

Abstract

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Chapter 1

Introduction

1.1 Overview

Fluid motions driven by buoyancy and frictional forces belongs to broad class of flows known as thermoconvective shear flows. These flows exhibit rich behaviour, and are of interest in both engineering and meteorology applications spanning across a broad range of length scales.

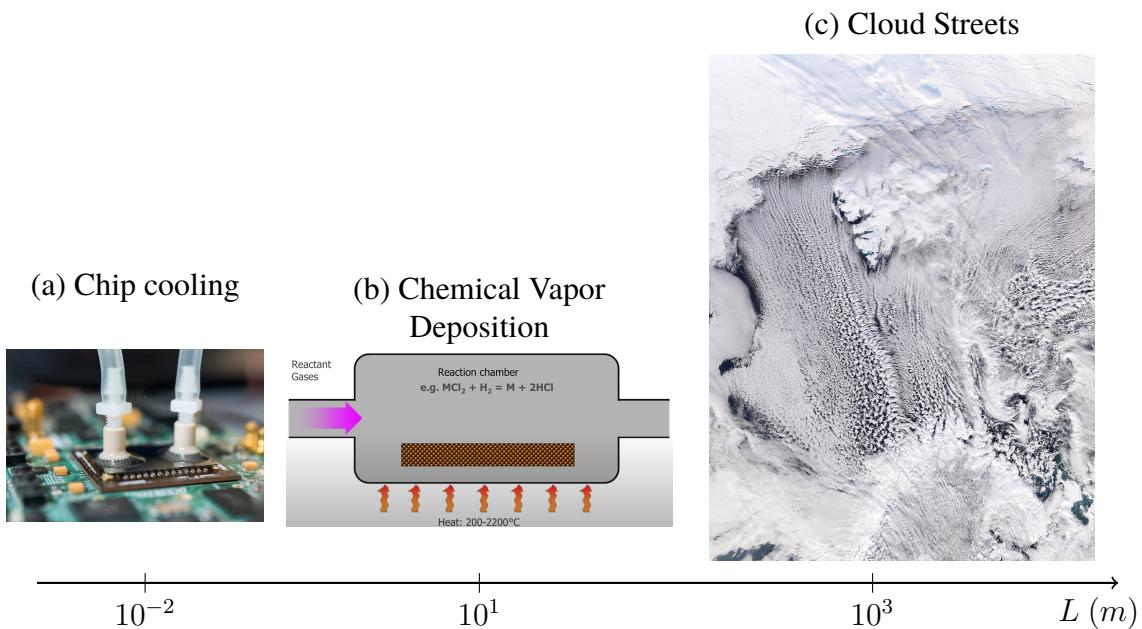


Figure 1.1: Thermoconvective shear flows driven by shear and buoyancy forces across length scales, $L \in [10^{-2} \text{m}, 10^3 \text{m}]$. Examples include (a) chip cooling, (b) chemical vapour deposition and (c) the formation of cloud streets.

At small scales, around $L \sim 10^{-2} \text{m}$, thermoconvective flows are relevant to the cooling of microprocessing chips. The fluid in such systems acting to dissipating heat, typically experiences shear and buoyancy forces from the confining walls, and heating. One of the major challenge in this industry is on increasing the density of transistors on a single chip, alluding to Moore's Law, which predicts the doubling of transistors on a single chip approximately every two years. However, one of the major limitations is the challenge of dissipating the excessive heat generated from the densely

packed transistors. Fluids, such as air, water or refrigerants, are often used to transport heat away from the components, and their fluid mechanical behaviour remains an open topic [Kennedy and Zebib, 1983, Ray and Srinivasan, 1992].

At intermediate length scales, $L \sim 1m$, the interaction between buoyancy and frictional forces is important in the fabrication of uniform thin films in chemical vapour deposition (CVD) [Evans and Greif, 1991, Jensen et al., 1991]. The CVD process typically involves a reactive gases carried by inert gases which flows through a channel with a heated substrate. Upon heating, the reactant gases react chemically on the substrate, depositing material and forming thin films, such as silicon layers. A key challenge in the CVD process is achieving a uniform deposition and maintaining sharp interfaces between layers. The interactions between shear and buoyancy forces often gives rise to boundary layers and thermoconvective rolls, which can disrupt uniform deposition, affecting film quality.

At larger length scales, $L \sim 10^3 m$, the thermoconvective shear flows can be observed in atmospheric flows such as the cloud streets over the Norwegian Sea. These parallel bands of cumulus clouds can stretch over hundreds of kilometres. They form when the relatively warmer sea surfaces heat up the colder air arriving from the North pole. As the colder air is heated, it rises upwards whilst carrying water vapour, condensing into visible clouds. This circulation is subsequently organised into parallel rotating parallel columns of air, forming distinct cloud streets.

The central focus of this thesis is on the investigation of fluid behaviour arising from the interaction between shear and buoyancy forces, a common thread among the examples discussed above. We note that by isolating our analysis to the interaction between shear and buoyancy forces, we might neglect other physical mechanisms such as phase change, chemical reactions and evaporation, which may be significant in the context of cooling microprocessors, chemical vapour deposition, and atmospheric boundary layers respectively [Vallis et al., 2019]. Nonetheless, the interaction between shear and buoyancy forces remains an open topic and will be the primary focus of this thesis, providing a foundation for future investigations that may include addition mechanisms.

