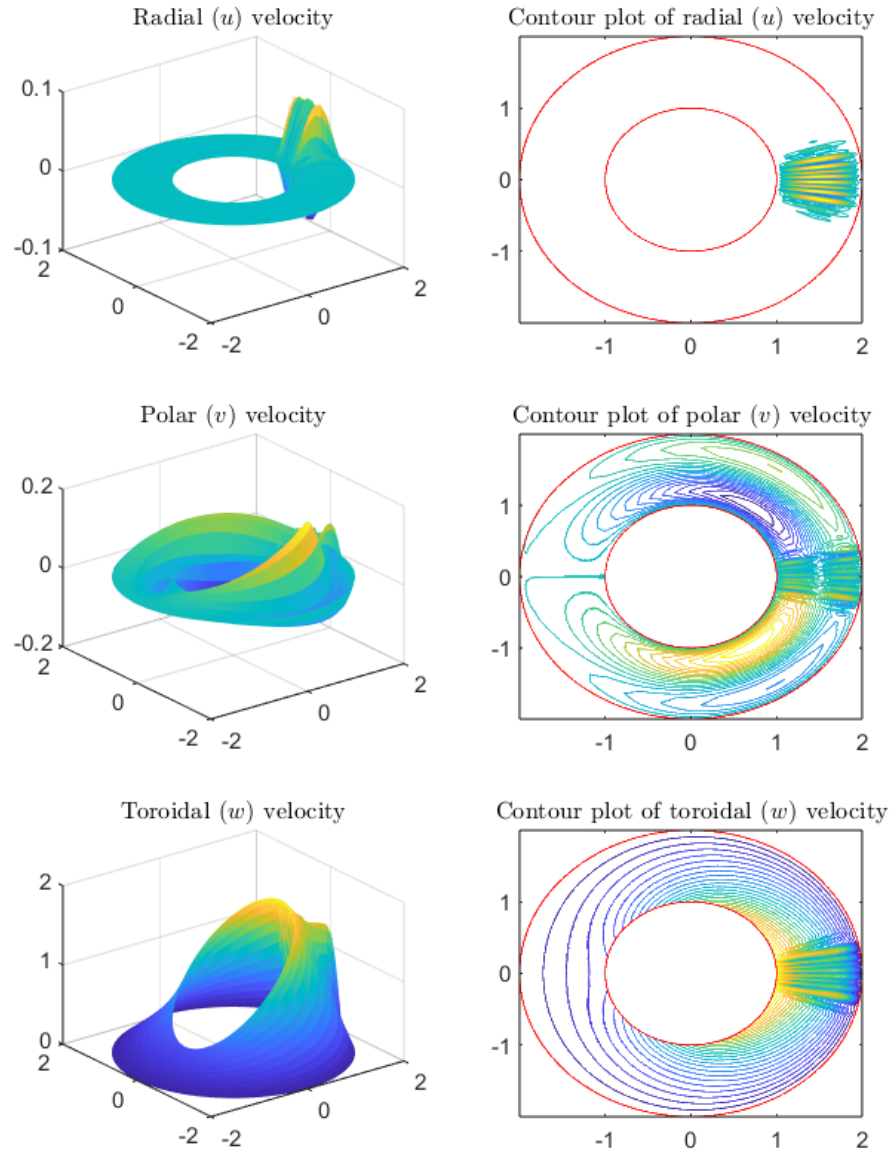


Figure 6.79: Velocity components at 1000s for $r_a = 0.75$, $r_b = 0.78$, $Re = 15000$

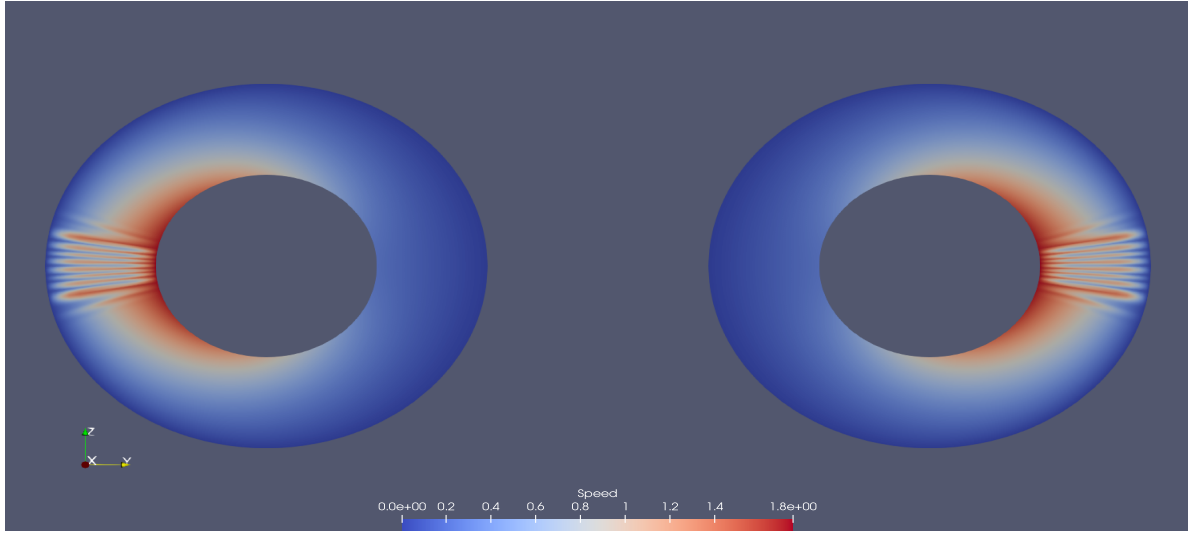


Figure 6.80: Speed at 1000s on $\phi = \frac{3\pi}{2}$ (left) and $\phi = \frac{\pi}{2}$ (right) for $r_a = 0.75$, $r_b = 0.78$, $Re = 15000$

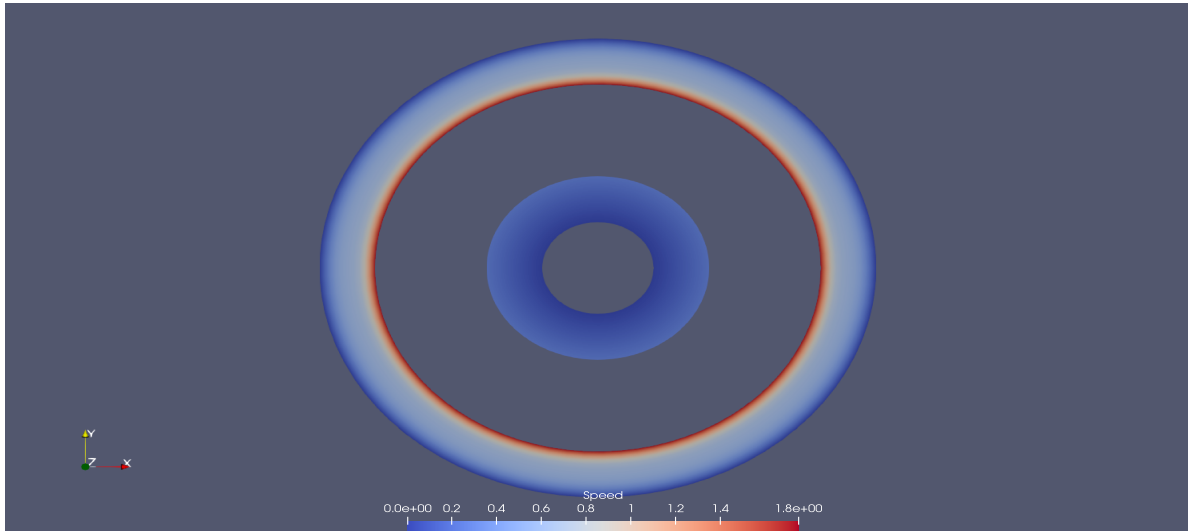


Figure 6.81: Speed at 1000s on the plane $\theta = 0$ for $r_a = 0.75$, $r_b = 0.78$, $Re = 15000$

6.4.3 Summary of results

The new position of the gap comes with new features. At the lower Reynolds number, $Re = 10000$, we have multiple fingers appearing with a narrow gap between them both at spin-up, see Figures 6.70, 6.71, 6.72 and in the long-term behaviour, see Figures 6.73, 6.74, 6.75. Additionally, the fingers occupy a larger region than the cases where $r_a = 0.25$ and $r_b = 0.28$.

At the higher Reynolds number, $Re = 15000$, the fingers are restricted to a smaller region at spin-up but are still numerous, see Figures 6.76, 6.77, 6.78. At $1000s$, the fingers undergo some noteworthy changes. The fingers are not all of the same thickness which is a feature that has not been observed before in any of the cases. There are several thin fingers separated by thin gaps bounded between two thicker fingers. This represents several slender bands of relatively high speed sandwiched between two thicker bands of even higher speeds outside of which the flow displays Couette properties, see Figures 6.79, 6.80, 6.81.

We again note the absence of ϕ -dependence in both cases. The number of points for the θ -grid has increased significantly for $r_a = 0.75$ and $r_b = 0.80$ because we need to resolve more oscillatory behaviour. With the increase in the number of fingers when $r_a = 0.75$, an obvious path for future work presents itself. It is possible to analyse the effect of changing r_a on the flow for a fixed gap width. As with the previous cases, the effect of increasing the number of radial points can also be explored in the future.

Chapter 7

Results: Oscillating flow

Oscillating flows bring us back to one of the main sources of motivation for this thesis. This chapter aims to provide insight into the behaviour of the fluid when both tori oscillate. In particular, we are interested in the torque exerted on the walls of both tori as a first step in determining the viability of fluidic ring actuators.

7.1 Torque

Torque is of particular interest when fluids rotate or turn in contact with a physical object. Heuristically, it is the amount of effort needed to rotate a physical object in contact with a fluid. The formal definition of torque is given below.

$$\mathbf{M} = \mathbf{L} \times \mathbf{F} \tag{7.1}$$

where $\mathbf{M}$ is the torque, $\mathbf{F}$ is the force applied and $\mathbf{L}$ is the ‘lever arm’ vector i.e. the vector connecting the axis of rotation to the point where the force is applied

In the case of fluid mechanics, the force, $\mathbf{F}$, needs to be appropriately represented. Morrison [95] has done the derivation for us.

$$\mathbf{F} = \iint_{\partial\Omega} [\hat{\mathbf{n}} \cdot \mathbf{T}]_{\text{on the surface}} dS \quad (7.2)$$

where $\hat{\mathbf{n}}$ is the unit normal to the surface which is in contact with the fluid and $\mathbf{T}$ is total stress tensor.

Therefore, the total torque, $\mathbf{M}$, on a surface, $\partial\Omega$, is given by

$$\mathbf{M} = \iint_{\partial\Omega} \mathbf{L} \times [\hat{\mathbf{n}} \cdot \mathbf{T}]_{\text{on the surface}} dS \quad (7.3)$$

We replicated the formula for the torque on concentric rotating spheres [96] using the aforementioned torque formula. With these ideas, we can derive the torque on concentric rotating (in the ϕ direction) tori found in this thesis.

7.1.1 Torque on concentric rotating tori

We need the following quantities to find the torque exerted by concentric rotating tori: $\mathbf{L}$, $\hat{\mathbf{n}}$ and $\mathbf{T}$.

We begin with the ‘lever arm’ vector, $\mathbf{L}$. Recall that this vector connects the axis of rotation with the point at which the force is applied. Therefore,

$$\mathbf{L} = h_\phi \cos \theta \hat{e}_r - h_\phi \sin \theta \hat{e}_\theta = h_\phi (\cos \theta, -\sin \theta, 0) \quad (7.4)$$

For now, we keep the stress tensor, $\mathbf{T}$, generic i.e.

$$\mathbf{T} = \begin{bmatrix} \tau_{rr} & \tau_{r\theta} & \tau_{r\phi} \\ \tau_{\theta r} & \tau_{\theta\theta} & \tau_{\theta\phi} \\ \tau_{\phi r} & \tau_{\phi\theta} & \tau_{\phi\phi} \end{bmatrix} \quad (7.5)$$

Finally, the unit normal to the surface, $\hat{\mathbf{n}}$, is obvious: $(1, 0, 0)$

With these three quantities, we can make progress by first calculating the quantity, $\hat{\mathbf{n}} \cdot \mathbf{T} = (\tau_{rr}, \tau_{r\theta}, \tau_{r\phi})$. However, we do not use this vector in the calculation of the torque. Instead, we take only the ϕ component of this vector because it is the only component that is in the direction of rotation. In other words, it is only this component of the force that is relevant for or causes the rotation. As a result, we have

$$\begin{aligned}\mathbf{M} &= - \iint_{\partial\Omega} \mathbf{L} \times [\hat{\mathbf{n}} \cdot \mathbf{T}]_{\text{on the surface}} dS \\ \mathbf{M} &= - \iint_{\partial\Omega} h_\phi (\cos \theta, -\sin \theta, 0) \times (0, 0, \tau_{r\phi}) dS \\ \mathbf{M} &= - \iint_{\partial\Omega} h_\phi \tau_{r\phi} \hat{\mathbf{z}} dS\end{aligned}\tag{7.6}$$

We pause here to explain several ideas in the above torque calculation. First, the minus sign is introduced because of the use of a cross product in a left-handed co-ordinate system. Second, the unit vector in the z -direction is $\sin \theta \hat{e}_r + \cos \theta \hat{e}_\theta$. The use of the vector $\hat{\mathbf{z}}$ is used to emphasize that the torque, $\mathbf{M}$, is indeed orthogonal to the lever arm vector and the force applied in the ϕ direction.

Therefore, the magnitude of the torque, M , is given by

$$M = \iint_{\partial\Omega} h_\phi \tau_{r\phi} dS\tag{7.7}$$

We can now proceed with the surface integral. First, note that $dS = rh_\phi d\theta d\phi$. Next, the limits of integration are between 0 and 2π in the θ direction and between 0 and π in the ϕ direction. These limits of integration only cover half of a torus so we need to double the integral to calculate the full torque.

$$M = 2 \int_0^\pi \int_0^{2\pi} rh_\phi^2 \tau_{r\phi} d\theta d\phi\tag{7.8}$$

At this point, we simplify the $\tau_{r\phi}$ component of the stress tensor.

$$\tau_{r\phi} = \frac{1}{2}\mu \left[\frac{\partial w}{\partial r} + \frac{1}{h_\phi} \left(\frac{\partial u}{\partial \phi} - w \cos \theta \right) \right] = \frac{1}{2}\mu \left[\frac{\partial w}{\partial r} - \frac{1}{h_\phi} w \cos \theta \right] \quad (7.9)$$

Clearly, $u = 0$ on the boundary and there is no change in u in the ϕ direction. Also, we expect $\frac{\partial w}{\partial r}$ to be non-zero due to the expected presence of boundary layers. We can now separate the surface integral into two parts and evaluate each individually numerically.

$$M = \mu \int_0^\pi \int_0^{2\pi} \frac{\partial w}{\partial r} r h_\phi^2 \, d\theta d\phi + \mu \int_0^\pi \int_0^{2\pi} r h_\phi w \cos \theta \, d\theta d\phi \quad (7.10)$$

7.2 Oscillating both tori

To study oscillating flow, we need to change the boundary conditions from that used in the previous chapter. Instead of rotating only the inner torus in the positive ϕ direction for all time, t , we switch the direction of rotation on *both* tori (not one) after a prescribed time has passed. For simplicity, we have regulated this change in direction with a sine function so that the direction of rotation will change every π seconds.

As in the cases studied in the previous chapter, in order to guarantee appropriate smoothness of the solution in a neighborhood of $t = 0$ (and hence preserve the high-order accuracy of the solutions for $t > 0$) we do not use impulsively-started boundary conditions. Instead, we make use of a smooth 'spin-up' function $f(t; 0, t_1)$ which smoothly transitions the velocities on the boundary from rest at $t = t_0 = 0$ to values at $t = t_1$, where t_1 is the spin-up time. A full description of the spin-up function is presented in Appendix C. With these considerations in mind, the boundary conditions enforced in this chapter are

$$\mathbf{u}(r, \theta, \phi, t) = \begin{cases} (0, 0, (1 - f(t; 0, t_1))(1 + r_a \cos \theta)) \sin(t), & r = r_a \\ (0, 0, (1 - f(t; 0, t_1))(1 + r_b \cos \theta)) \sin(t), & r = r_b \end{cases} \quad (7.11)$$

We present the results of numerical simulations with these new boundary conditions below.

We study the same cases as in the previous chapter with one notable difference. The spin-up time was shortened to $100s$ because we are interested in observing the flow after both tori have reached their maximum speed. The parameters used are listed in Table 7.1 and we observe the flow up to $400s$.

N_r	N_θ	N_ϕ	Re	r_a	r_b	R_0	Spin-up	Sub-section	Figures
15	255	40	15000	0.25	0.28	1.0	100s	Case 1	7.1, 7.2, 7.3, 7.4, 7.25
15	255	40	15000	0.25	0.30	1.0	100s	Case 2	7.5, 7.6, 7.7, 7.8, 7.25
15	255	40	20000	0.25	0.28	1.0	100s	Case 3	7.9, 7.10, 7.11, 7.12, 7.26
15	255	40	20000	0.25	0.30	1.0	100s	Case 4	7.13, 7.14, 7.15, 7.16, 7.26
20	255	40	25000	0.25	0.28	1.0	100s	Case 5	7.17, 7.18, 7.19, 7.20, 7.27
20	255	40	25000	0.25	0.30	1.0	100s	Case 6	7.21, 7.22, 7.23, 7.24, 7.27

Table 7.1: Parameters used to study the effect of oscillating tori

7.2.1 Case 1, $r_a = 0.25$, $r_b = 0.28$, $Re = 15000$

At 100s

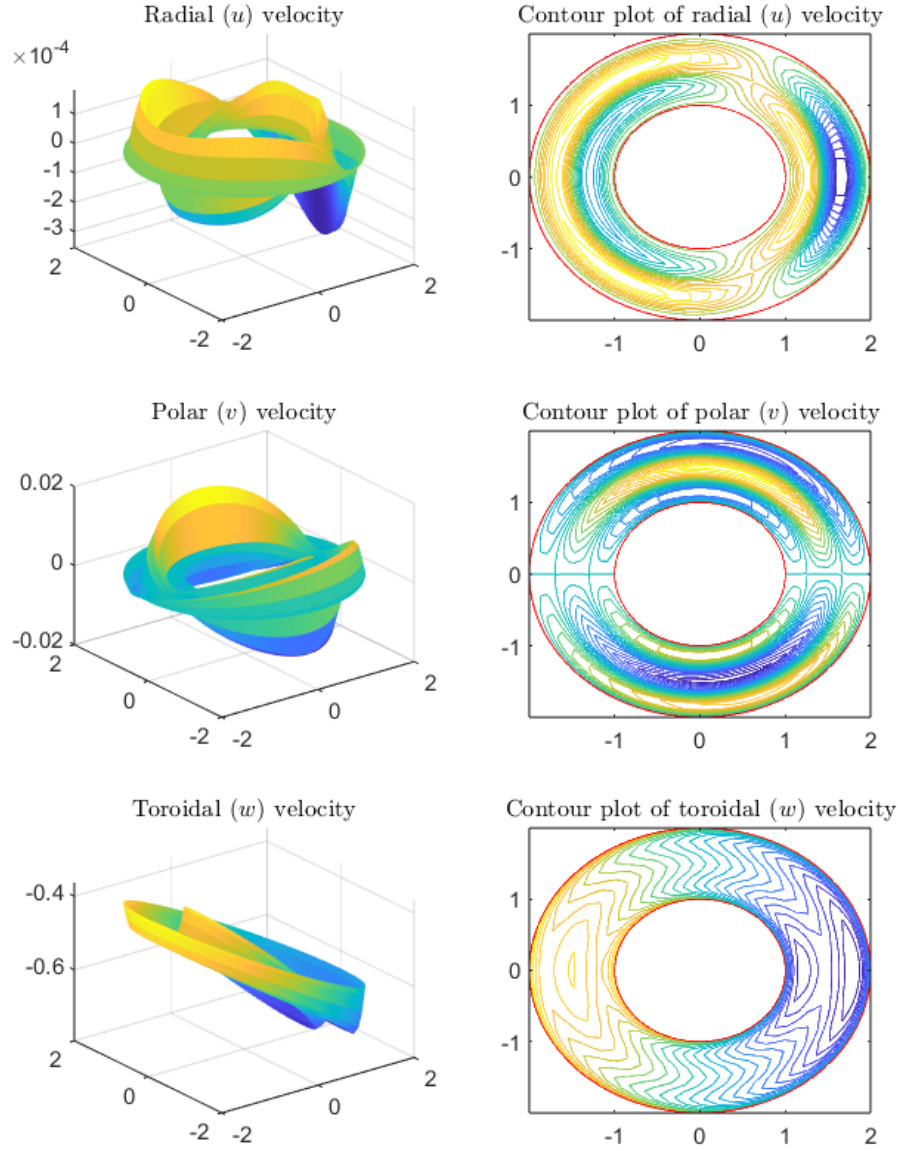


Figure 7.1: Velocity components at 100s for $r_a = 0.25$, $r_b = 0.28$, $Re = 15000$

At 400s

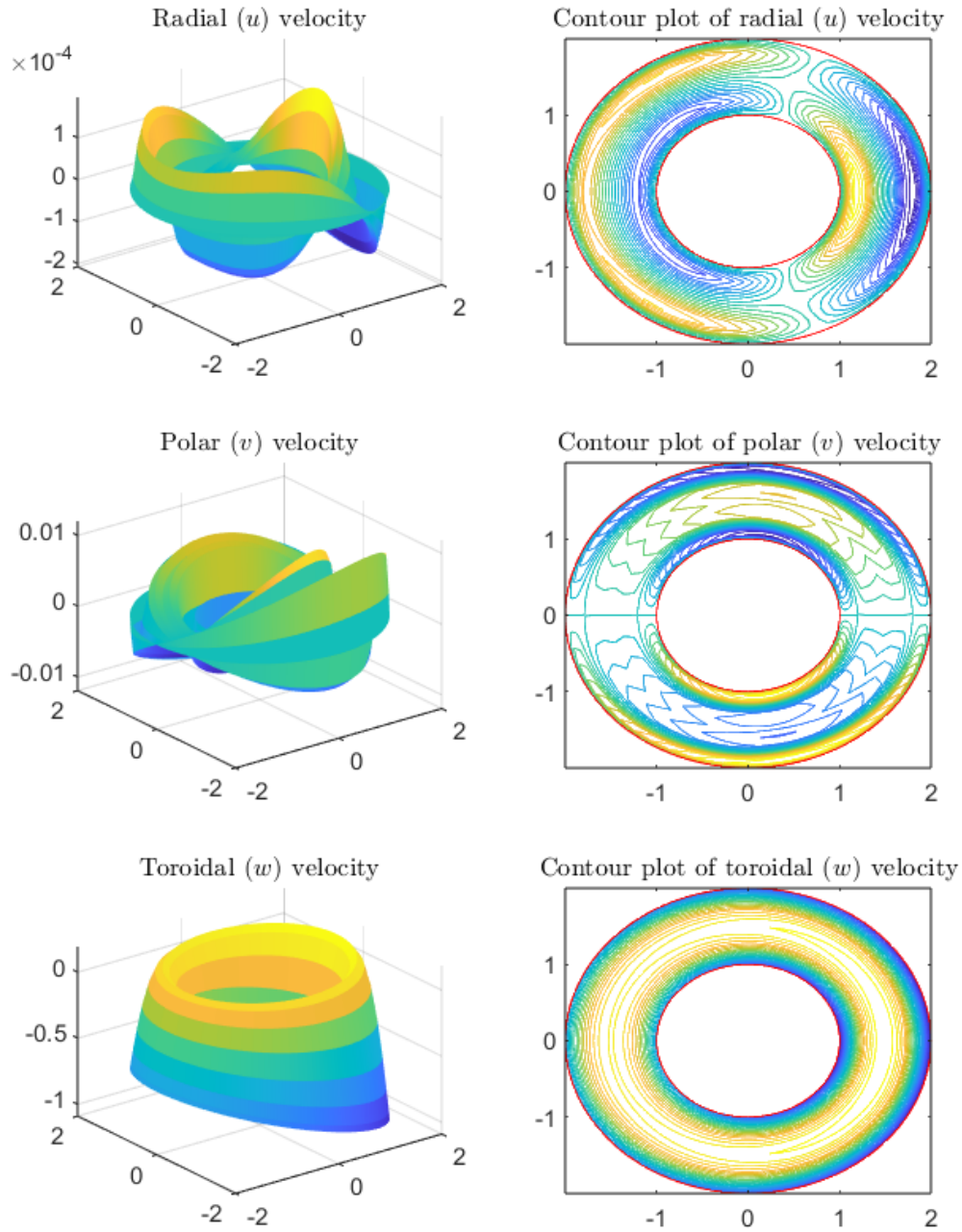


Figure 7.2: Velocity components at 400s for $r_a = 0.25$, $r_b = 0.28$, $Re = 15000$

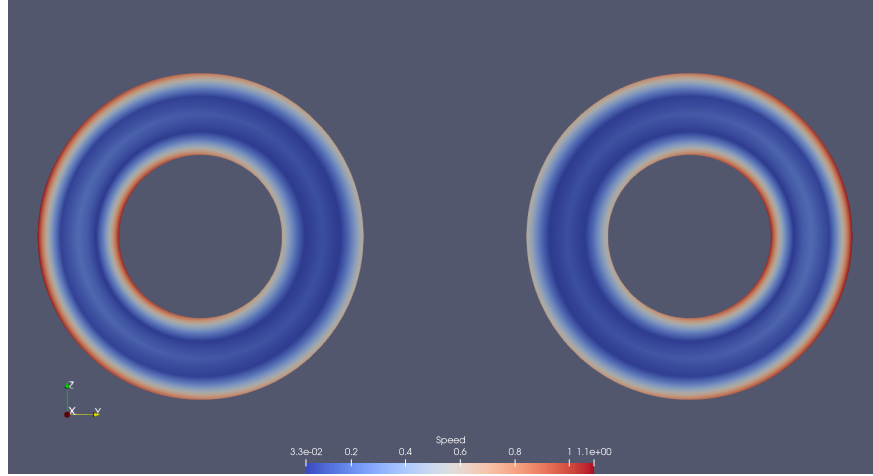


Figure 7.3: Speed at 400s on $\phi = \frac{3\pi}{2}$ (left) and $\phi = \frac{\pi}{2}$ (right) for $r_a = 0.25$, $r_b = 0.28$, $Re = 15000$

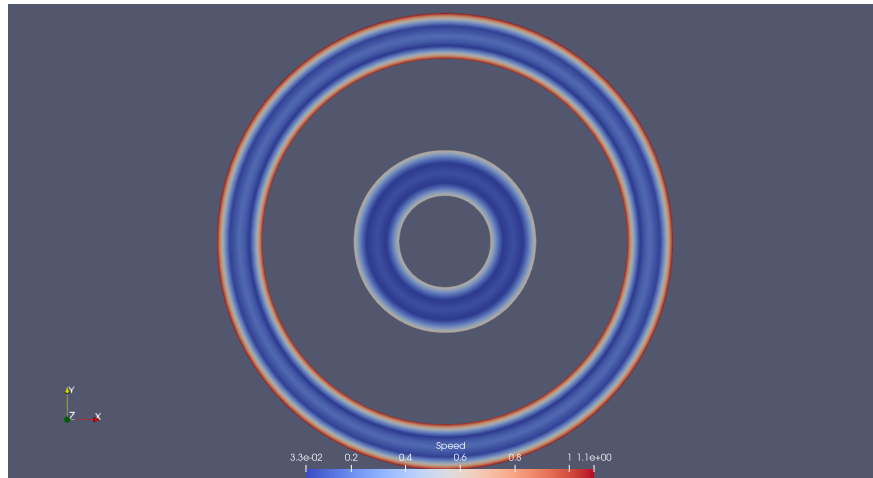


Figure 7.4: Speed at 400s on the plane $\theta = 0$ for $r_a = 0.25$, $r_b = 0.28$, $Re = 15000$

7.2.2 Case 2, $r_a = 0.25$, $r_b = 0.30$, $Re = 15000$

At 100s

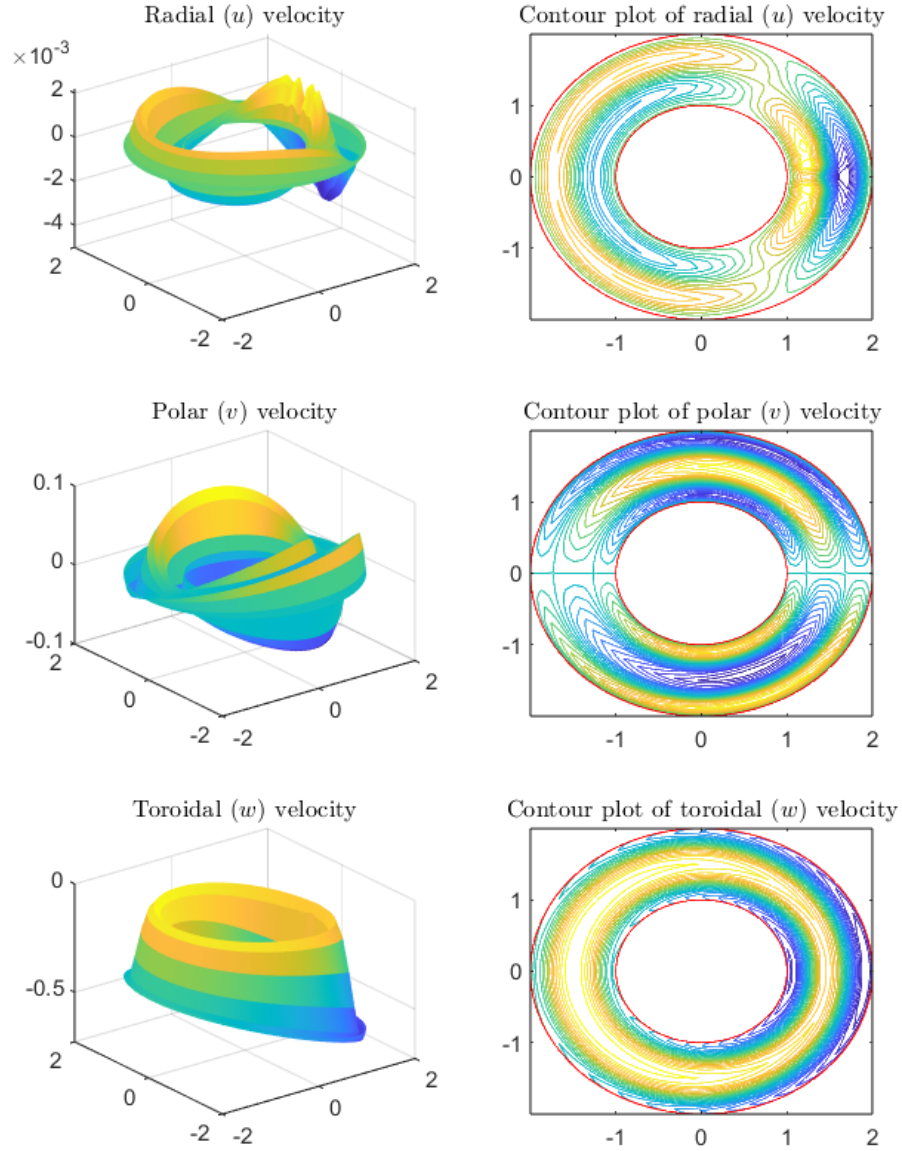


Figure 7.5: Velocity components at 100s for $r_a = 0.25$, $r_b = 0.30$, $Re = 15000$

At 400s

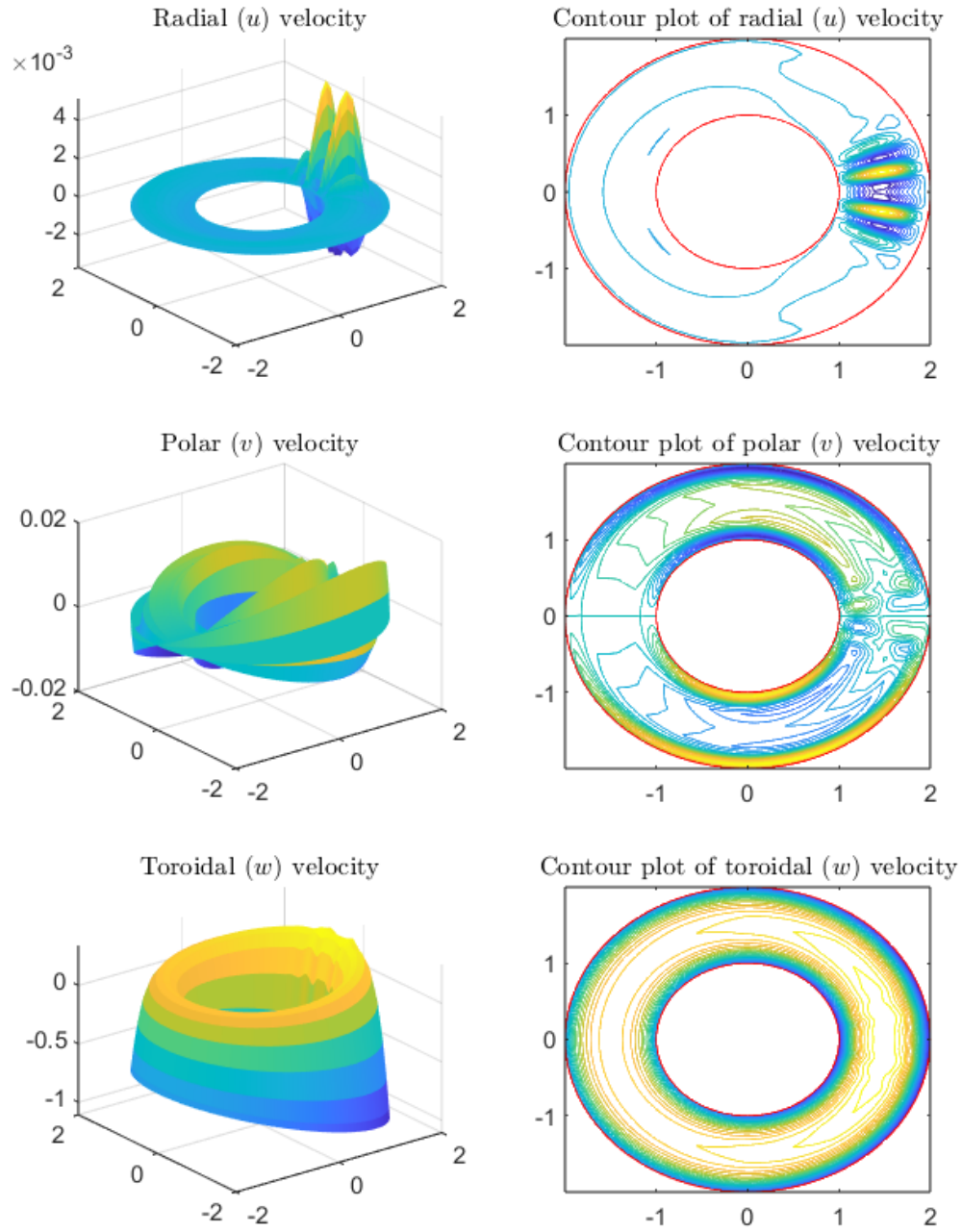


Figure 7.6: Velocity components at 400s for $r_a = 0.25$, $r_b = 0.30$, $Re = 15000$