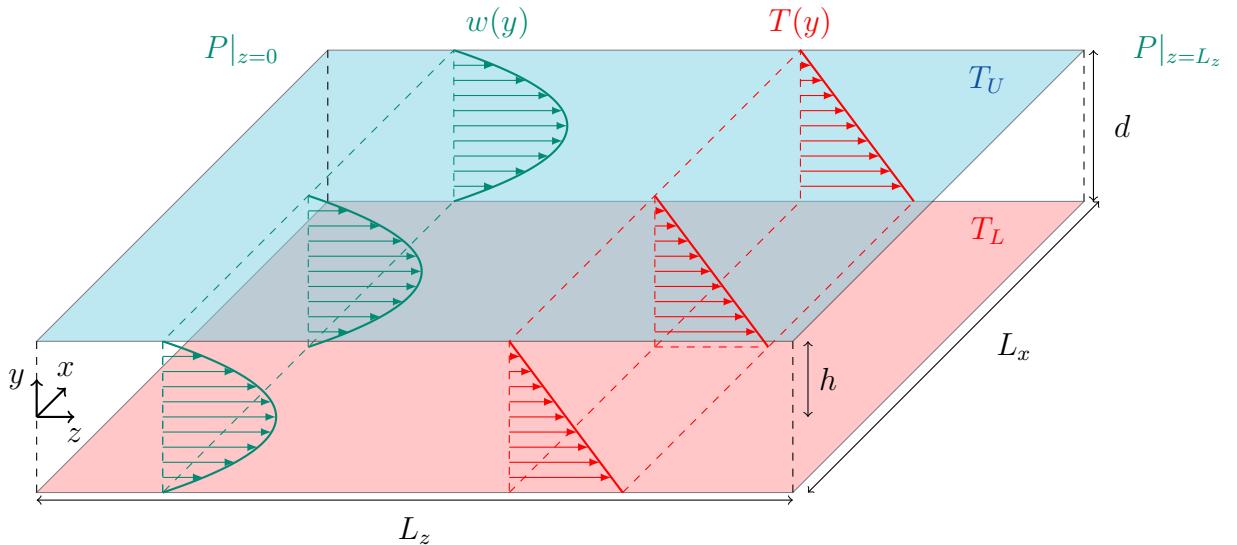


Figure 1.2: The Rayleigh-Bénard Poiseuille (RBP) flow configuration.

To consider this interaction, we consider an idealised setup, known as the Rayleigh-Bénard-

Poiseuille (RBP) flow. This RBP system describes the fluid motion confined between two infinitely extended parallel plates, heated from below and cooled from the top, with an additional pressure gradient driving the flow. The RBP configuration combines the two paradigmatic flow configurations; the classical Rayleigh-Bénard convection (RBC), driven purely by buoyancy, and plane Poiseuille flow (PPF), driven purely by shear. While the onset of convection in RBC, and the transition to subcritical shear-driven turbulence in PPF have been both extensively studied, the transitional regime in which both forces interact remains less understood. Understanding their transitional behaviour and their transport properties could have implications for the applications mentioned above.

The RBP configuration is illustrated in figure 1.1, where z, y, x refer to the stream-, spanwise and wall normal coordinates and L_z, L_x, d, h the length, span, depth and half-height of the domain respectively. We note that the domain is biperiodic along z and x . The flow is driven by a pressure gradient along the streamwise z direction, $\Delta P = P|_{z=0} - P|_{z=L_z} < 0$, leading to a laminar Poiseuille flow, $w(y) = 1 - y^2$, if ΔP is kept small such that flow remains laminar. We will consider a fully developed flow, where the boundary layer from the top and the bottom wall meets at the midplane $y = 0$ and entrance effects are therefore neglected. Like the RBC system, the RBP system is unstably stratified. The temperature difference between the lower, T_L , and upper wall, T_U , is always positive, $\Delta T = T_L - T_U > 0$, leading to a stable linear conduction layer along the wall-normal direction, $T(y)$, if ΔT is kept sufficiently small.

In the absence of a pressure gradient, the RBP configuration reduces to the classical Rayleigh-Bénard convection problem, bringing about buoyancy-driven convection for a sufficiently large unstable stratification. In the limiting case without unstable stratification, $\Delta T = 0$, the system reduces to the wall-bounded plane Poiseuille flow (PPF), where the transition towards subcritical shear-driven turbulence may be expected for a sufficiently large pressure gradient. We focus on the transitional regime, by investigating if buoyancy forces promote the transition to shear-driven turbulence and the effect of shear on convection in large domains.

We describe the structure of the introductory chapter as follows. We begin our discussion on the development of hydrodynamic stability theory of wall-bounded shear flows in §1.2. Theoretical frameworks used in the study of stability of flow such as linear modal/non-modal stability, nonlinear dynamical systems and the spatiotemporal character of transitional shear flows will be discussed. Throughout this discussion, we also highlight examples of PPF which is relevant to the RBP system. This followed by the developments of Rayleigh-Bénard convection (RBC) in §1.3, where theoretical concepts from §1.2 will be utilised. After which, we describe the developments of RBP flows §1.4, before concluding this chapter with an outline of the thesis in §1.5.

1.2 Transitional wall-bounded shear flows

Wall-bounded shear flows concerns the motion of the fluid flowing in parallel to walls, typically bounded by one or more walls. Near the wall, the fluid comes to rest due to the no-slip boundary condition, resulting in a velocity gradient perpendicular to the wall, giving rise to shear within the fluid - hence the term *wall-bounded shear flows*. Examples include the pressure-driven plane Poiseuille

flow (channel flow), Hagen-Poiseuille flow (pipe flow), plane Couette flow and flat plate boundary layers. These geometrically simple configurations provides a convenient framework amenable to the mathematical analysis of fluid motion subjected to shear. Depending on the degree of shear, the fluid motion can be either laminar, where the fluid layers move in smooth parallel 'laminates', or turbulent, characterised by chaotic eddying motions. We also note that there is a transitional regime where both states can coexist discuss later. A central question is predicting the transition from the laminar regime to the turbulence.

The first investigation into this transition was conducted by [Reynolds \[1883\]](#). In his experimental setup, the flow speed through the pipe could be controlled by regulating the inlet pressure, while injecting dye to visualise the flow, as illustrated in figure 1.3(a). At low speeds, the fluid remained laminar, resulting to a single streak of steady dye in figure 1.3(b). As the speed increased, the dye begin to exhibit irregular 'sinuous' motions interspersed with laminar regions shown in figure 1.3(c). This is now referred to as the transitional/intermittent regime, alternating between the laminar and turbulent states. Beyond a critical speed, the dye breaks down entirely into chaotic 'eddies', mixing with the surrounding fluid and discolouring the flow with dye downstream in figure 1.3(d). This regime is now identified as turbulence.

Reynolds proposed that the threshold between the laminar, transitional and turbulent regimes could be characterised by a non-dimensional parameter, now referred to as the Reynolds number,

$$Re = UD/\nu, \quad (1.1)$$

where U is the centerline velocity in the pipe, D , the pipe diameter and ν , the kinematic viscosity. He observed that flow through the pipe remained 'stable' and laminar for $Re < 1900$, while it became 'unstable' and turbulent for $Re > 2000$ [[Reynolds, 1895](#)]. These findings introduced the concept of flow stability.