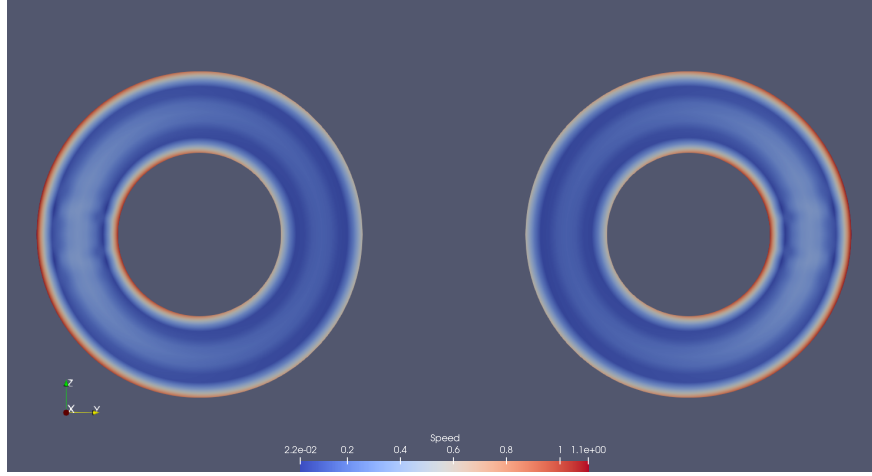


Figure 7.7: Speed at 400s on $\phi = \frac{3\pi}{2}$ (left) and $\phi = \frac{\pi}{2}$ (right) for $r_a = 0.25$, $r_b = 0.30$, $Re = 15000$

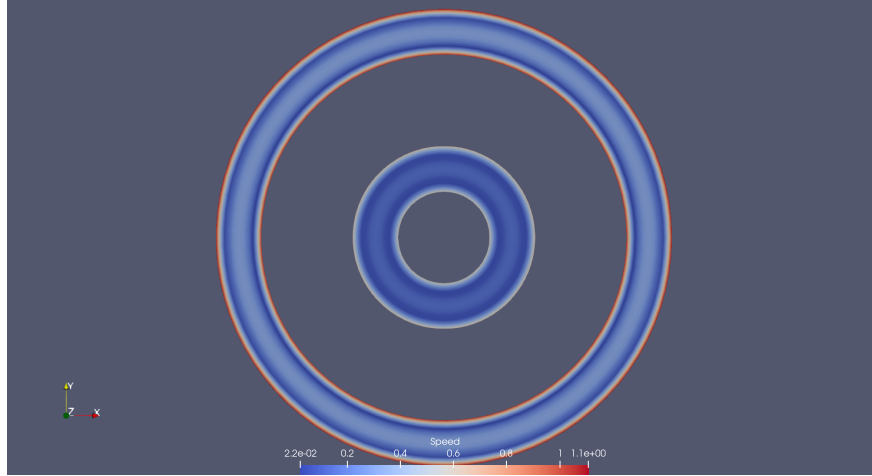


Figure 7.8: Speed at 400s on the plane $\theta = 0$ $r_a = 0.25$, $r_b = 0.30$, $Re = 15000$

Discussion

Case 1 presents us with our first oscillating flow and there are a number of features to point out. First, there is a significant difference in the flow at spin-up, see Figure 7.1 and after spin-up, see Figure 7.2. The ϕ velocity, see Figure 7.2, and the speed, see Figure 7.3, appear different from their counterparts in Figure 6.25, for instance, where only the inner torus rotated. The most obvious difference is the absence of bands of high and low speed. Instead, we have a distinctly different shape for and negative velocities in the ϕ -component of the

flow. The negative velocities are expected given that the direction of rotation changes every π seconds. There are only minor contributions from the other components of the flow so the entire flow is very close to its ϕ -component. Finally, the velocity appears uniform in both the θ and ϕ directions, see Figure 7.4.

Widening the gap in Case 2 has resulted in the faint appearance of the now familiar bands of high and low velocity in both the r - and θ - components seen in Figure 7.6 after 400s. However, the overall flow pattern is nothing like those observed in the previous chapter. There is a faint appearance of a sinusoidal wave of low speed in the middle of the gap centred around $\theta = 0$ and $\theta = \pi$. Once again, there is a significant difference at 100s, see Figure 7.5, and at 400s. Finally, there is no ϕ -dependence in either Case 1 or Case 2.

7.2.3 Case 3, $r_a = 0.25$, $r_b = 0.28$, $Re = 20000$

At 100s

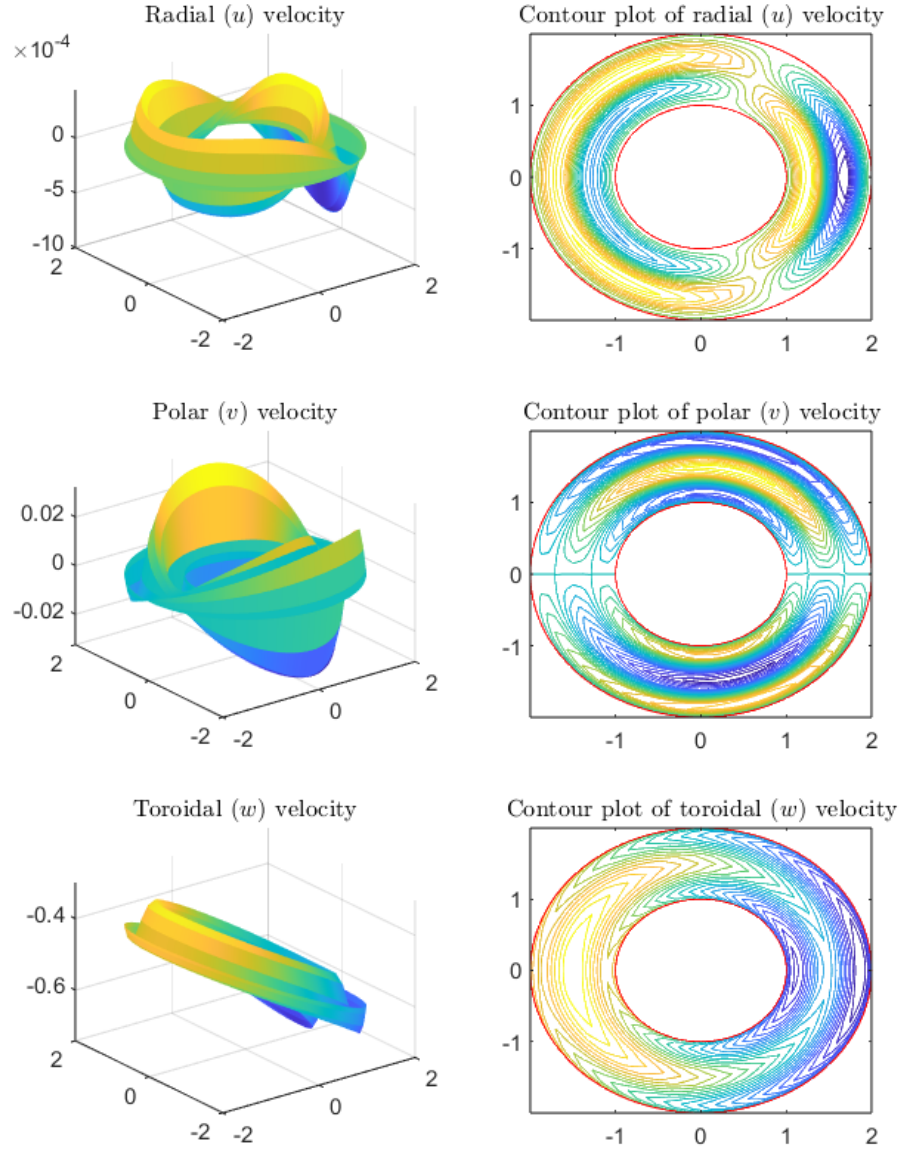


Figure 7.9: Velocity components at 100s for $r_a = 0.25$, $r_b = 0.28$, $Re = 20000$

At 400s

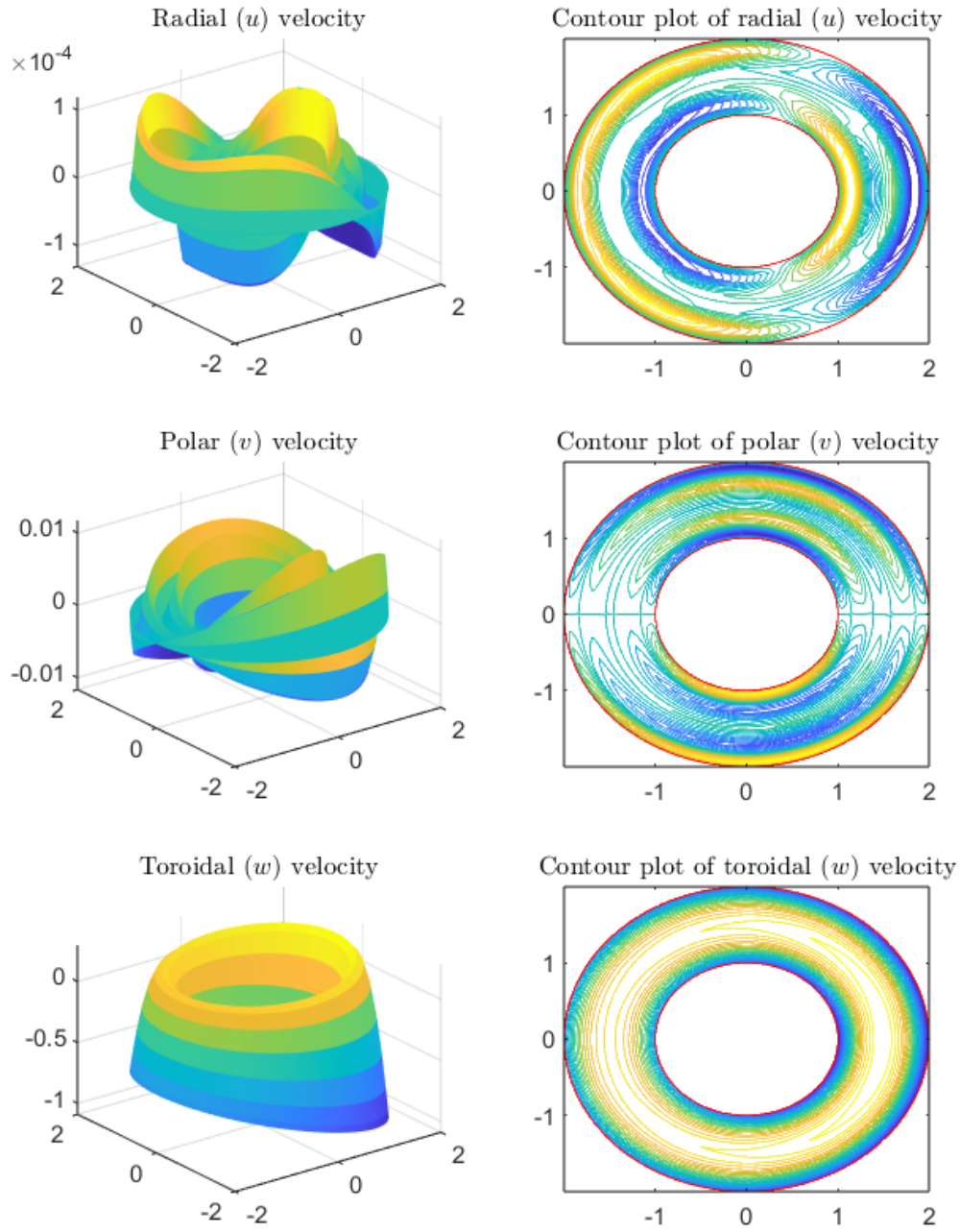


Figure 7.10: Velocity components at 400s for $r_a = 0.25$, $r_b = 0.28$, $Re = 20000$

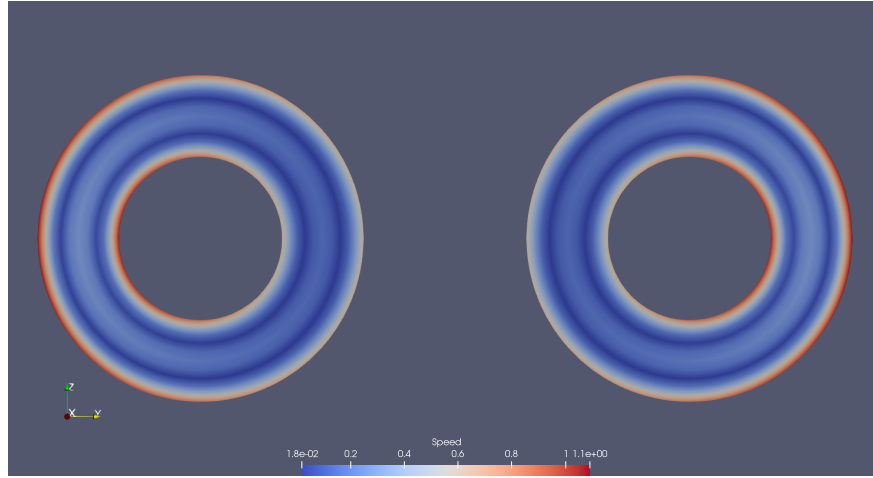


Figure 7.11: Speed at 400s on $\phi = \frac{3\pi}{2}$ (left) and $\phi = \frac{\pi}{2}$ (right) for $r_a = 0.25$, $r_b = 0.28$, $Re = 20000$

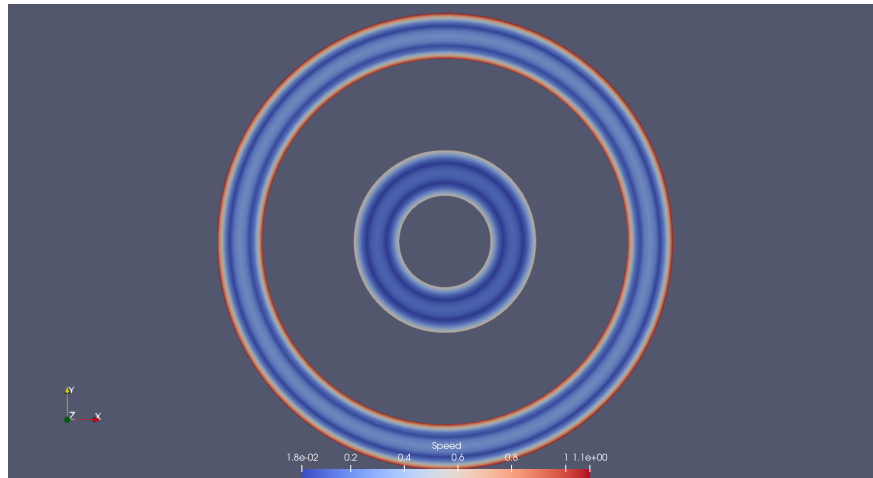


Figure 7.12: Speed at 400s on the plane $\theta = 0$ for $r_a = 0.25$, $r_b = 0.28$, $Re = 20000$

7.2.4 Case 4, $r_a = 0.25$, $r_b = 0.30$, $Re = 20000$

At 100s

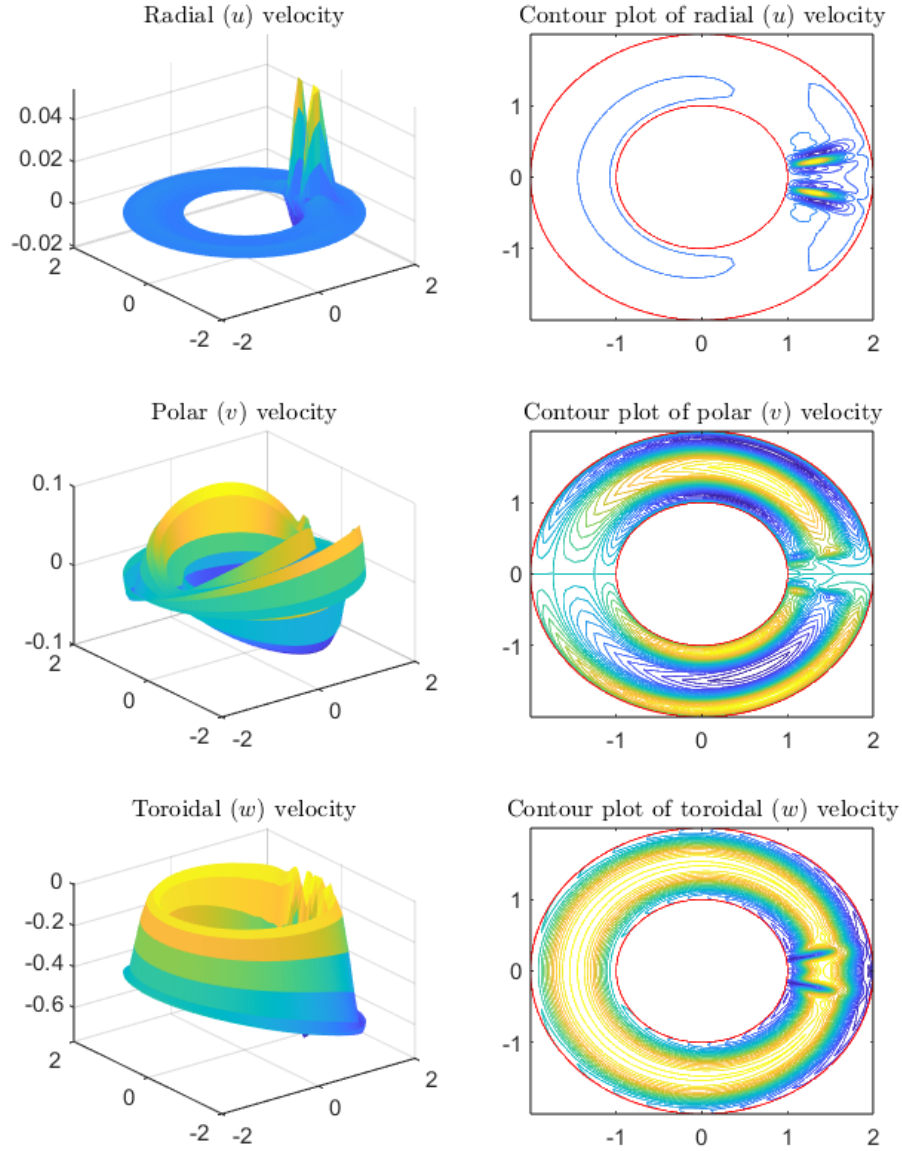


Figure 7.13: Velocity components at 100s for $r_a = 0.25$, $r_b = 0.30$, $Re = 20000$

At 400s

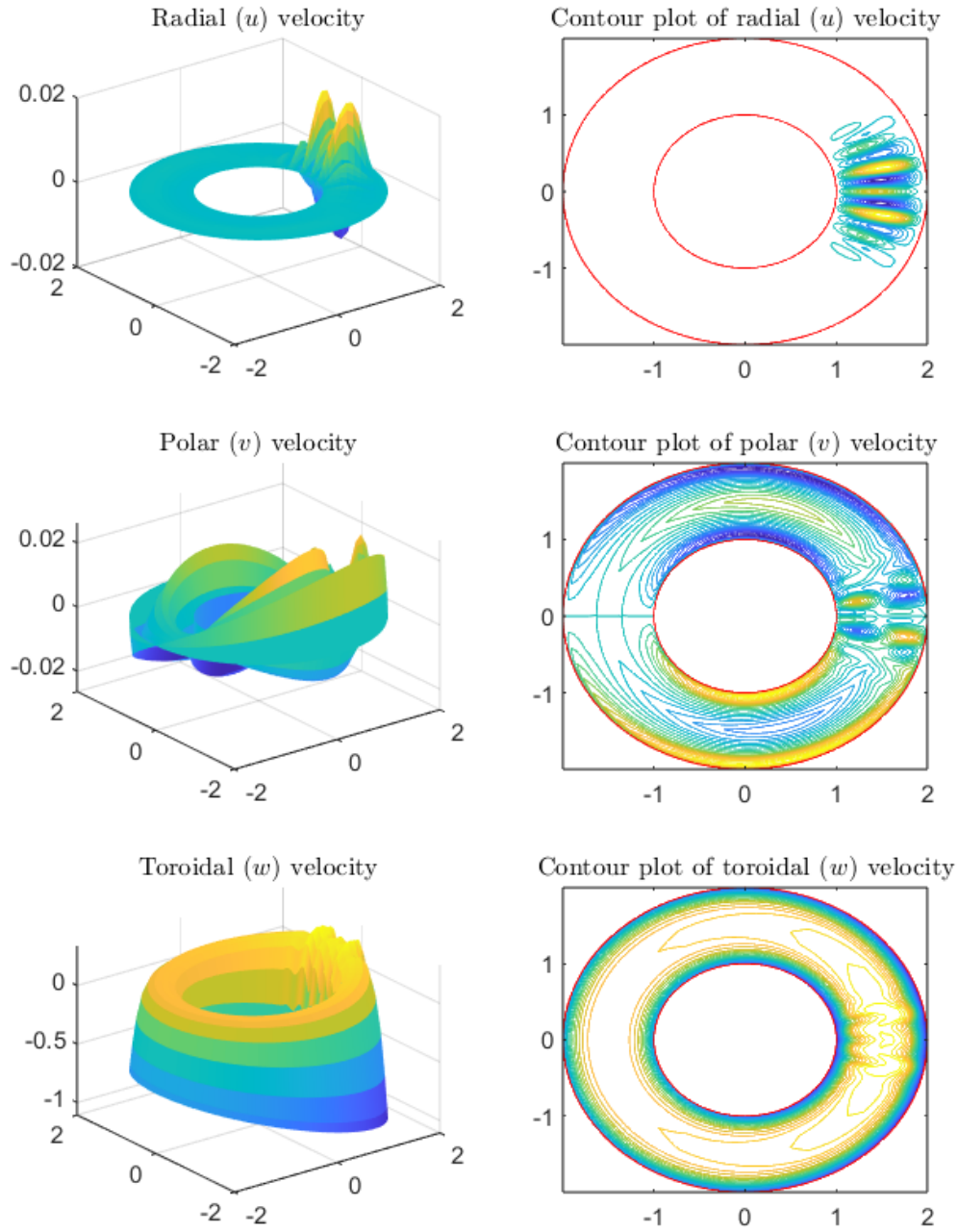


Figure 7.14: Velocity components at 400s for $r_a = 0.25$, $r_b = 0.30$, $Re = 20000$

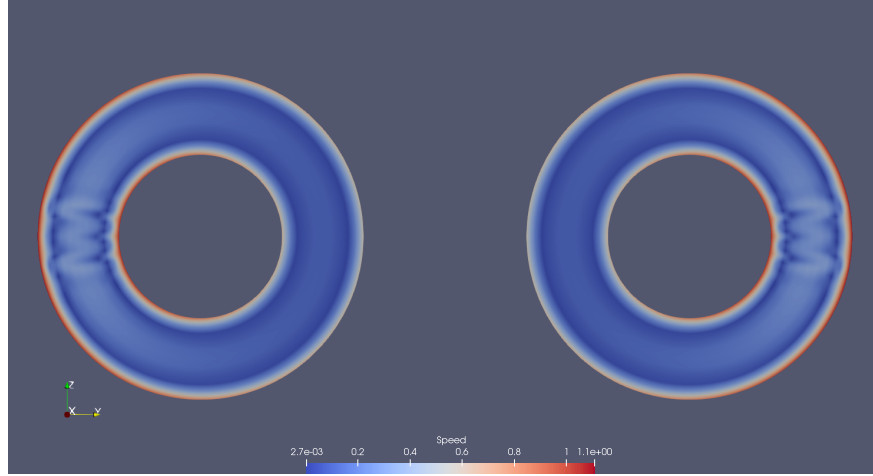


Figure 7.15: Speed at 400s on $\phi = \frac{3\pi}{2}$ (left) and $\phi = \frac{\pi}{2}$ (right) for $r_a = 0.25$, $r_b = 0.30$, $Re = 20000$

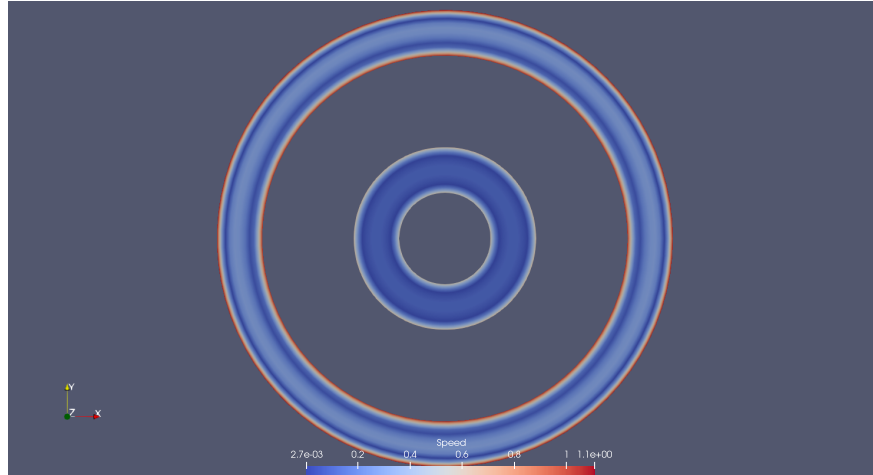


Figure 7.16: Speed at 400s on the plane $\theta = 0$ for $r_a = 0.25$, $r_b = 0.30$, $Re = 20000$

Discussion

Case 4 shows a more pronounced sinusoidal variation in the middle of the gap than that found in Case 2, see Figure 7.15. Its presence is also expressed in the toroidal velocity in Figure 7.14 similar to the fingers we have already seen. Finally, there is no ϕ -dependence in either flow, see Figure 7.12 and Figure 7.16.

7.2.5 Case 5, $r_a = 0.25$, $r_b = 0.28$, $Re = 25000$

At 100s

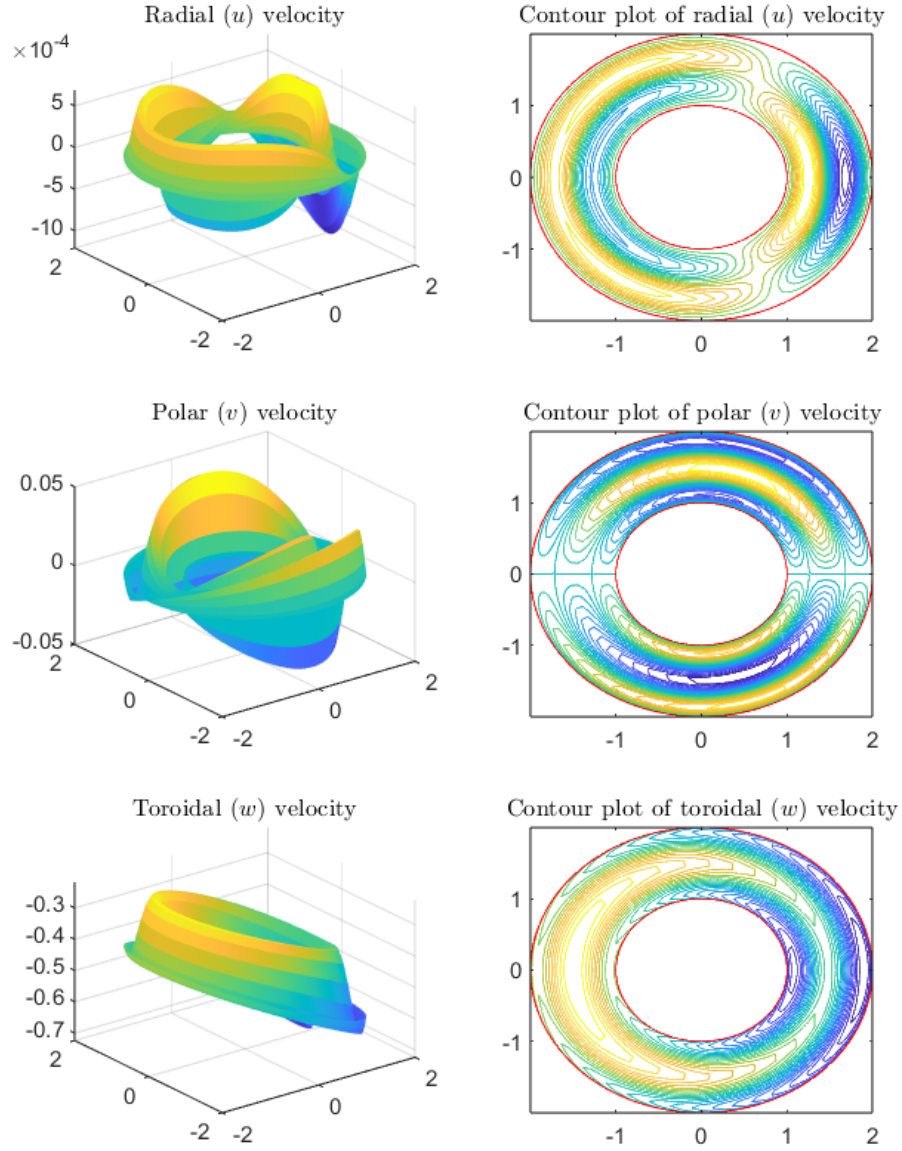


Figure 7.17: Velocity components at 100s for $r_a = 0.25$, $r_b = 0.28$, $Re = 25000$

At 400s

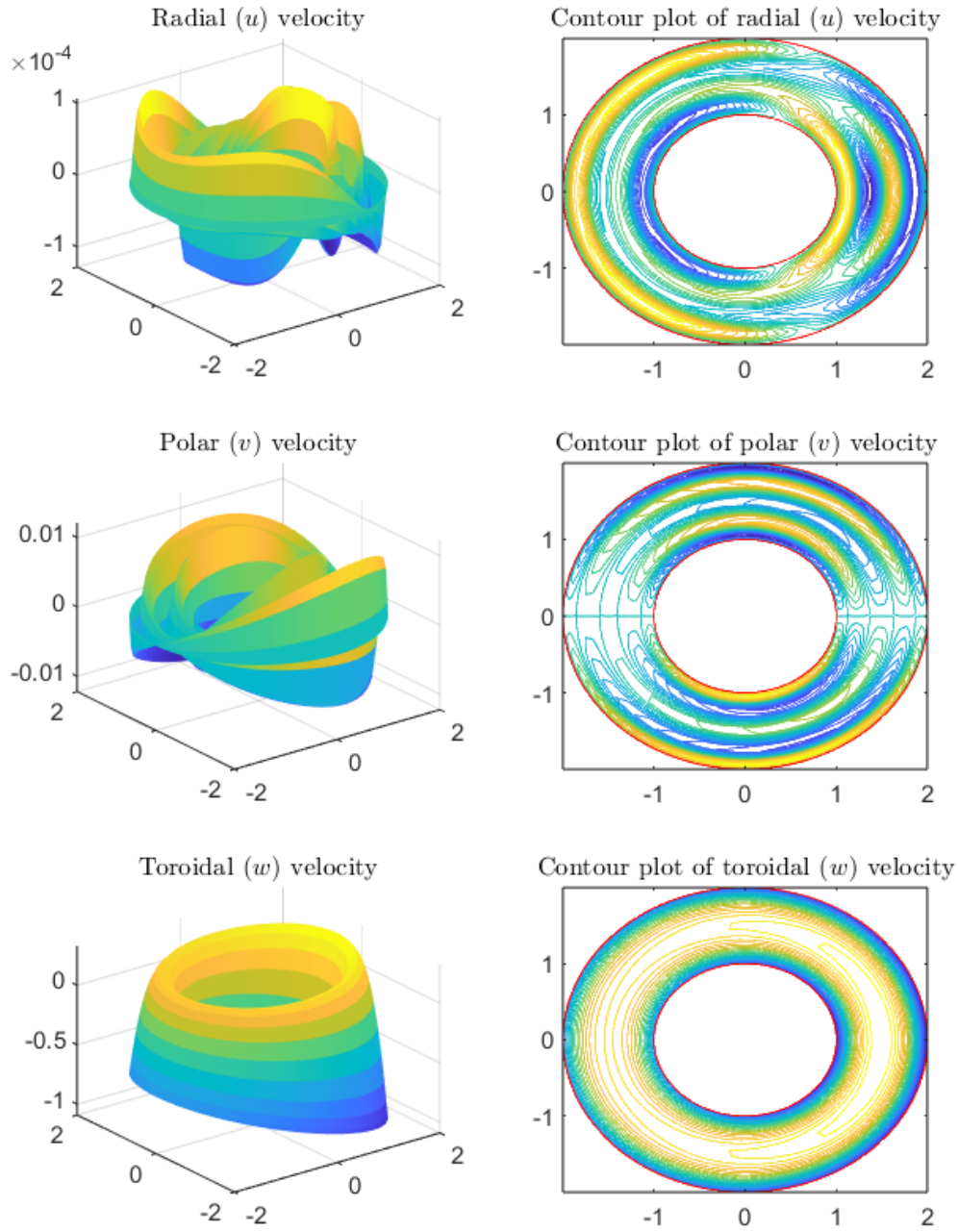


Figure 7.18: Velocity components at 400s for $r_a = 0.25$, $r_b = 0.28$, $Re = 25000$

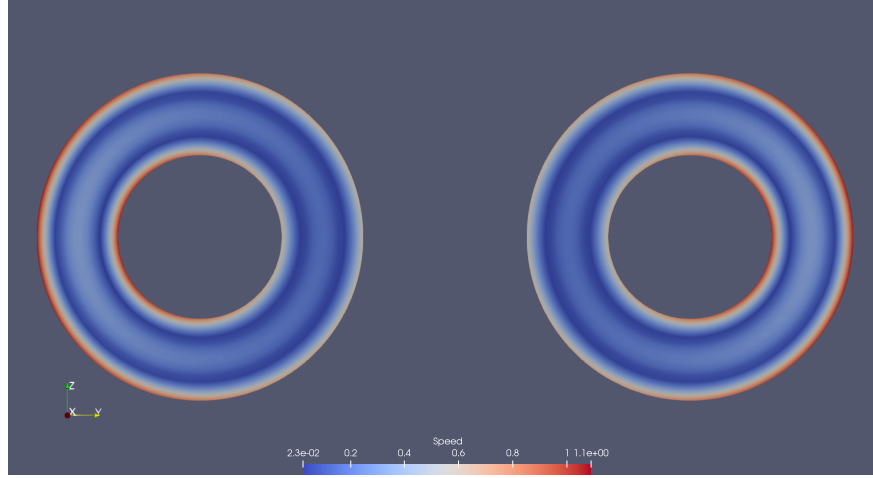


Figure 7.19: Speed at 400s on $\phi = \frac{3\pi}{2}$ (left) and $\phi = \frac{\pi}{2}$ (right) for $r_a = 0.25$, $r_b = 0.28$, $Re = 25000$

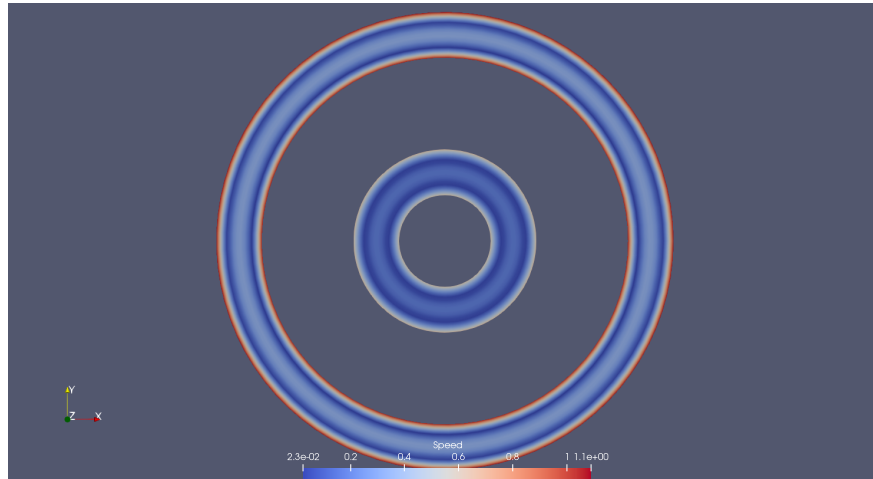


Figure 7.20: Speed at 400s on the plane $\theta = 0$ for $r_a = 0.25$, $r_b = 0.28$, $Re = 25000$