1.2.1 Linear Stability Analysis

Following Reynolds' experiment, interest towards the mathematical analysis of the stability of laminar flows grew in early 20st century. The mathematical approach typically begins by decomposing the velocity field, $\mathbf{u}(\mathbf{x}, t)$, into a laminar (base) state, $U(y)$, and the velocity perturbations, $\mathbf{u}'(\mathbf{x}, t)$, with pressure similarly decomposed as,

$$\mathbf{u}(\mathbf{x}) = U(y) + \mathbf{u}'(\mathbf{x}, t), \quad \text{and} \quad p(\mathbf{x}, t) = P(x) + p'(\mathbf{x}, t). \quad (1.2)$$

Substituting into the Navier-Stokes equations and linearising (neglecting nonlinear terms), we get,

$$\frac{\partial \mathbf{u}'}{\partial t} + (U \cdot \nabla) \mathbf{u}' + (\mathbf{u}' \cdot \nabla) U = -\nabla p' + \frac{1}{Re} \nabla^2 \mathbf{u}', \quad (1.3a)$$

$$\nabla \cdot \mathbf{u}' = 0, \quad (1.3b)$$

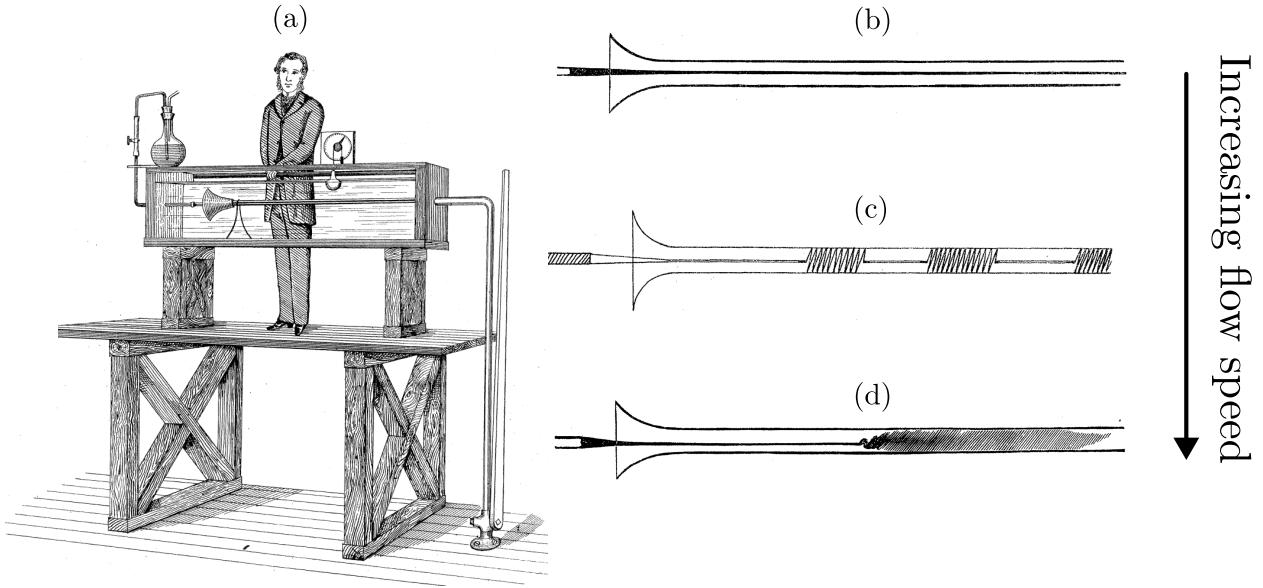


Figure 1.3: (a) Osbourne Reynolds pipe experiment with the dye injection apparatus, illustrating the (b) laminar flow, (c) intermittent regime and (d) turbulent flow as the flow speed is increased, taken from [Reynolds, 1883].

known as the linearised Navier-Stokes equations. This commonly followed by introducing a wavelike ansatz (mode) defined by streamwise and spanwise wavenumbers, α, β and complex frequency, ω . In general two ways to analysis the linearised Navier-Stokes equations by considering the behaviour of each mode independently in §1.2.1 and their coupled dynamics in §1.2.1

Modal analysis

It is convenient to eliminate the pressure terms by reformulating equation (1.3) using the wall-normal perturbation velocity, v' , and wall-normal vorticity, $\eta' = \partial u'/\partial z - \partial w'/\partial x$, variables. Using (v, η) , we introduce a modal ansatz for them,

$$v'(\mathbf{x}, t) = \tilde{v}(y)e^{i(\alpha x + \beta z - \omega t)}, \quad \text{and} \quad \eta'(\mathbf{x}, t) = \tilde{\eta}(y)e^{i(\alpha x + \beta z - \omega t)}. \quad (1.4)$$

where α, β, ω denotes the streamwise and spanwise wavenumbers, and complex frequency (i.e. $\omega = \omega_r + i\omega_i$), respectively. Substituting this ansatz into linearised equations lead to the classical Orr-Sommerfeld and Squire equations [Orr, 1907, Sommerfeld, 1909, Squire, 1933, Schmid and Henningson, 2001],

$$\begin{pmatrix} \mathcal{L}_{OS} & 0 \\ i\beta U' & \mathcal{L}_{SQ} \end{pmatrix} \begin{pmatrix} \tilde{v} \\ \tilde{\eta} \end{pmatrix} = i\omega \begin{pmatrix} k^2 - \mathcal{D}^2 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \tilde{v} \\ \tilde{\eta} \end{pmatrix}. \quad (1.5a)$$

with

$$\mathcal{L}_{OS} = i\alpha U(k^2 - \mathcal{D}^2) + i\alpha U'' + \frac{1}{Re}(k^2 - \mathcal{D}^2)^2, \quad \mathcal{L}_{SQ} = i\alpha U + \frac{1}{Re}(k^2 - \mathcal{D}^2). \quad (1.5b)$$

where $\mathcal{D} = d/dy$, $k^2 = \alpha^2 + \beta^2$ and U'' is the second derivative of $U(y)$. Equation (1.5a) is a generalised eigenvalue problem with eigenvalue $i\omega$, which determines the growth of perturbations. The goal of modal stability analysis is to determine the critical Reynolds number Re_c , defined as the lowest value of Re , for all α and β in which $\Im[\omega] = 0$. For $Re > Re_c$, perturbations can grow exponentially, indicating instability. Squire's theorem states that for every unstable three-dimensional perturbation, there exist an unstable two-dimensional perturbation, with a lower Re_c [Squire, 1933]. This implies that the most linearly unstable perturbation of wall-bounded flows is two dimensional. Calculations by Tollmien [1928] and Schlichting [1933] for a flat-plate boundary layer flow yielded a critical Reynolds number based on streamwise distance x of $Re_{x,c} = Ux_c/\nu = 520$ [Schlichting and Gersten, 2017]. These two dimensional unstable eigenmodes are known as Tollmien-Schlichting (T.S) waves. In plane Poiseuillw flow, the critical Reynolds number is $Re_c = 5772.2$ with a critical wavenumber of $\alpha_c = 1.02$ [Orszag, 1971]. However, experiments reveal that transition to turbulence can occur at must lower Reynolds number, around, $Re \sim 1000 - 2000$ [Davies and White, 1928, Patel and Head, 1969, Dean, 1978, Iida and Nagano, 1998, Tsukahara et al., 2014a], highlighting a key limitation of modal analysis. Similar discrepancies are observed in plane Couette and pipe flows [Meseguer and Trefethen, 2003], where the laminar state is linearly stable for all Re , yet transition to turbulence occurs. Despite these limitations, modal analysis predicts instabilities in other flows such as Rayleigh-Bénard convection and Taylor-Couette flow [Chandrasekhar, 1968]. Further extensions of modal stability, including spatial instability analysis [Huerre and Monkewitz, 1990], and secondary instability [Orszag and Patera, 1983] are well established and are beyond the scope of this thesis.

Non-modal stability

One of a major limitations of modal analysis is that it treats each eigenmode independently. However, the interaction between decaying eigenmodes can lead to a transient growth, where perturbations amplify temporarily before decaying asymptotically. To demonstrate an example of transient growth, we consider a two-dimensional toy model governing the time-evolution of $\mathbf{q} = (v, \eta)^T$,

$$\frac{d}{dt} \begin{pmatrix} v \\ \eta \end{pmatrix} = \begin{pmatrix} -\frac{1}{Re} & -1 \\ 0 & -\frac{2}{Re} \end{pmatrix} \begin{pmatrix} v \\ \eta \end{pmatrix}, \quad (1.6)$$

where Re refers to the Reynolds number. The toy model has negative eigenvalues, $(\lambda_1, \lambda_2) = (-1/Re, -2/Re)$, indicating asymptotic decay. At $Re = 15$, the eigenvectors, $\mathbf{x}_1 = (1, 0)$, $\mathbf{x}_2 = (1, \frac{1}{\sqrt{Re^2+1}})$, are highly non-orthogonal, becoming almost parallel shown in figure 1.4(a). Notably, we become increasingly linearly dependent as $Re \rightarrow \infty$. For a particular initial condition, the energy $\|\mathbf{q}\|^2 = \sqrt{v^2 + \eta^2}$, is amplified four times before decaying in blue trajectory, shown in Figure 1.4(b). Yet for another choice of initial condition, the trajectory decays asymptotically as the green trajectory indicates. Despite decaying eigenmodes, the toy model highlights the significance of transient growth, which depends on the choice of initial condition.

The aim of non-modal stability analysis is find the initial conditions, $\tilde{\mathbf{q}}_0$, that leads to the maximum

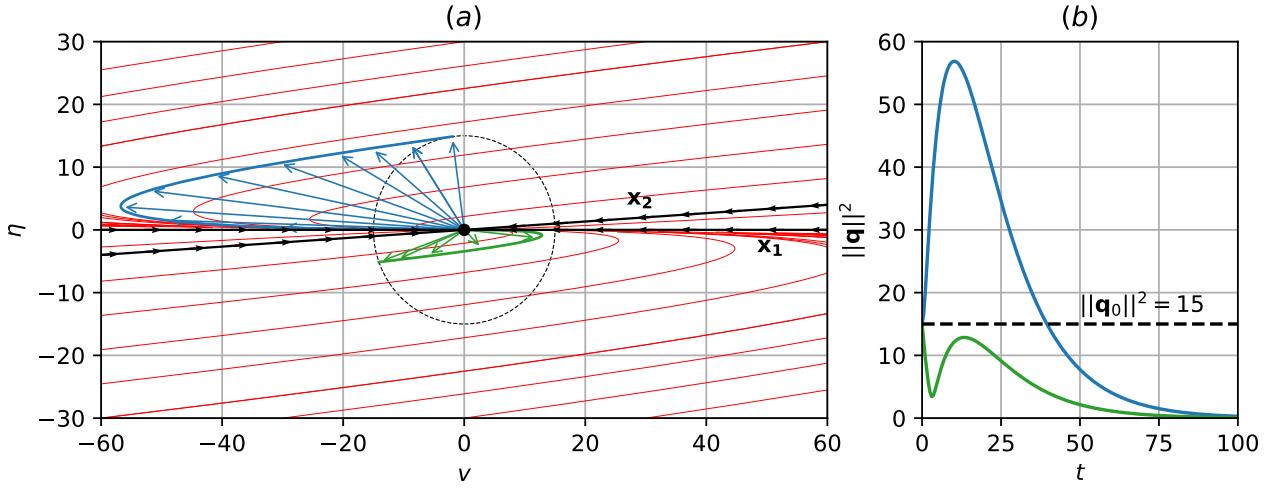


Figure 1.4: (a) The phase portrait of the toy model with $Re = 15$, where red lines are phase lines of the toy model. The blue trajectory lead to transient growth and the green trajectory do not (b) Time history of blue and green trajectory.

amplification, $G(\tau)$, over a time horizon τ . This is posed as an optimistaion problem,

$$G(\tau) = \max_{\tilde{\mathbf{q}}_0 \neq 0} \frac{\langle \tilde{\mathbf{q}}(\tau), \tilde{\mathbf{q}}(\tau) \rangle}{\langle \tilde{\mathbf{q}}_0, \tilde{\mathbf{q}}_0 \rangle}, \quad \text{s.t. } \langle \tilde{\mathbf{q}}_0, \tilde{\mathbf{q}}_0 \rangle = 1, \quad (1.7)$$

where, $\langle \cdot, \cdot \rangle$ denotes the inner-product,

$$\langle \mathbf{x}, \mathbf{y} \rangle = \int_{\Omega} \mathbf{x}^H \mathbf{y} \, d\Omega, \quad (1.8)$$

and \mathbf{x}^H refers to the complex conjugate transpose of \mathbf{x} . By considering the linearised operator of (1.5a), we can define a linear time invariant operator given as,

$$\tilde{\mathbf{q}}(\tau) = \mathcal{A}(\tau) \tilde{\mathbf{q}}_0, \quad (1.9)$$