7.2.6 Case 6, $r_a = 0.25$, $r_b = 0.30$, $Re = 25000$

At 100s

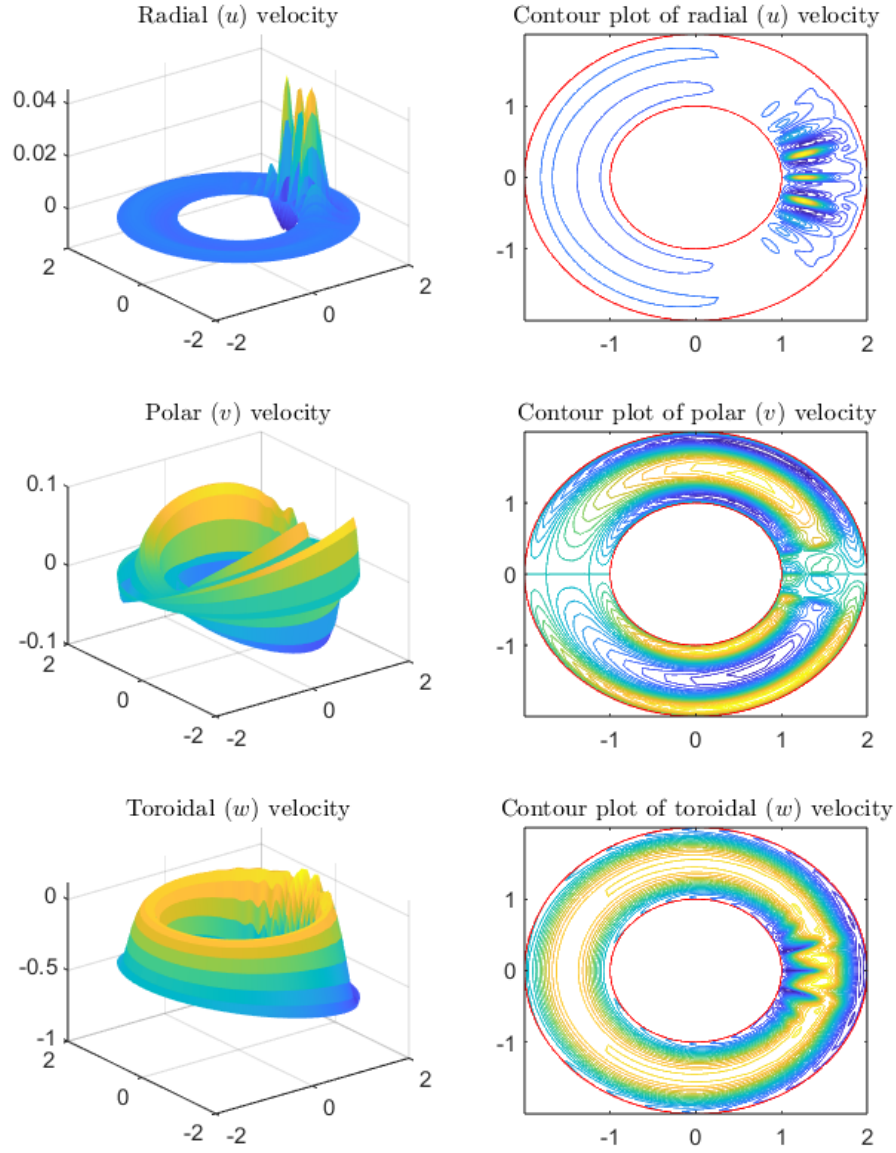


Figure 7.21: Velocity components at 100s for $r_a = 0.25$, $r_b = 0.30$, $Re = 25000$

At 400s

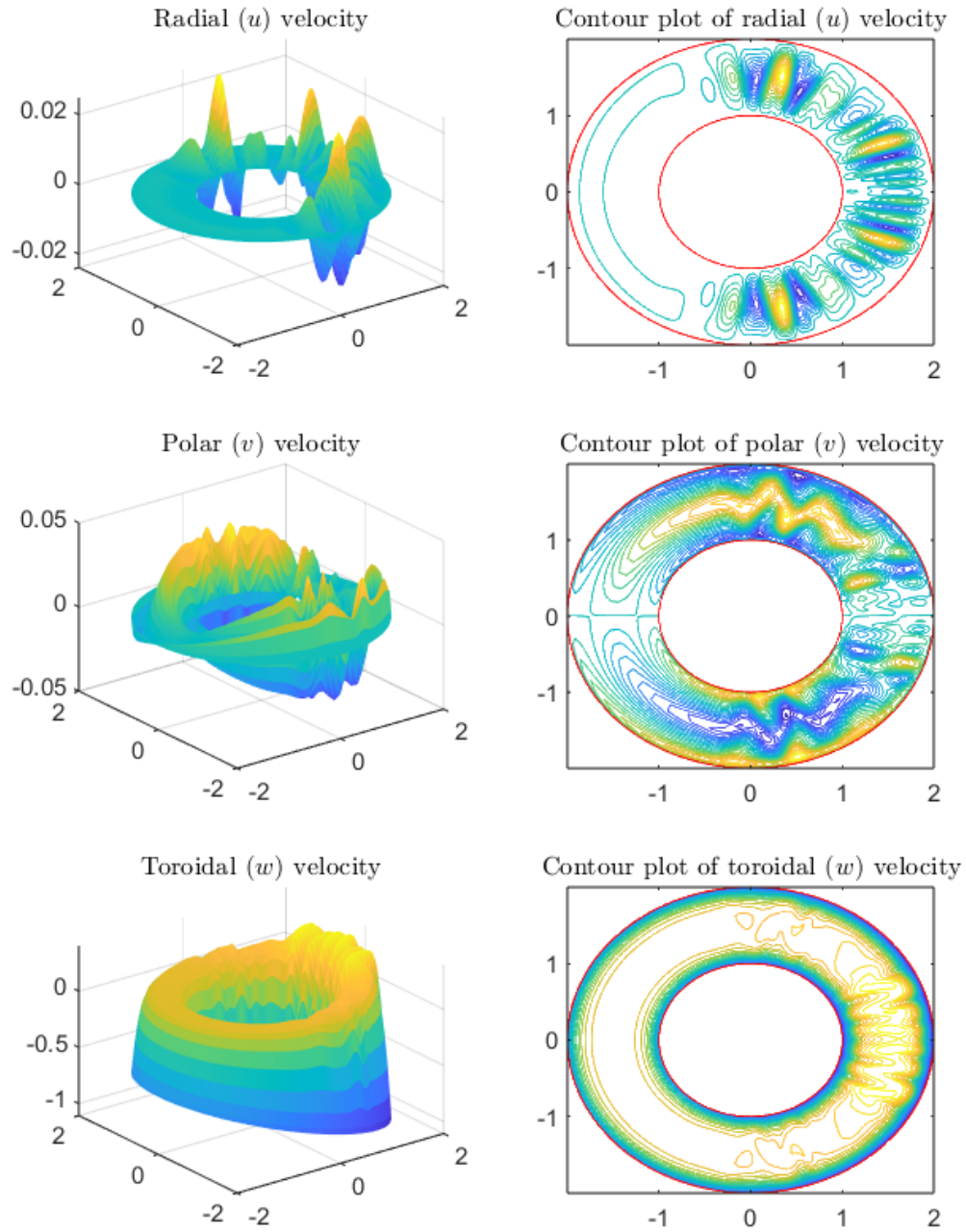


Figure 7.22: Velocity components at 400s for $r_a = 0.25$, $r_b = 0.30$, $Re = 25000$

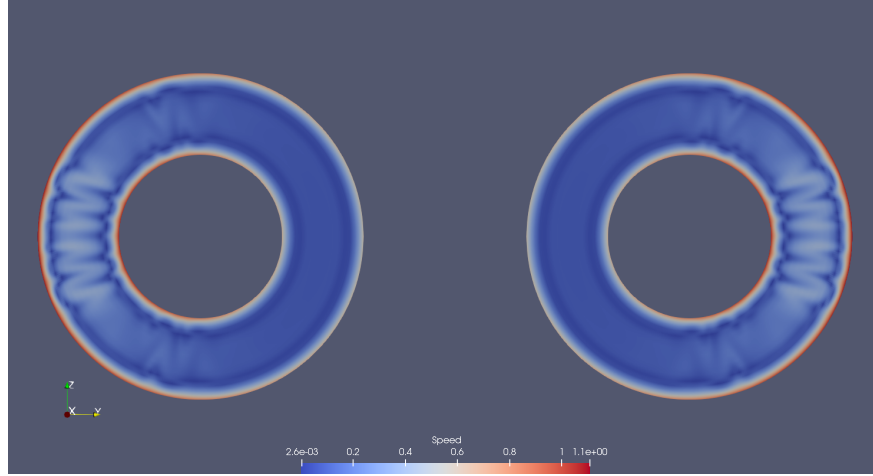


Figure 7.23: Speed at 400s on $\phi = \frac{3\pi}{2}$ (left) and $\phi = \frac{\pi}{2}$ (right) for $r_a = 0.25$, $r_b = 0.30$, $Re = 25000$

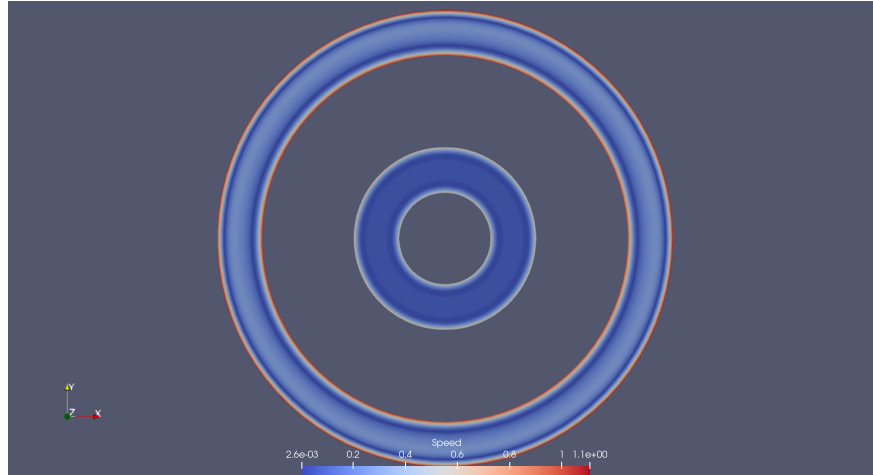


Figure 7.24: Speed at 400s on the plane $\theta = 0$ for $r_a = 0.25$, $r_b = 0.30$, $Re = 25000$

Discussion

Case 5 is again similar to Case 3 and Case 1 in that there is only radial deviation in the flow, see Figures 7.18, 7.19, 7.20. In Case 6, not only is the sinusoidal pattern discernible but also has increased its range and appears to leave a wake, see Figure 7.23. Again, there is no ϕ -dependence, see Figure 7.24.

7.2.7 Numerically calculated torque

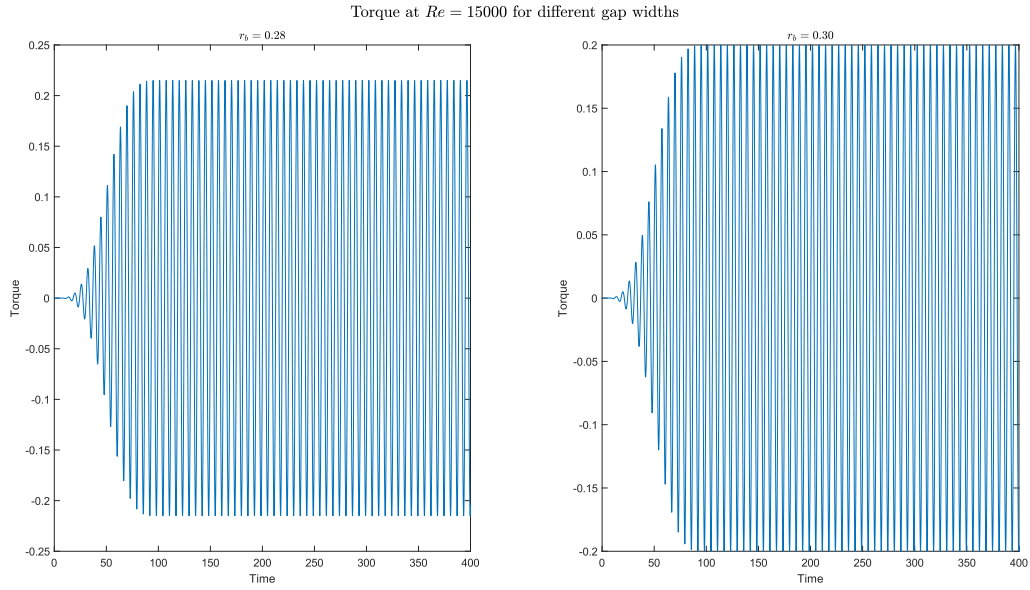


Figure 7.25: Torque for different gap widths at $Re = 15000$

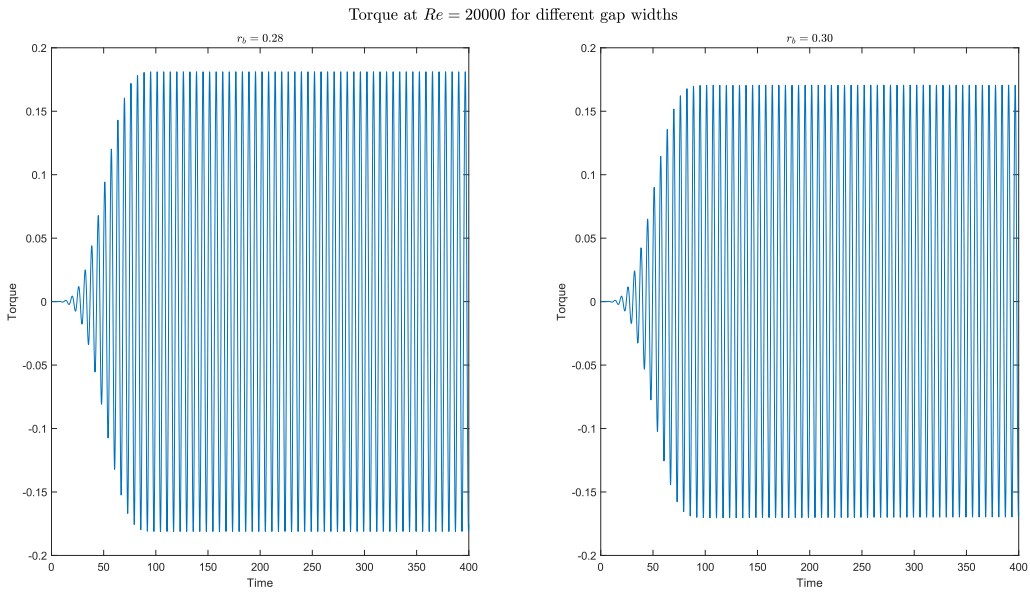


Figure 7.26: Torque for different gap widths at $Re = 20000$

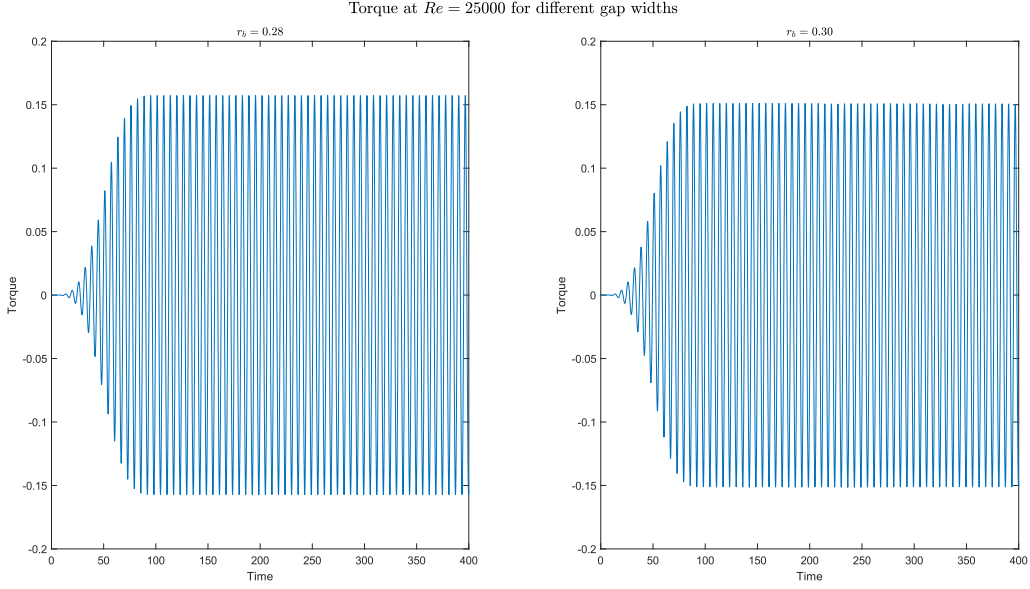


Figure 7.27: Torque for different gap widths at $Re = 25000$

Discussion

We now turn our attention to the torque on the walls of both tori shown in Figures 7.25, 7.26, 7.27. The torque is unsurprisingly oscillatory due to the oscillatory boundary conditions and achieves its maximum value only after the spin-up time of 100s has elapsed. Next, the amplitude of the torque is slightly lower at larger gap widths (on the right of Figures 7.25, 7.26, 7.27) at all the Reynolds numbers observed. This is similar to plane Couette flows where the force to push the top plate is known to be inversely proportional to the gap width. Finally, the most peculiar result is that the amplitude of the torque decreases as the Reynolds number increases for both gap widths.

7.2.8 Summary of results

Oscillating both tori in the same direction produces two distinct flow patterns, both of which are distinct from the flow patterns that develop when only the inner torus rotated in one direction while the outer torus was stationary.