which takes the solution from initial conditions, $\tilde{\mathbf{q}}_0$, to $\tilde{\mathbf{q}}(\tau)$ at time τ . Subtituting the expression above into equation (1.7),

$$G(\tau) = \max_{\tilde{\mathbf{q}}_0 \neq 0} \frac{\langle \mathcal{A}(\tau) \tilde{\mathbf{q}}_0, \mathcal{A}(\tau) \tilde{\mathbf{q}}_0 \rangle}{\langle \tilde{\mathbf{q}}_0, \tilde{\mathbf{q}}_0 \rangle} = \langle \tilde{\mathbf{q}}_0, \mathcal{A}^\dagger(\tau) \mathcal{A}(\tau) \tilde{\mathbf{q}}_0 \rangle = \lambda_{max}(\mathcal{A}(\tau)^\dagger \mathcal{A}(\tau)) \quad (1.10)$$

where \mathcal{A}^\dagger refers to the adjoint of $\mathcal{A}(t)$. The maximum amplification factor $\max G(t)$ is the largest eigenvalue of $\mathcal{A}^\dagger(\tau) \mathcal{A}(\tau)$. The eigenvalue problem is given as,

$$\mathcal{A}^\dagger(t) \mathcal{A}(t) \tilde{\mathbf{q}}_0 = \lambda \tilde{\mathbf{q}}_0, \quad (1.11)$$

where $\tilde{\mathbf{q}}_0$ refers to the eigenvector denoting the optimal initial condition. For a detailed derivation of the optimal initial conditions or forcing, the reader is referred to [Butler and Farrell, 1992, Schmid, 2007].

An alternative method of computing the optimal transient growth is by analysing the pseudospectral of linear operators discussed in [Trefethen, 1997], but is outside the scope of this thesis.

Both two-, and three-dimensional non-modal analyses reveal mechanisms for transient growth. In two-dimensions, the optimal initial conditions are in the form of near wall vortices tilted upstream, which amplifies transiently via the Orr-mechanism [Orr, 1907, Farrell, 1988, Reddy et al., 1993]. In three-dimensions, streamwise vortices are optimal, leading to the the amplification of streamwise streaks via the lift-up effect [Ellingsen and Palm, 1975, Reddy and Henningson, 1993]. Notably, the spacing of these streaks analysed using non-modal analysis at higher Reynolds number has been consistently reported to occur around 100 wall units [Del Álamo and Jiménez, 2006, Pujals et al., 2009, Hwang and Cossu, 2010], which supports experimental observations of streak spacing in turbulent boundary layers [Kline et al., 1967, Smith and Metzler, 1983]. The main results from non-modal analysis is that three dimensional perturbations can lead to strong transient growth at subcritical Reynolds numbers, contradicting the two dimensional TS waves from modal analysis. Both modal and non-modal mechanisms highlight important insights into the linear mechanisms which might be responsible for the transition from laminar to turbulent flows.

1.2.2 Nonlinear dynamical systems

In the previous section, we have examined the laminar to turbulent transition using linear frameworks. However, the the transition process is ultimately described by the nonlinear Navier-Stokes equations, which motivates the development and adoption of mathematical frameworks beyond linear methbods.

In the context of shear flow turbulence, there has been a growing interesting in adopting techniques from nonlinear dynamical systems, interpreting turbulence as a chaotic trajectories which evolves within a finite-dimensional phase space. This phase space refers to a set of solutions satisfying the Navier-Stokes equations, conjectured to be infinite dimensional by Hopf [1948]. Hopf [1948] further conjectured that within the infinite dimension phase space lie a finite dimensional manifold, whose properties depended on viscosity. For large viscosities (i.e. low Re), this finite dimensional space corresponds to a single point, the laminar state. This point may become unstable at a certain critical Reynolds number, bifurcating to form new manifolds, as viscosity is decreased (i.e. Re is increased) further, potentially leading to chaos. The set of such manifolds is referred to *inertial manifolds*, and its existence under certain properties has been established [Foias et al., 1988]. A implication of this is that the transition to turbulence could be viewed as successive bifurcations from the laminar state, govern by a single control parameter (i.e. the Reynolds numnber), generalised by the so called *routes to chaos* scenarios.

Landau [1944] proposed that the transition to turbulence may occur through a sequence of Hopf bifurcations, each introducing a new incommensurate frequency, resulting in quasi-periodic motions on a high-dimensional torus. However, this model did not capture the essential ingredients of turbulence, such as sensitivity of initial conditions and mixing [John et al., 1993]. Ruelle and Takens [1971] later show that a *strange attractor* exhibit key features of chaos can emerge after three successive Hopf bifurcations from a stationary state, referred to as the *Ruelle-Takens* route to chaos. This scenario has been have been observed in Taylor-Couette flow [Gollub and Swinney, 1975], and Rayleigh-Bénard

convection [Swinney and Gollub, 1978]. Other routes to chaos scenarios, such as periodic-doubling [Feigenbaum, 1979], and intermittency Manneville and Pomeau [1979] scenarios have been proposed. For a review of these routes to chaos scenarios, the reader is referred to John et al. [1993]. Nonetheless, the transition to turbulence is subcritical in shear flow configurations, meaning that the route of chaos scenarios do not necessarily apply through bifurcations from the laminar state.