The first flow pattern occurs at the smaller gap width when $r_a = 0.25, r_b = 0.28$ and has only radial dependence regardless of a change in Reynolds number. The second flow pattern occurs when $r_a = 0.25, r_b = 0.30$ is far more interesting and appears to be made of two parts: one that is only radially dependent and one that has both radial and polar dependence. The polar dependence manifests as sinusoidal pattern in the region where the speed is largest in the gap. The gap width appears to be responsible for the appearance of this flow while the Reynolds numbers appears to be responsible for the region this flow occupies. We summarise these results in Table 7.2 below.

	$r_b = 0.28$	$r_b = 0.30$
$Re = 15000$	r -variation	r - and θ -variation
$Re = 20000$	r -variation	r - and θ -variation
$Re = 25000$	r -variation	r - and θ -variation

Table 7.2: Variation in oscillating tori when $r_a = 0.25$

Chapter 8

Conclusions and future work

8.1 Conclusions

The most obvious conclusion from Chapter 6 is that laminar flow, which occurs at low Reynolds numbers, transitions into the first manifestation or the first category of stable Taylor-Couette flow when the inner torus is rotated and the outer torus is stationary. The first category of Taylor-Couette flow is two-dimensional i.e. it is invariant in the ϕ -direction. It is characterised by alternating bands of high and low velocity in the region of the gap where the speed is greatest and laminar flow everywhere else. The number and size of the alternating bands of high and low velocity and the region they occupy varies depending on the Reynolds number, the gap width and its position relative to the axis of rotation.

The chapter on oscillating flows presented distinct flows and demonstrated an apparent dependence on the gap width (not so much the Reynolds number) for the appearance of a kind of Taylor-Couette flow. The smaller gap width showed only radial dependence while the larger gap width showed both radial and polar dependence in the region where speed is highest. The appearance of distinct flow in this region is reminiscent of the Taylor-Couette flow observed in Chapter 6. We also observed that the torque on both toroidal walls is inversely proportional to both the gap width and the Reynolds number.

8.2 Future work

Our results have presented us with many ideas for future work. The most obvious path is to attempt to establish a critical Reynolds number for which the flow transitions from laminar to its first Taylor-Couette form for a specified set of parameters. For example, we know that the transition occurs between $Re = 5000$ and $Re = 8000$ for $r_a = 0.25, r_b = 0.28$. More simulations can be conducted at within this range of Reynolds numbers to determine its critical value for which the flow transitions from laminar to its first Taylor-Couette flow. Similarly, other critical transitions, such as the transition between three bands of high speed to five bands of high speed and vice-versa, can be experimentally deduced.

Another obvious path is to continue the search for three-dimensional instabilities. Presumably, if the Reynolds numbers is increased beyond 25000 (the largest considered in this thesis), then other, likely three-dimensional, categories of Taylor-Couette flow would present themselves. This would be similar to what has been observed in the cylindrical and spherical counterparts.

One idea not explored in this thesis is the simulation of the flow as $r_a \rightarrow 0$ to compare with the work already done with fluid rotating in a single torus. Additionally, different positions of the gap width can be explored to determine its effect on the appearance of Taylor-Couette flow. We examined only two instances of the gap width of 0.03 in this thesis with $r_a = 0.25$ and $r_a = 0.75$. We observed that the number of bands are significantly greater and the bands have much less space between them for $r_a = 0.75$ than for $r_a = 0.25$. For enough runs of different values of r_a , it may be possible to establish a relationship between the type of Taylor-Couette flow and the inner radius, r_a , and similar progress can be made for gap widths of different sizes.

Oscillating flows present us with another rich area of future study. More extensive studies can be performed with the ideas for the case with only the inner torus rotating. Gap widths, gap positions, length of oscillations and Reynolds numbers can be altered and their impact on the flow and torque can be observed. For oscillating flows, the torque is an important quantity to consider since it has direct consequences for practical application. Ideally, a

thorough study will provide an understanding of both the expected flow pattern and how to maximise torque with a given set of parameters.

Appendix A

Vector Calculus in Toroidal Coordinates

A.1 Coordinate system

The toroidal co-ordinate system (sometimes known as ‘simple’ toroidal coordinates [38]) is described by

$$\begin{aligned}x(r, \theta, \phi) &= (R_0 + r \cos \theta) \cos \phi \\y(r, \theta, \phi) &= (R_0 + r \cos \theta) \sin \phi \\z(r, \theta, \phi) &= r \sin \theta\end{aligned}\tag{A.1}$$

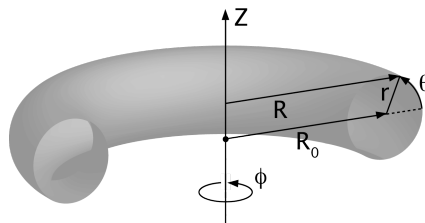


Figure A.1: Simple toroidal coordinates

where r is the polar radius, θ is the polar angle, R_0 is the toroidal radius and ϕ is the toroidal angle. x , y and z are from the (usual) Cartesian co-ordinate system. The coordinate ranges are $-\pi < \theta \leq \pi$, $0 \leq r < R_0$ and $0 \leq \phi < 2\pi$. This geometry is also used to describe tokamaks [97].

The following expressions are taken from ‘A Primer on Tensor Calculus’ [98]. We have verified our expressions by comparing against those produced by Maple’s Vector Calculus package.

Another well known set of toroidal coordinates [99] which we briefly mention here is obtained by the following change of variables:

$$\begin{aligned} x &= \frac{a \sinh \tau}{\cosh \tau - \cos \theta} \cos \phi \\ y &= \frac{a \sinh \tau}{\cosh \tau - \cos \theta} \sin \phi \\ z &= \frac{a \sin \sigma}{\cosh \tau - \cos \theta}. \end{aligned} \tag{A.2}$$

The coordinate ranges are $-\pi < \sigma \leq \pi$, $0 \leq \tau < +\infty$ and $0 \leq \phi < 2\pi$. In essence, this is the classic two dimensional bipolar coordinate system (obtained from solutions of the Laplace equation corresponding to potential and stream lines arising from two point sources of opposite sign) rotated about the angle ϕ . The surfaces of constant σ are the spheres

$$(x^2 + y^2) + (z - a \cot \sigma)^2 = \frac{a^2}{\sin^2 \sigma}, \tag{A.3}$$

while the surfaces of constant τ are the tori

$$z^2 + \left(\sqrt{x^2 + y^2} - \frac{a}{\sinh \tau} \right)^2 = a^2 \coth^2 \tau. \tag{A.4}$$

Importantly for our purposes, the spheres and tori are not concentric; therefore, we would not be able to prescribe boundary conditions on two concentric tori (the subject of this work) along coordinate lines of this system. A remarkable aspect of this system, however, is that

Laplace's equation $\nabla^2 u = 0$ is partially separable, giving rise to solutions of the form

$$u = \sqrt{\cosh \tau - \cos \sigma} e^{i\nu\sigma} e^{i\mu\phi} T_{\mu\nu}(\tau) \quad (\text{A.5})$$

where $T_{\mu\nu}(\tau)$ are the so-called toroidal harmonics, given explicitly in terms of the associated Legendre functions of the first and second kinds [100].

A.2 The Scale Factors

In what follows, it is helpful to frame our discussion in a slightly more general context that will allow us to leverage well-known results related to the change of variables from one orthogonal coordinate system to another. Suppose we define a one-to-one coordinate transformation from $\mathbb{R}^3$ to $\mathbb{R}^3$ that maps a bounded region in Cartesian (x, y, z) -space onto a bounded region in (ξ_1, ξ_2, ξ_3) -space:

$$\begin{aligned} x &= x(\xi_1, \xi_2, \xi_3) \\ y &= y(\xi_1, \xi_2, \xi_3) \\ z &= z(\xi_1, \xi_2, \xi_3) \end{aligned} \quad (\text{A.6})$$

A simple application of the chain rule to (A.6) shows that differential elements are related according to

$$\begin{bmatrix} dx \\ dy \\ dz \end{bmatrix} = J \begin{bmatrix} d\xi_1 \\ d\xi_2 \\ d\xi_3 \end{bmatrix}, \quad (\text{A.7})$$

where

$$J = \frac{\partial(x, y, z)}{\partial(\xi_1, \xi_2, \xi_3)} = \begin{bmatrix} \frac{\partial x}{\partial \xi_1} & \frac{\partial x}{\partial \xi_2} & \frac{\partial x}{\partial \xi_3} \\ \frac{\partial y}{\partial \xi_1} & \frac{\partial y}{\partial \xi_2} & \frac{\partial y}{\partial \xi_3} \\ \frac{\partial z}{\partial \xi_1} & \frac{\partial z}{\partial \xi_2} & \frac{\partial z}{\partial \xi_3} \end{bmatrix} \quad (\text{A.8})$$

is the Jacobian matrix of the coordinate transformation. Making explicit use of basis vectors for the clarity of our exposition, the differential displacement is given by

$$d\mathbf{r} = dx\hat{\mathbf{x}} + dy\hat{\mathbf{y}} + dz\hat{\mathbf{z}}, \quad (\text{A.9})$$

where $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$ and $\hat{\mathbf{z}}$ are the standard Cartesian (unit) basis vectors. It should be clear that equation (A.7) states that (A.9) may be written as

$$d\mathbf{r} = d\xi_1 \frac{\partial}{\partial \xi_1} \mathbf{r} + d\xi_2 \frac{\partial}{\partial \xi_2} \mathbf{r} + d\xi_3 \frac{\partial}{\partial \xi_3} \mathbf{r}. \quad (\text{A.10})$$

The vector quantities on the right-hand side of (A.10) are the column vectors of the Jacobian matrix. Let $\hat{\mathbf{e}}_1$, $\hat{\mathbf{e}}_2$ and $\hat{\mathbf{e}}_3$ be the orthogonal unit vectors in the ξ_1 -, ξ_2 - and ξ_3 -directions, respectively; these quantities are given by

$$\hat{\mathbf{e}}_i = \frac{1}{h_i} \frac{\partial}{\partial \xi_i} \mathbf{r} \quad i = 1, 2, 3. \quad (\text{A.11})$$

The differential displacement vector (A.10) thus becomes

$$d\mathbf{r} = h_1 d\xi_1 \hat{\mathbf{e}}_1 + h_2 d\xi_2 \hat{\mathbf{e}}_2 + h_3 d\xi_3 \hat{\mathbf{e}}_3. \quad (\text{A.12})$$

The *scale factors* appearing in equations (A.11) and (A.12) are the Euclidean norms of the column vectors of the Jacobian matrix (A.8):

$$h_i = \sqrt{\left(\frac{\partial x}{\partial \xi_i}\right)^2 + \left(\frac{\partial y}{\partial \xi_i}\right)^2 + \left(\frac{\partial z}{\partial \xi_i}\right)^2}, \quad i = 1, 2, 3. \quad (\text{A.13})$$

In terms of the scale factors, we can present formulas for all of the differential operators of vector calculus required in this thesis.

As is easily verified, the scale factors for the toroidal change of variables (A.1) are given by

$$h_r = 1, \quad h_\theta = r, \quad \text{and} \quad h_\phi = R_0 + r \cos \theta. \quad (\text{A.14})$$

From equation (A.11) the unit vectors corresponding to the toroidal coordinate system are then given by

$$\hat{\mathbf{e}}_r = \cos \theta \cos \phi \hat{\mathbf{x}} + \cos \theta \sin \phi \hat{\mathbf{y}} + \sin \theta \hat{\mathbf{z}} \quad (\text{A.15})$$

$$\hat{\mathbf{e}}_\theta = -\sin \theta \cos \phi \hat{\mathbf{x}} - \sin \theta \sin \phi \hat{\mathbf{y}} + \cos \theta \hat{\mathbf{z}} \quad (\text{A.16})$$

$$\hat{\mathbf{e}}_\phi = -\sin \phi \hat{\mathbf{x}} + \cos \phi \hat{\mathbf{y}} \quad (\text{A.17})$$

It should be noted that the result is a left-handed orthogonal coordinate system, as can be seen by the simple cross-product relations

$$\hat{\mathbf{e}}_r \times \hat{\mathbf{e}}_\theta = -\hat{\mathbf{e}}_\phi, \quad \hat{\mathbf{e}}_\theta \times \hat{\mathbf{e}}_\phi = -\hat{\mathbf{e}}_r, \quad \hat{\mathbf{e}}_\phi \times \hat{\mathbf{e}}_r = -\hat{\mathbf{e}}_\theta. \quad (\text{A.18})$$

The important takeaway from the fact that the coordinate system is left-handed is that $\hat{\mathbf{e}}_r$ is a normal vector to the surface of a torus *pointing inwards* to the centre of the body. The fact that the coordinate system is left-handed is not of great concern to us, but if one were determined to work with a right-handed coordinate system, then the remedy is, in equation (A.1), (i) place a negative sign in front of the transformation of the y -variable or (ii) place a negative sign in front of the transformation of the z -variable.

We can now immediately compute useful quantities such as the volume element (required for volume integrals):

$$dV = |J| dr d\theta d\phi = r h_\phi dr d\theta d\phi, \quad (\text{A.19})$$

where $|J|$ represents the determinant of the Jacobian matrix. It may be shown that an

element of surface area of a torus of radius r is given by

$$dS = \left\| \frac{\partial}{\partial \theta} \mathbf{r} \times \frac{\partial}{\partial \phi} \mathbf{r} \right\| = rh_\phi \|\hat{\mathbf{e}}_\theta \times \hat{\mathbf{e}}_\phi\| d\theta d\phi = rh_\phi d\theta d\phi, \quad (\text{A.20})$$

where $\|\cdot\|$ represents the Euclidean norm. As a sanity check (and we have needed several), we can integrate the elemental volume and surface areas over the range of the variables to produce well known formulas for the volume and surface area of a torus:

$$V = 2\pi^2 R_0 r^2 \quad \text{and} \quad S = 4\pi^2 R_0 r. \quad (\text{A.21})$$

A.3 Gradient (scalar)

This formula is given by Morse and Feshbach equation [1.4.2] Given a scalar function, $f = f(\xi_1, \xi_2, \xi_3)$, its gradient is given by

$$\nabla f = \left(\frac{1}{h_1} \partial_1 f, \frac{1}{h_2} \partial_2 f, \frac{1}{h_3} \partial_3 f \right), \quad (\text{A.22})$$

where, as is customary, we use the shorthand $\partial_i f = \partial f / (\partial \xi_i)$. In terms of our toroidal coordinates, the gradient of the scalar function $f = f(r, \theta, \phi)$ is given by

$$\nabla f = \frac{\partial f}{\partial r} \hat{\mathbf{e}}_r + \frac{1}{r} \frac{\partial f}{\partial \theta} \hat{\mathbf{e}}_\theta + \frac{1}{h_\phi} \frac{\partial f}{\partial \phi} \hat{\mathbf{e}}_\phi \quad (\text{A.23})$$

where $\hat{\mathbf{e}}_r$, $\hat{\mathbf{e}}_\theta$ and $\hat{\mathbf{e}}_\phi$ are unit vectors in the r -, θ - and ϕ -directions, respectively. Since it appears so frequently, we maintain the notation $h_\phi = R_0 + r \cos \theta$ in equation (A.23) and throughout this appendix.

A.4 Divergence

Given a vector, $\vec{A} = (A_1, A_2, A_3)$, its divergence is given by

$$\nabla \cdot \vec{A} = \frac{1}{h_1 h_2 h_3} \sum_i \partial_i \left(\frac{h_1 h_2 h_3}{h_i} A_i \right)$$

This formula is given by Morse and Feshbach equation [1.4.6]

In toroidal co-ordinates, given a vector $\mathbf{u} = (u, v, w)$, its divergence is given by

$$\nabla \cdot \mathbf{u} = \frac{\partial u}{\partial r} + \frac{u}{r} + \frac{1}{r} \frac{\partial v}{\partial \theta} + \frac{1}{h_\phi} \left(u \cos \theta - v \sin \theta + \frac{\partial w}{\partial \phi} \right). \quad (\text{A.24})$$

Next, defining the vector

$$\mathbf{q} = (q_r, q_\theta, q_\phi) = \nabla (\nabla \cdot \mathbf{u}) \quad (\text{A.25})$$

we see that a consequence of the relationships above is

$$\begin{aligned} q_r &= \frac{\partial^2 u}{\partial r^2} + \frac{1}{r} \frac{\partial u}{\partial r} - \frac{1}{r^2} \left(u + \frac{\partial v}{\partial \theta} \right) + \frac{1}{h_\phi} \left(\frac{\partial u}{\partial r} \cos \theta - \frac{\partial v}{\partial r} \sin \theta \right) \\ &\quad - \frac{\cos \theta}{h_\phi^2} \left(u \cos \theta - v \sin \theta + \frac{\partial w}{\partial \phi} \right) + \frac{1}{r} \frac{\partial^2 v}{\partial r \partial \theta} + \frac{1}{h_\phi} \frac{\partial^2 w}{\partial r \partial \phi} \end{aligned} \quad (\text{A.26})$$

$$\begin{aligned} q_\theta &= \frac{1}{r^2} \left(\frac{\partial u}{\partial \theta} + \frac{\partial^2 v}{\partial \theta^2} \right) + \frac{1}{r h_\phi} \left(\frac{\partial u}{\partial \theta} \cos \theta - \frac{\partial v}{\partial \theta} \sin \theta \right) - \frac{1}{r h_\phi} (u \sin \theta + v \cos \theta) \\ &\quad + \frac{\sin \theta}{h_\phi^2} \left(u \cos \theta - v \sin \theta + \frac{\partial w}{\partial \phi} \right) + \frac{1}{r} \frac{\partial^2 u}{\partial \theta \partial r} + \frac{1}{r h_\phi} \frac{\partial^2 w}{\partial \theta \partial \phi} \end{aligned} \quad (\text{A.27})$$

$$\begin{aligned} q_\phi &= \frac{1}{r h_\phi} \frac{\partial u}{\partial \phi} + \frac{1}{h_\phi^2} \left(\frac{\partial u}{\partial \phi} \cos \theta - \frac{\partial v}{\partial \phi} \sin \theta + \frac{\partial^2 w}{\partial \phi^2} \right) \\ &\quad + \frac{1}{h_\phi} \frac{\partial^2 u}{\partial \phi \partial r} + \frac{1}{r h_\phi} \frac{\partial^2 v}{\partial \phi \partial \theta} \end{aligned} \quad (\text{A.28})$$

A.5 Laplacian (scalar)

Given a scalar function, $u = u(r, \theta, \phi)$, its Laplacian is given by

$$\nabla^2 u = \nabla \cdot \nabla u = \frac{1}{h_1 h_2 h_3} \sum_i \partial_i \left(\frac{h_1 h_2 h_3}{h_i^2} \partial_i u \right) \quad (\text{A.29})$$

This formula is given by Morse and Feshbach 1.5.11. In toroidal co-ordinates, given a scalar function, f , its Laplacian is given by

$$\nabla^2 u = \frac{1}{r h_\phi} \frac{\partial}{\partial r} \left(r h_\phi \frac{\partial u}{\partial r} \right) + \frac{1}{r^2 h_\phi} \frac{\partial}{\partial \theta} \left(h_\phi \frac{\partial u}{\partial \theta} \right) + \frac{1}{h_\phi^2} \frac{\partial^2 u}{\partial \phi^2} \quad (\text{A.30})$$

This can be expanded to give

$$\nabla^2 u = \frac{\partial^2 u}{\partial r^2} + \left(\frac{1}{r} + \frac{\cos \theta}{h_\phi} \right) \frac{\partial u}{\partial r} - \frac{\sin \theta}{r h_\phi} \frac{\partial u}{\partial \theta} + \frac{1}{r^2} \frac{\partial^2 u}{\partial \theta^2} + \frac{1}{h_\phi^2} \frac{\partial^2 u}{\partial \phi^2} \quad (\text{A.31})$$

A.6 Curl

Given a vector, $\vec{A}$, its curl is given by

$$\nabla \times \vec{A} = \left(\frac{\partial_2(h_3 A_3) - \partial_3(h_2 A_2)}{h_2 h_3}, \frac{\partial_3(h_1 A_1) - \partial_1(h_3 A_3)}{h_3 h_1}, \frac{\partial_1(h_2 A_2) - \partial_2(h_1 A_1)}{h_1 h_2} \right) \quad (\text{A.32})$$

This formula is given by Morse and Feshbach equation [1.4.10] For velocity field $\mathbf{u} = (u, v, w)$ the curl of the field is therefore given by

$$\begin{aligned} \nabla \times \mathbf{u} &= \left(\frac{1}{r} \frac{\partial w}{\partial \theta} - \frac{w \sin \theta}{h_\phi} - \frac{1}{h_\phi} \frac{\partial v}{\partial \phi} \right) \hat{\mathbf{e}}_r + \left(\frac{1}{h_\phi} \frac{\partial u}{\partial \phi} - \frac{w \cos \theta}{h_\phi} - \frac{\partial w}{\partial r} \right) \hat{\mathbf{e}}_\theta \\ &+ \left(\frac{v}{r} + \frac{\partial v}{\partial r} - \frac{1}{r} \frac{\partial u}{\partial \theta} \right) \hat{\mathbf{e}}_\phi \end{aligned} \quad (\text{A.33})$$

Next, defining the vector

$$\mathbf{q} = (q_r, q_\theta, q_\phi) = \nabla \times \nabla \times \mathbf{u} \quad (\text{A.34})$$

we have

$$\begin{aligned}
q_r &= \frac{1}{r^2} \left(\frac{\partial v}{\partial \theta} - \frac{\partial^2 u}{\partial \theta^2} \right) + \frac{\sin \theta}{h_\phi} \left(\frac{1}{r} \frac{\partial u}{\partial \theta} - \frac{\partial v}{\partial r} - \frac{v}{r} \right) - \frac{1}{h_\phi^2} \left(\frac{\partial^2 u}{\partial \phi^2} - \cos \theta \frac{\partial w}{\partial \phi} \right) \\
&+ \frac{1}{r} \frac{\partial^2 v}{\partial \theta \partial r} + \frac{1}{h_\phi} \frac{\partial^2 w}{\partial \phi \partial r}
\end{aligned} \tag{A.35}$$

$$\begin{aligned}
q_\theta &= \frac{1}{r} \left(\frac{\cos \theta}{h_\phi} - \frac{1}{r} \right) \left(\frac{\partial u}{\partial \theta} - v \right) - \left(\frac{\cos \theta}{h_\phi} + \frac{1}{r} \right) \frac{\partial v}{\partial r} - \frac{1}{h_\phi^2} \left(\frac{\partial^2 v}{\partial \phi^2} + \sin \theta \frac{\partial w}{\partial \phi} \right) \\
&- \frac{\partial^2 v}{\partial r^2} + \frac{1}{r} \frac{\partial^2 u}{\partial r \partial \theta} + \frac{1}{r h_\phi} \frac{\partial^2 w}{\partial \phi \partial \theta}
\end{aligned} \tag{A.36}$$

$$\begin{aligned}
q_\phi &= -\frac{1}{h_\phi} \left(\frac{\cos \theta}{h_\phi} - \frac{1}{r} \right) \frac{\partial u}{\partial \phi} - \left(\frac{\cos \theta}{h_\phi} + \frac{1}{r} \right) \frac{\partial w}{\partial r} - \frac{\partial^2 w}{\partial r^2} - \frac{1}{r^2} \frac{\partial^2 w}{\partial \theta^2} + \frac{w}{h_\phi^2} \\
&+ \frac{\sin \theta}{h_\phi} \left(\frac{1}{r} \frac{\partial w}{\partial \theta} + \frac{1}{h_\phi} \frac{\partial v}{\partial \phi} \right) + \frac{1}{h_\phi} \frac{\partial^2 u}{\partial r \partial \phi} + \frac{1}{r h_\phi} \frac{\partial^2 v}{\partial \theta \partial \phi}
\end{aligned} \tag{A.37}$$

A.7 Vector Laplacian

Given a vector $\vec{A} = (u, v, w)$ its vector Laplacian is given by

$$\nabla^2 \vec{A} = \nabla(\nabla \cdot \vec{A}) - \nabla \times (\nabla \times \vec{A}) \tag{A.38}$$

Defining the vector

$$\mathbf{q} = (q_r, q_\theta, q_\phi) = \nabla^2 \mathbf{u} \tag{A.39}$$

assuming continuous second derivatives so that the order of the partials may be reversed, we have, from equations above,

$$q_r = \nabla^2 u - \frac{u}{r^2} - \frac{2}{r^2} \frac{\partial v}{\partial \theta} - \frac{\cos \theta}{h_\phi^2} \left(u \cos \theta - v \sin \theta + 2 \frac{\partial w}{\partial \phi} \right) + \frac{v \sin \theta}{r h_\phi} \tag{A.40}$$

$$q_\theta = \nabla^2 v - \frac{v}{r^2} + \frac{2}{r^2} \frac{\partial u}{\partial \theta} + \frac{\sin \theta}{h_\phi^2} \left(u \cos \theta - v \sin \theta + 2 \frac{\partial w}{\partial \phi} \right) - \frac{u \sin \theta}{r h_\phi} \quad (\text{A.41})$$

$$q_\phi = \nabla^2 w + \frac{1}{h_\phi^2} \left(2 \cos \theta \frac{\partial u}{\partial \phi} - 2 \sin \theta \frac{\partial v}{\partial \phi} - w \right) \quad (\text{A.42})$$

As is customary, we have defined the components of the vector Laplacian in terms of the scalar Laplacian.

A.8 Gradient (vector)

The vector gradient is a rank 2 tensor. This formula is given by Morse and Feshbach 1.6.13. Given a vector, $\vec{A}$, its gradient is given by

$$(\nabla \vec{A})_{ij} = \begin{cases} \partial_i \left(\frac{A_i}{h_i} \right) + \frac{1}{h_i} \vec{A} \cdot \nabla h_i, & i = j \\ \frac{1}{h_i} (\partial_i A_j - \frac{A_i}{h_j} \partial_j h_i), & i \neq j \end{cases}$$

In toroidal co-ordinates, given a vector $\mathbf{u} = (u, v, w)$, its gradient is given by the dyad

$$\nabla \mathbf{u} = \begin{bmatrix} \frac{\partial u}{\partial r} & \frac{\partial v}{\partial r} & \frac{\partial w}{\partial r} \\ \frac{1}{r} \left(\frac{\partial u}{\partial \theta} - v \right) & \frac{1}{r} \left(\frac{\partial v}{\partial \theta} + u \right) & \frac{1}{r} \frac{\partial w}{\partial \theta} \\ \frac{1}{h_\phi} \left(\frac{\partial u}{\partial \phi} - w \cos \theta \right) & \frac{1}{h_\phi} \left(\frac{\partial v}{\partial \phi} + w \sin \theta \right) & \frac{1}{h_\phi} \left(\frac{\partial w}{\partial \phi} + u \cos \theta - v \sin \theta \right) \end{bmatrix}. \quad (\text{A.43})$$

Note that the trace of the tensor is

$$\text{Tr}(\nabla \mathbf{u}) = \sum_{i=1}^3 (\nabla \mathbf{u})_{ii} = \nabla \cdot \mathbf{u}. \quad (\text{A.44})$$

Next, defining the vector

$$\mathbf{q} = (q_r, q_\theta, q_\phi) = \mathbf{u} \cdot \nabla \mathbf{u} \quad (\text{A.45})$$

as an immediate consequence of the above we have

$$q_r = u \frac{\partial u}{\partial r} + \frac{v}{r} \left(\frac{\partial u}{\partial \theta} - v \right) + \frac{w}{h_\phi} \left(\frac{\partial u}{\partial \phi} - w \cos \theta \right) \quad (\text{A.46})$$

$$q_\theta = u \frac{\partial v}{\partial r} + \frac{v}{r} \left(\frac{\partial v}{\partial \theta} + u \right) + \frac{w}{h_\phi} \left(\frac{\partial v}{\partial \phi} + w \sin \theta \right) \quad (\text{A.47})$$

$$q_\phi = u \frac{\partial w}{\partial r} + \frac{v}{r} \frac{\partial w}{\partial \theta} + \frac{w}{h_\phi} \left(\frac{\partial w}{\partial \phi} + u \cos \theta - v \sin \theta \right) \quad (\text{A.48})$$

A.9 Strain rate tensor

For a vector $\mathbf{u} = (u, v, w)$, the strain rate tensor is given by

$$\begin{aligned} & \frac{1}{2} \left(\nabla \vec{u} + (\nabla \vec{u})^T \right) \\ &= \frac{1}{2} \begin{bmatrix} \frac{\partial u}{\partial r} & \frac{\partial v}{\partial r} & \frac{\partial w}{\partial r} \\ \frac{1}{r} \left(\frac{\partial u}{\partial \theta} - v \right) & \frac{1}{r} \left(\frac{\partial v}{\partial \theta} + u \right) & \frac{1}{r} \frac{\partial w}{\partial \theta} \\ \frac{1}{h_\phi} \left(\frac{\partial u}{\partial \phi} - w \cos \theta \right) & \frac{1}{h_\phi} \left(\frac{\partial v}{\partial \phi} + w \sin \theta \right) & \frac{1}{h_\phi} \left(\frac{\partial w}{\partial \phi} + u \cos \theta - v \sin \theta \right) \end{bmatrix} \\ &+ \frac{1}{2} \begin{bmatrix} \frac{\partial u}{\partial r} & \frac{1}{r} \left(\frac{\partial u}{\partial \theta} - v \right) & \frac{1}{h_\phi} \left(\frac{\partial u}{\partial \phi} - w \cos \theta \right) \\ \frac{\partial v}{\partial r} & \frac{1}{r} \left(\frac{\partial v}{\partial \theta} + u \right) & \frac{1}{h_\phi} \left(\frac{\partial v}{\partial \phi} + w \sin \theta \right) \\ \frac{\partial w}{\partial r} & \frac{1}{r} \frac{\partial w}{\partial \theta} & \frac{1}{h_\phi} \left(\frac{\partial w}{\partial \phi} + u \cos \theta - v \sin \theta \right) \end{bmatrix} \\ &= \frac{1}{2} \begin{bmatrix} 2 \frac{\partial u}{\partial r} & \frac{\partial v}{\partial r} + \frac{1}{r} \left(\frac{\partial u}{\partial \theta} - v \right) & \frac{\partial w}{\partial r} + \frac{1}{h_\phi} \left(\frac{\partial u}{\partial \phi} - w \cos \theta \right) \\ \frac{\partial v}{\partial r} + \frac{1}{r} \left(\frac{\partial u}{\partial \theta} - v \right) & \frac{2}{r} \left(\frac{\partial v}{\partial \theta} + u \right) & \frac{1}{r} \frac{\partial w}{\partial \theta} + \frac{1}{h_\phi} \left(\frac{\partial v}{\partial \phi} + w \sin \theta \right) \\ \frac{\partial w}{\partial r} + \frac{1}{h_\phi} \left(\frac{\partial u}{\partial \phi} - w \cos \theta \right) & \frac{1}{r} \frac{\partial w}{\partial \theta} + \frac{1}{h_\phi} \left(\frac{\partial v}{\partial \phi} + w \sin \theta \right) & \frac{2}{h_\phi} \left(\frac{\partial w}{\partial \phi} + u \cos \theta - v \sin \theta \right) \end{bmatrix} \quad (\text{A.49}) \end{aligned}$$

A.10 Stress tensor

From the previous section (Strain rate tensor), we can easily deduce the stress tensor, σ , by including pressure, p , terms along the diagonal.

$$\frac{1}{2} \begin{bmatrix} -p + 2\frac{\partial u}{\partial r} & \frac{\partial v}{\partial r} + \frac{1}{r} \left(\frac{\partial u}{\partial \theta} - v \right) & \frac{\partial w}{\partial r} + \frac{1}{h_\phi} \left(\frac{\partial u}{\partial \phi} - w \cos \theta \right) \\ \frac{\partial v}{\partial r} + \frac{1}{r} \left(\frac{\partial u}{\partial \theta} - v \right) & -p + \frac{2}{r} \left(\frac{\partial v}{\partial \theta} + u \right) & \frac{1}{r} \frac{\partial w}{\partial \theta} + \frac{1}{h_\phi} \left(\frac{\partial v}{\partial \phi} + w \sin \theta \right) \\ \frac{\partial w}{\partial r} + \frac{1}{h_\phi} \left(\frac{\partial u}{\partial \phi} - w \cos \theta \right) & \frac{1}{r} \frac{\partial w}{\partial \theta} + \frac{1}{h_\phi} \left(\frac{\partial v}{\partial \phi} + w \sin \theta \right) & -p + \frac{2}{h_\phi} \left(\frac{\partial w}{\partial \phi} + u \cos \theta - v \sin \theta \right) \end{bmatrix} \quad (\text{A.50})$$

A.11 Navier-Stokes equations

Denoting the vector velocity field as $\mathbf{u} = (u, v, w)$, the full three-dimensional Navier-Stokes equations corresponding to the momentum balance of an incompressible Newtonian fluid are

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \frac{1}{\text{Re}} \nabla^2 \mathbf{u} \quad (\text{A.51})$$

Based on the vector differential operators developed in this appendix, in toroidal coordinates the Navier-Stokes equations are, on a component basis:

$$\begin{aligned} & \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial r} + \frac{v}{r} \left(\frac{\partial u}{\partial \theta} - v \right) + \frac{w}{h_\phi} \left(\frac{\partial u}{\partial \phi} - w \cos \theta \right) = -\frac{\partial p}{\partial r} \\ & + \frac{1}{\text{Re}} \left[\nabla^2 u - \frac{u}{r^2} - \frac{2}{r^2} \frac{\partial v}{\partial \theta} - \frac{\cos \theta}{h_\phi^2} \left(u \cos \theta - v \sin \theta + 2 \frac{\partial w}{\partial \phi} \right) + \frac{v \sin \theta}{r h_\phi} \right] \end{aligned} \quad (\text{A.52})$$

$$\begin{aligned} & \frac{\partial v}{\partial t} + u \frac{\partial v}{\partial r} + \frac{v}{r} \left(\frac{\partial v}{\partial \theta} + u \right) + \frac{w}{h_\phi} \left(\frac{\partial v}{\partial \phi} + w \sin \theta \right) = -\frac{1}{r} \frac{\partial p}{\partial \theta} \\ & + \frac{1}{\text{Re}} \left[\nabla^2 v - \frac{v}{r^2} + \frac{2}{r^2} \frac{\partial u}{\partial \theta} + \frac{\sin \theta}{h_\phi^2} \left(u \cos \theta - v \sin \theta + 2 \frac{\partial w}{\partial \phi} \right) - \frac{u \sin \theta}{r h_\phi} \right] \end{aligned} \quad (\text{A.53})$$

$$\begin{aligned}
& \frac{\partial w}{\partial t} + u \frac{\partial w}{\partial r} + \frac{v}{r} \frac{\partial w}{\partial \theta} + \frac{w}{h_\phi} \left(\frac{\partial w}{\partial \phi} + u \cos \theta - v \sin \theta \right) \\
= & -\frac{1}{h_\phi} \frac{\partial p}{\partial \phi} + \frac{1}{\text{Re}} \left[\nabla^2 w + \frac{1}{h_\phi^2} \left(2 \cos \theta \frac{\partial u}{\partial \phi} - 2 \sin \theta \frac{\partial v}{\partial \phi} - w \right) \right]
\end{aligned} \tag{A.54}$$

where $h_\phi = R_0 + r \cos \theta$ is the ϕ scale factor. The scalar Laplacian, which appears in each of the three momentum equations is defined as (for example)

$$\nabla^2 u \equiv \frac{\partial^2 u}{\partial r^2} + \left(\frac{1}{r} + \frac{\cos \theta}{h_\phi} \right) \frac{\partial u}{\partial r} - \frac{\sin \theta}{r h_\phi} \frac{\partial u}{\partial \theta} + \frac{1}{r^2} \frac{\partial^2 u}{\partial \theta^2} + \frac{1}{h_\phi^2} \frac{\partial^2 u}{\partial \phi^2} \tag{A.55}$$

The momentum equations are supplemented by the mass continuity equation

$$\nabla \cdot \mathbf{u} = \frac{\partial u}{\partial r} + \frac{u}{r} + \frac{1}{r} \frac{\partial v}{\partial \theta} + \frac{1}{h_\phi} \left(u \cos \theta - v \sin \theta + \frac{\partial w}{\partial \phi} \right) = 0. \tag{A.56}$$

On the boundaries of the domain, we impose no-slip conditions, as usual.