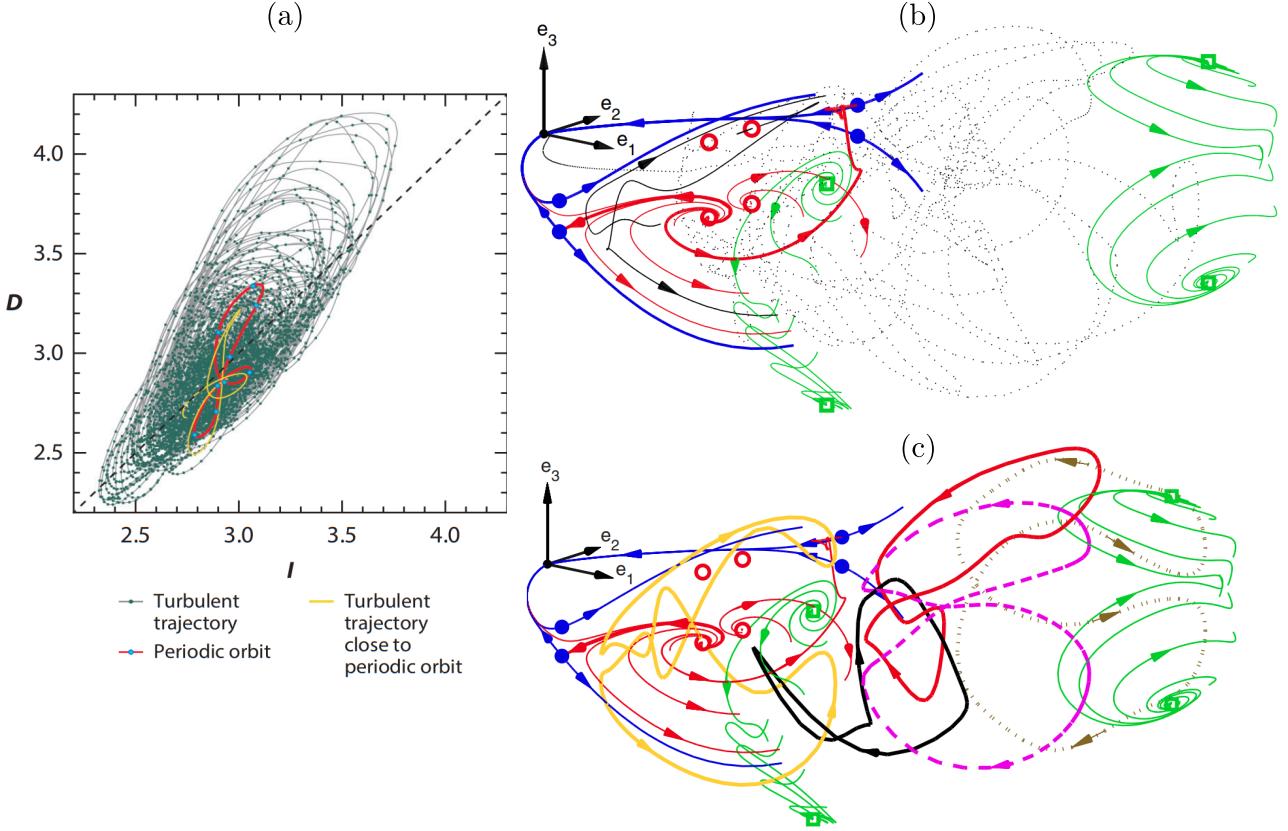


Figure 1.5: (a) Chaotic trajectories of turbulence of plane Couette flow at $Re = 400$, approaching the an unstable periodic orbit (red) highlighted as yellow, adopted from Kawahara and Kida [2001]. (b) State space organisation of turbulence trajectories (black dots) confined around equilibria (circles, dots and squares) and their unstable manifolds (solid lines), heteroclinic connections between them are shown in red. The coordinate system is centered on the laminar state, using a linear combination of the upper branch invariant state. (c) State space projection of five periodic orbits (coloured solid lines), embedded within the same space where turbulence evolves in (b), adopted from [Cvitanović and Gibson, 2010].

A major development came with the identification of a pair of non-trivial, unstable equilibrium states in plane Couette flow [Nagata, 1990]. This pair referred to as the *lower* and *upper* branches, emerging from a saddle node bifurcation which is disconnected from the stable laminar state. The *lower* branch lies closer to the laminar state, while the *upper* branch resides further away in state space. Later, a travelling-wave solution in plane Couette flow also later found by the same author [Nagata, 1997]. A family of equilibrium and travelling-wave solutions was found later for plane Couette and plane Poiseuille flows under different boundary conditions (i.e. stress-free, slip and no-slip) were identified by [Waleffe, 2001, 2003], sometimes referred to as *exact coherent states*. Additional equilibria and travelling-wave solutions were identified by Gibson et al. [2008, 2009],

along with their heteroclinic connections between them [Halcrow et al., 2009]. In the context of pipe flow, multiple travelling-wave solutions have also been reported [Faisst and Eckhardt, 2003, Wedin and Kerswell, 2004, Kerswell and Tutty, 2007, Wang et al., 2007, Duguet et al., 2008, Pringle et al., 2009]. The set of equilibria, and travelling waves, shows good agreement with the statistical quantities (e.g. mean and fluctuations) with direct numerical simulations. However, since they are equilibria, and travelling-waves (relative equilibria), they do no capture the temporal dynamics of turbulence such as the *self-sustaining process* (SSP) [Hamilton et al., 1995]. While these unstable solutions demonstrate good agreements with results from DNS such as the spanwise length scales, and mean and fluctuations, they do not capture the dynamical processes.

The next breakthrough was on the identification of time-dependent invariant solutions in the form of periodic orbits. Kawahara and Kida [2001] computed a pair of periodic orbits in plane Couette, with one exhibiting a single regeneration cycle similar to the SSP while the other exhibits mild modulation of streaks. These periodic orbits are connected via heteroclinic trajectories. In plane Poiseuille flow, Toh and Itano [2003] also identified periodic orbits displaying bursting behaviour. Using a Newton–Krylov iteration with a hook-step modification, Viswanath [2007] computed multiply relative periodic orbits. These studies conceptualise that the chaotic trajectories of turbulence as being embedded within a set of unstable periodic orbits, evolving along their unstable manifolds [Viswanath, 2007, Gibson et al., 2008, 2009, Halcrow et al., 2009, Graham and Floryan, 2021]. An example is shown in figure 1.5, where the chaotic trajectories in figure 1.5(b), reside within the same state space as the periodic orbits, enclosed by equilibria and their heteroclinic connections shown in figure 1.5(c). The set of equilibria, travelling waves and their relative counterparts, are referred to as *invariant solutions* offering a building block description of turbulence. However, they do not provide insight into the transition process, since these solutions already reside in the turbulent attractor.

The transition to turbulence in canonical shear flow configurations are typically subcritical, emerging from the invariant solutions described above, accompanied by an underlying stable laminar state. A consequence of this is that the laminar and turbulent states form a bistable attractors in phase space. The laminar and turbulent states coexist as stable attractors, with a boundary—known as the *edge*, separating their respective basins of attraction. Attractors that sit along this edge have been identified and found to possess a saddle-like structure, attracting trajectories within the edge and repelling them toward either the laminar or turbulent state, known as *edge states*. The algorithm to identify such states, known as edge tracking, was first employed in pipe flow experiments Schneider et al. [2007], where it is chaotic. Time-averaging of this chaotic attractor revealed a close resemblance to the unstable lower branch travelling-wave solutions, suggesting that the edge separating basin of attraction between the laminar and turbulent states consist of the lower branch solutions and their symmetries [Duguet et al., 2008, Pringle et al., 2009]. As Reynolds number increases, the edge and the turbulent attractor moves apart [Schneider and Eckhardt, 2009]. In the context of pipe flows, it was recognised that the edge consists of a set of unstable travelling-wave solutions connected to the lower branch. A graphical representation of the edge, and edge states, separating the laminar and turbulent states is shown in figure 1.6. Near the onset of subcritical turbulence, turbulence appear to be transient, decaying towards the laminar solution after a finite lifetime [Bottin et al., 1998, Faisst and Eckhardt, 2004, Hof et al.,

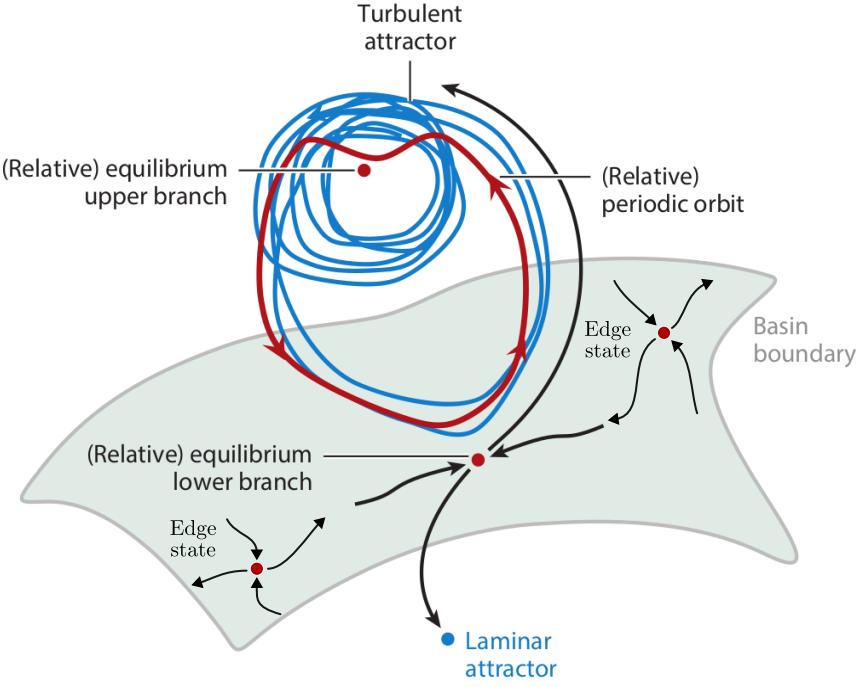


Figure 1.6: A graphical representation of the edge (grey surface) separating the basin of boundary of the laminar and turbulent attractor, consisting of attractors, known as edge states, adapted from [Graham and Floryan \[2021\]](#).

[2006](#)] This may be interpreted as the turbulent attractor colliding with the lower branch solution (i.e. the edge) through a *boundary crisis* [[Lai and Tél, 2011](#)], where the chaotic attractor becomes *leaky*, providing an avenue for the solution trajectory towards relaminarisation [[Kreilos and Eckhardt, 2012](#), [Zammert and Eckhardt, 2015](#)].

1.2.3 Spatiotemporal transitional flows

This section describes the inherent spatiotemporal structure of subcritical turbulence near the onset commonly reported in large extended domains. In this regime, turbulence is characterised by the coexistence of turbulent and laminar structures. Examples of such are found in canonical shear flow systems such as plane Couette flows [[Prigent et al., 2003](#), [Barkley and Tuckerman, 2005, 2007](#), [Tuckerman and Barkley, 2011](#), [Duguet et al., 2010](#), [Reetz et al., 2019](#)], Taylor-Couette flows [[Prigent and Dauchot, 2002](#), [Prigent et al., 2003](#)], pipe flows [[Avila et al., 2010, 2011](#), [Song et al., 2017](#), [Avila et al., 2023](#)] and plane Poiseuille flows [[Tsukahara et al., 2014a,c](#), [Tuckerman et al., 2014](#), [Tsukahara et al., 2014b](#), [Gomé et al., 2020](#), [Paranjape, 2019](#), [Paranjape et al., 2020, 2023](#)].

We will focus on the plane Poiseuille flow configuration, where the spatiotemporal intermittent patterns are referred to as oblique turbulent-laminar bands illustrated in figure 1.7 at $Re = 1400$ for $L/h = 16\pi$. The bright and dark regions highlight coexisting spatially localised turbulent and laminar regions. These turbulent-laminar bands occur over a range of Reynolds numbers, and its precise range is likely dependent on the domain's aspect ratio [[Tsukahara et al., 2014b](#), [Tuckerman et al., 2014](#), [Paranjape et al., 2023](#)]. Near the upper Re threshold of this regime, the domain is fully engulfed by