Appendix B

Fourier series

B.1 Two dimensional Fourier series

The Fourier series representation for a function, f of two variables, θ and ϕ can be expressed as follows

$$\begin{aligned} f(\theta, \phi) = & \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \alpha_{mn} \cos(m\theta) \cos(n\phi) \\ & + \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \beta_{mn} \cos(m\theta) \sin(n\phi) \\ & + \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \gamma_{mn} \sin(m\theta) \cos(n\phi) \\ & + \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \delta_{mn} \sin(m\theta) \sin(n\phi) \end{aligned}$$

where $\alpha_{mn}, \beta_{mn}, \gamma_{mn}, \delta_{mn}$ are the respective Fourier coefficients. Using the exponential representation of complex numbers, we can re-write this Fourier series.

$$\begin{aligned} f(\theta, \phi) = & \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \alpha_{mn} \left(\frac{1}{2} e^{im\theta} + \frac{1}{2} e^{-im\theta} \right) \left(\frac{1}{2} e^{in\phi} + \frac{1}{2} e^{-in\phi} \right) \\ & + \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \beta_{mn} \left(\frac{1}{2} e^{im\theta} + \frac{1}{2} e^{-im\theta} \right) \left(-\frac{1}{2} i e^{in\phi} + \frac{1}{2} i e^{-in\phi} \right) \end{aligned}$$

$$\begin{aligned}
& + \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \gamma_{mn} \left(-\frac{1}{2}ie^{im\theta} + \frac{1}{2}ie^{-im\theta} \right) \left(\frac{1}{2}e^{in\phi} + \frac{1}{2}e^{-in\phi} \right) \\
& + \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \delta_{mn} \left(-\frac{1}{2}ie^{im\theta} + \frac{1}{2}ie^{-im\theta} \right) \left(-\frac{1}{2}ie^{in\phi} + \frac{1}{2}ie^{-in\phi} \right)
\end{aligned}$$

Expanding,

$$\begin{aligned}
f(\theta, \phi) = & \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \alpha_{mn} \left(\frac{1}{4}e^{im\theta}e^{in\phi} + \frac{1}{4}e^{im\theta}e^{-in\phi} + \frac{1}{4}e^{-im\theta}e^{in\phi} + \frac{1}{4}e^{-im\theta}e^{-in\phi} \right) \\
& + \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \beta_{mn} \left(-\frac{1}{4}ie^{im\theta}e^{in\phi} + \frac{1}{4}ie^{im\theta}e^{-in\phi} - \frac{1}{4}ie^{-im\theta}e^{in\phi} + \frac{1}{4}ie^{-im\theta}e^{-in\phi} \right) \\
& + \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \gamma_{mn} \left(-\frac{1}{4}ie^{im\theta}e^{in\phi} - \frac{1}{4}ie^{im\theta}e^{-in\phi} + \frac{1}{4}ie^{-im\theta}e^{in\phi} + \frac{1}{4}ie^{-im\theta}e^{-in\phi} \right) \\
& + \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \delta_{mn} \left(-\frac{1}{4}e^{im\theta}e^{in\phi} + \frac{1}{4}e^{im\theta}e^{-in\phi} + \frac{1}{4}e^{-im\theta}e^{in\phi} - \frac{1}{4}e^{-im\theta}e^{-in\phi} \right)
\end{aligned}$$

Note that we have organised the Fourier basis functions in the following order for each double sum:

$$\left(e^{im\theta}e^{in\phi}, e^{im\theta}e^{-in\phi}, e^{-im\theta}e^{in\phi}, e^{-im\theta}e^{-in\phi} \right)$$

To combine these four double sums into a single sum, let us investigate different parts of the double sums. **m=0,n=0**

$$f(\theta, \phi) = \alpha_{00}$$

m=0,n≠0

$$\begin{aligned}
f(\theta, \phi) = & \alpha_{0n} \sum_{n=0}^{\infty} \left(\frac{1}{2}e^{in\phi} + \frac{1}{2}e^{-in\phi} \right) + \sum_{n=0}^{\infty} \beta_{0n} \left(-\frac{1}{2}ie^{in\phi} + \frac{1}{2}ie^{-in\phi} \right) \\
= & \sum_{n=0}^{\infty} \left(\frac{1}{2}\alpha_{0n} - \frac{1}{2}\beta_{0n}i \right) e^{in\phi} + \left(\frac{1}{2}\alpha_{0n} + \frac{1}{2}\beta_{0n}i \right) e^{-in\phi}
\end{aligned}$$

Note the pair of complex conjugates. **m≠0,n=0**

$$f(\theta, \phi) = \sum_{m=0}^{\infty} \alpha_{m0} \left(\frac{1}{2}e^{im\theta} + \frac{1}{2}e^{-im\theta} \right) + \sum_{m=0}^{\infty} \gamma_{m0} \left(-\frac{1}{2}ie^{im\theta} + \frac{1}{2}ie^{-im\theta} \right)$$

$$= \sum_{m=0}^{\infty} \left(\frac{1}{2} \alpha_{m0} - \frac{1}{2} \gamma_{m0} i \right) e^{im\theta} + \left(\frac{1}{2} \alpha_{m0} + \frac{1}{2} \gamma_{m0} i \right) e^{-im\theta}$$

Note the pair of complex conjugates.

$$\begin{aligned} f(\theta, \phi) &= \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \left(\frac{1}{4} \alpha_{mn} - \frac{1}{4} \delta_{mn} \right) e^{im\theta} e^{in\phi} - \left(\frac{1}{4} \beta_{mn} i + \frac{1}{4} \gamma_{mn} i \right) e^{im\theta} e^{in\phi} \\ &+ \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \left(\frac{1}{4} \alpha_{mn} - \frac{1}{4} \delta_{mn} \right) e^{-im\theta} e^{-in\phi} + \left(\frac{1}{4} \beta_{mn} i + \frac{1}{4} \gamma_{mn} i \right) e^{-im\theta} e^{-in\phi} \\ &+ \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \left(\frac{1}{4} \alpha_{mn} + \frac{1}{4} \delta_{mn} \right) e^{im\theta} e^{-in\phi} + \left(\frac{1}{4} \beta_{mn} i - \frac{1}{4} \gamma_{mn} i \right) e^{im\theta} e^{-in\phi} \\ &+ \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \left(\frac{1}{4} \alpha_{mn} + \frac{1}{4} \delta_{mn} \right) e^{-im\theta} e^{in\phi} + \left(\frac{1}{4} \gamma_{mn} i - \frac{1}{4} \beta_{mn} i \right) e^{-im\theta} e^{in\phi} \end{aligned}$$

Note the pairs of complex conjugates. We can now condense this information into a single term.

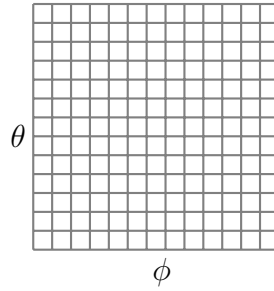
$$f(\theta, \phi) = \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} c_{mn} e^{im\theta} e^{in\phi}$$

where

$$c_{mn} = \begin{cases} \left(\frac{1}{4}\alpha_{mn} - \frac{1}{4}\delta_{mn} \right) - \left(\frac{1}{4}\beta_{mn}i + \frac{1}{4}\gamma_{mn}i \right) & m>0, n>0 \\ \left(\frac{1}{4}\alpha_{mn} - \frac{1}{4}\delta_{mn} \right) + \left(\frac{1}{4}\beta_{mn}i + \frac{1}{4}\gamma_{mn}i \right) & m<0, n<0 \\ \left(\frac{1}{4}\alpha_{mn} + \frac{1}{4}\delta_{mn} \right) + \left(\frac{1}{4}\beta_{mn}i - \frac{1}{4}\gamma_{mn}i \right) & m>0, n<0 \\ \left(\frac{1}{4}\alpha_{mn} + \frac{1}{4}\delta_{mn} \right) + \left(\frac{1}{4}\gamma_{mn}i - \frac{1}{4}\beta_{mn}i \right) & m<0, n>0 \\ \left(\frac{1}{2}\alpha_{0n} - \frac{1}{2}\beta_{0n}i \right) & m=0, n>0 \\ \left(\frac{1}{2}\alpha_{0n} + \frac{1}{2}\beta_{0n}i \right) & m=0, n<0 \\ \left(\frac{1}{2}\alpha_{m0} - \frac{1}{2}\gamma_{m0}i \right) & m>0, n=0 \\ \left(\frac{1}{2}\alpha_{m0} + \frac{1}{2}\gamma_{m0}i \right) & m<0, n=0 \\ \alpha_{00} & m=0, n=0 \end{cases}$$

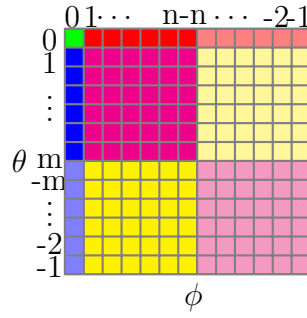
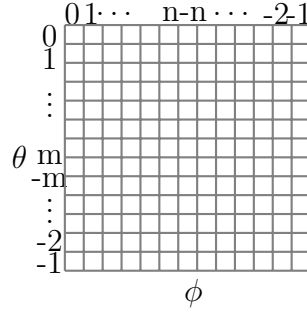
B.2 MATLAB representation of 2-D Fourier series

Suppose we have a matrix, A, of data points on $f(\theta, \phi)$ in MATLAB arranged as shown below. The rows contain data in the θ direction and the columns contain data in the ϕ direction.



Using the native MATLAB function, `ifft2`, on A returns a matrix of the same size, `Aifft2`, with the 2-D complex Fourier coefficients (from the previous section) arranged as shown below.

Using the information about the complex Fourier coefficients from the previous section, we can label the respective parts of `Aifft2` with colour.



The colours are arranged as such to show the location of the Fourier coefficients with respect to their conjugates. For example, the data points that are covered by the red blocks (first row) are complex conjugates of the data points that are covered by the light red blocks (adjacent to the red blocks, also in the first row). Similarly, the yellow and light yellow blocks, magenta and light magenta blocks and blue and light blue blocks are complex conjugates of each other. Finally, the green block represents the c_{00} Fourier coefficient (this has only a real part).

Knowing this orientation of the Fourier coefficients, we can clearly see what would data points we need to complete the matrix, Aifft2. For instance, if we only know the Fourier coefficients in the the first $n + 1$ columns, then we can populate the remainder of the matrix.

There is no smaller set of data points that we can use to populate Aifft2 (assuming $m = n$).

Appendix C

The Spin-Up Function

In this appendix, we provide details on the spin-up function used in this thesis to smoothly transition stationary initial states on the boundary of the domain to steady state values. The use of such a function (in this work at least) allows us to avoid using impulsively started conditions, which result in low order convergence in the time-stepping due to the non-smoothness of these conditions in the time variable.

Our spin-up function is a smooth transition between data points (t_0, f_0) and (t_1, f_1) and has the form

$$f(t; t_0, t_1) = (f_1 - f_0)U(t) + f_0, \quad t_0 \leq t \leq t_1, \quad (\text{C.1})$$

where the function $U(t)$ smoothly transitions the data between points $(t_0, 0)$ and $(t_1, 1)$. The spin-up function we use in this work is essentially related to well-known windowing functions used in other application areas. We will review a few examples that are widely-used in the literature and then derive a windowing function of our own that offers advantages in the present work.

C.1 A brief review of windowing functions

While there are many such examples, we will review two windowing functions from the literature with properties that differ in important ways. A widely-used windowing function described in [101, pg. 75] is obtained by setting (for a chosen integer value $p \geq 2$)

$$U(t) = \frac{[v(t)]^p}{[v(t)]^p + [1 - v(t)]^p}, \quad (\text{C.2})$$

where

$$v(t) = \left(\frac{1}{2} - \frac{1}{p}\right) \left(\frac{2t - t_1 - t_0}{t_1 - t_0}\right)^3 + \frac{1}{p} \left(\frac{2t - t_1 - t_0}{t_1 - t_0}\right) + \frac{1}{2}, \quad (\text{C.3})$$

for $t_0 \leq t \leq t_1$. Derivatives are explicitly computed using the simple relation

$$v(t)[1 - v(t)]U'(t) = pU(t)[1 - U(t)]v'(t), \quad t_0 \leq t \leq t_1, \quad (\text{C.4})$$

which follows from equation (C.2). It is readily verified that $U(t) = \mathcal{O}(t - t_0)^p$ and $1 - U(t) = \mathcal{O}(t_1 - t)^p$; that is, this windowing function ensures that the first $p - 1$ derivatives vanish at the endpoints $t = t_0$ and $t = t_1$ (the p -th derivatives of $U(t)$ are non-zero at the endpoints). This version of the windowing function is useful since it gives us direct control over how many derivatives we want to be zero at the endpoints; this is important since the more derivatives that vanish at the endpoints, the larger the derivative of the windowing function will be in the center of the domain, which can present its own computational issues in a time-stepping procedure. A minor downside in the use of this windowing function is that it can be a little more expensive to compute than another method we derive in this appendix.

Another widely-used windowing function, used in reference [102] and elsewhere, is given by

$$U(t) = 1 - \exp\left(\frac{2e^{-1/x}}{x - 1}\right) \quad \text{with} \quad x = \frac{t - t_0}{t_1 - t_0}, \quad (\text{C.5})$$

for $t_0 \leq t \leq t_1$. This windowing function is interesting since it ensures that the transition between points $(t_0, 0)$ and $(t_1, 1)$ is infinitely differentiable. In doing this, the windowing

function ensures that all derivatives vanish at the endpoints $t = t_0$ and $t = t_1$; as a result, the derivative of $U(t)$ can be extremely large in the middle of the domain, and this large derivative would need to be resolved with extremely small time steps if it were used in our work.

C.2 A new windowing function

We now outline a new windowing function that we have derived that, in our view, improves on the deficiencies of the previous two cases. The function $U(t)$ is defined on the interval $[t_0, t_1]$ as the truncated cosine series

$$U(t) = \frac{1}{2} - \sum_{k=1}^n b_{2k-1}^{(n)} \cos \left[\frac{(2k-1)\pi(t-t_0)}{t_1-t_0} \right]. \quad (\text{C.6})$$

Enforcing $U(t_0) = 0$ and $U(t_1) = 1$ and the vanishing of all of the derivatives of (C.6) leads to an $n \times n$ linear system of the form $V_n \mathbf{b} = \mathbf{d}$ where

$$V_n = \begin{bmatrix} 1 & 1 & 1 & \cdots & 1 \\ 1 & \alpha_1^2 & \alpha_2^2 & \cdots & \alpha_{n-1}^2 \\ 1 & \alpha_1^4 & \alpha_2^4 & \cdots & \alpha_{n-1}^4 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & \alpha_1^{2n-2} & \alpha_2^{2n-2} & \cdots & \alpha_{n-1}^{2n-2} \end{bmatrix},$$

is a Vandermonde-type matrix and

$$\mathbf{b} = [b_1, b_3, \dots, b_{2n-1}]^T \quad \text{and} \quad \mathbf{d} = [1/2, 0, \dots, 0]^T.$$

While these matrices are known to be very ill-conditioned, explicit formulas exist for computing the inverse. Since all but the first element of $\mathbf{d}$ is zero, in order to compute $\mathbf{b}$ we are only

interested in the first column of the inverse given by the column vector with elements

$$V_n^{-1}(1, 1) = \frac{\prod_{k=1}^{n-1} \alpha_k^2}{\prod_{k=1}^{n-1} (\alpha_k + 1)(\alpha_k - 1)}$$

and

$$V_n^{-1}(j + 1, 1) = \frac{\prod_{k=1, k \neq j}^{n-1} \alpha_k^2}{(\alpha_j + 1)(\alpha_j - 1) \prod_{k=1, k \neq j}^{n-1} (\alpha_k + \alpha_j)(\alpha_k - \alpha_j)}; \quad j = 1, 2, \dots, n - 1.$$

With $\alpha_i = 2i + 1$, $i = 1, 2, \dots, n - 1$, the expansion coefficients of our windowing function are easily determined as

$$b_{2j+1}^{(n)} = \frac{2}{\pi} \frac{(-1)^j [\Gamma(n + 1/2)]^2}{(2j + 1)(n - j - 1)!(n + j)!}; \quad j = 0, 2, \dots, n - 1, \quad (\text{C.7})$$

where

$$\Gamma(n + 1/2) = \frac{1 \cdot 3 \cdot 5 \cdots (2n - 1)}{2^n} \Gamma(1/2) = \frac{\sqrt{\pi} (2n)!}{2^{2n} n!}.$$

A stable recursion relation for the coefficients is easily derived from (C.7) by simplifying a ratio of successive terms. We thus obtain

$$b_{2j+3}^{(n)} = \frac{(j - n + 1)(2j + 1)}{(j + n + 1)(2j + 3)} b_{2j+1}^{(n)}, \quad b_1 = \frac{8}{n} \frac{[(2n - 1)!]^2}{[2^n(n - 1)!]^4}, \quad (\text{C.8})$$

for $j = 0, 2, \dots, n - 2$. With the coefficients so defined, it may be shown that the first $2n - 1$ derivatives of $U(t)$ vanish on each of the interval endpoints $t = t_0$ and $t = t_1$. As a point of interest, in the limit $n \rightarrow \infty$ we have $b_1^{(\infty)} = 2/\pi$ and

$$b_{2j+1}^{(\infty)} = \frac{2}{\pi} \frac{(-1)^j}{2j + 1}; \quad j = 1, 2, \dots$$

This is the Fourier series of the square waveform. Our new windowing function allows us to control the number of vanishing derivatives on the endpoints and is expressed in a form that allows the use of fast transforms, so that values may be very efficiently calculated at each

point in the domain, if desired.

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