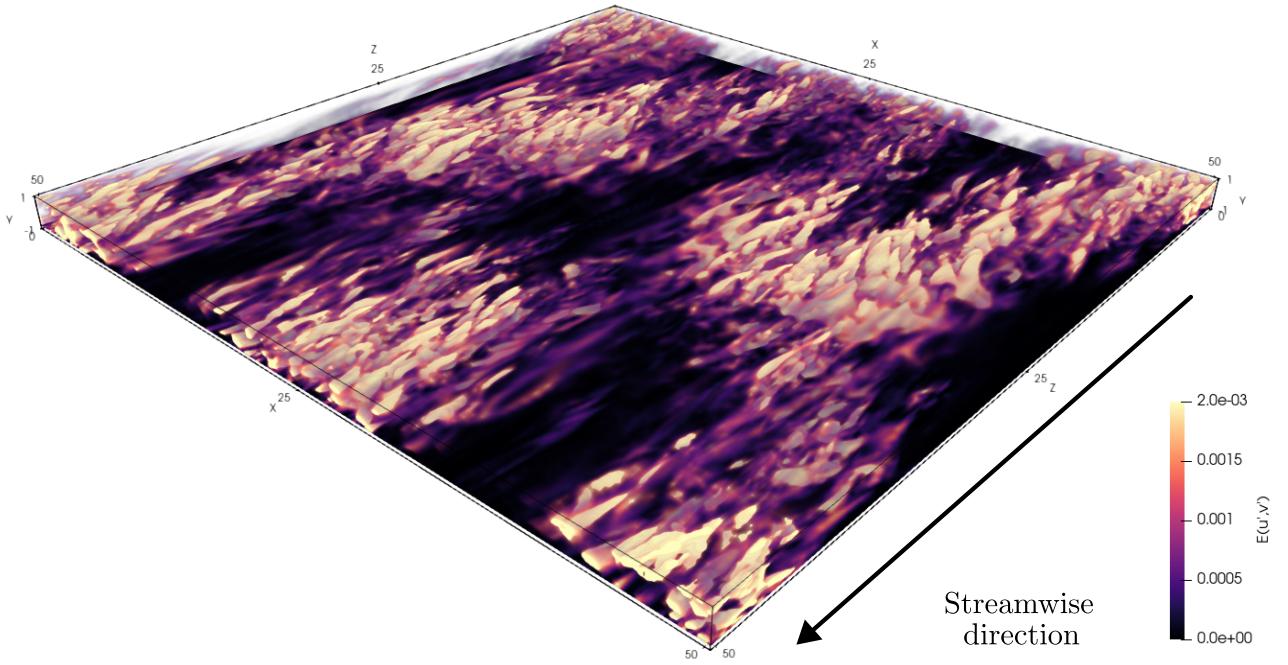


Figure 1.7: A snapshot of turbulent-laminar bands at $Re = 1400$ in a large domain $L/d = 8\pi$, depicting its spatiotemporal intermittent nature. Isovolumetric renderings are based on the spanwise, u' , and wall-normal, v' , perturbation kinetic energy, $E(u', v') = 1/2(u'^2 + v'^2)$, where the perturbation velocities are defined about the laminar state $\mathbf{u}'(\mathbf{x}, t) = \mathbf{u}(\mathbf{x}, t) - U_{lam}(y)$.

developed turbulent regions, referred to as uniform, featureless turbulence appearing at $Re = 1800$ in figure 1.7(a). As Re decreases towards $Re = 1050$, spatiotemporal turbulent and laminar structures known as turbulent-laminar bands persist in between $Re \in [1050, 1600]$ shown in figures 1.8(b-f). In particular, these turbulent-laminar bands appear to have a preferred inclined angle, between $20^\circ \sim 30^\circ$, with streamwise wavelengths of $\sim 60h$, and spanwise wavelengths of $\sim 20h - 30h$ [Tsukahara et al., 2014b]. Kashyap et al. [2022] considered the linear response of the fluctuating turbulent field, and showed that the preferred band angle emerges near 23.2° . In the minimal band unit (MBU) studies of plane Poiseuille flows, the turbulent bands convect at about $\sim 1\%$ of the bulk velocity, propagating either upstream or downstream, depending on Re [Tuckerman et al., 2014, Gomé et al., 2020]. Notably, the spanwise lengths of the bands are much wider than the half-heights and depend on Re , appearing at $\lambda_z \sim 20h$ for $Re \gtrsim 1400$ and $\lambda_z \sim 40h$ for $Re \lesssim 1100$. Interestingly, the bands alternate between both spanwise lengths between the Re range, merging and splitting continuously [Tuckerman et al., 2014], reminiscent of a puff splitting in pipe flows [Avila et al., 2011]. An example of this could be observed in $Re = 1050$, where the band appears to alternate between different spanwise wavelengths in figure 1.8(f). As Re falls below a certain Re threshold, turbulent bands spontaneously decay and relaminarise [Tuckerman et al., 2014, Gomé et al., 2020]. An example is shown in figure 1.8(g).

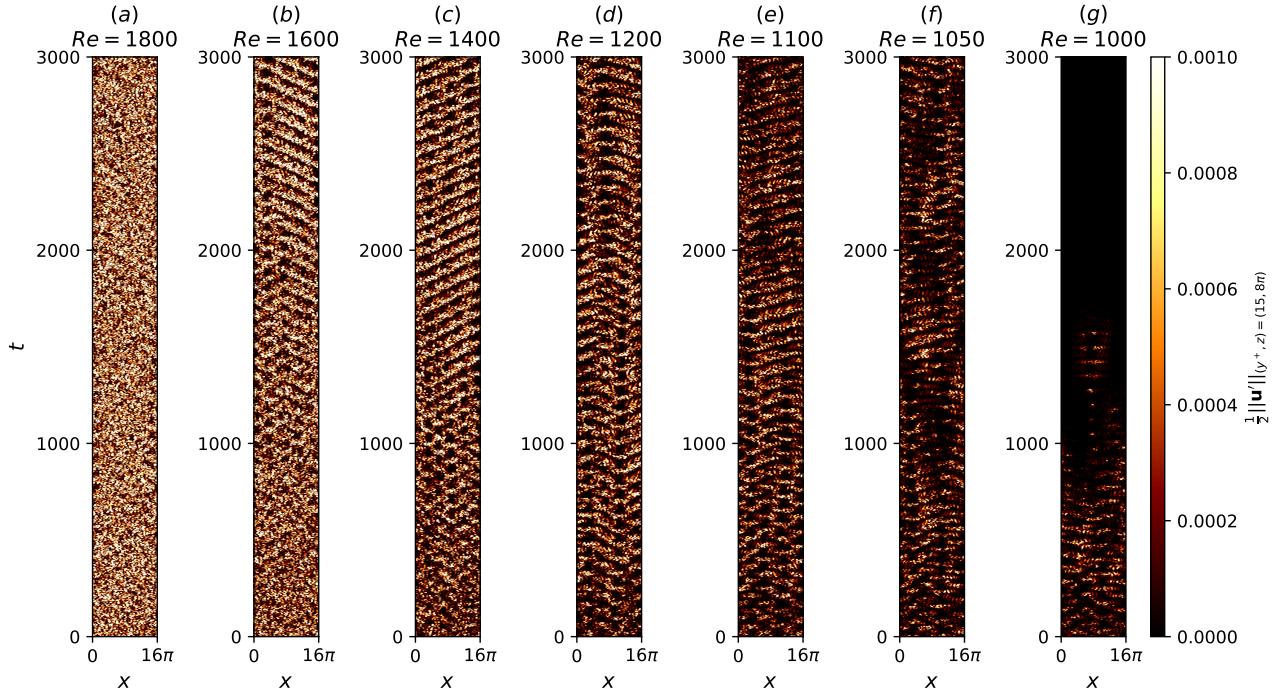


Figure 1.8: Turbulent-laminar bands for $t \in [0, 3000]$ in large domains $(L_x, L_z) = (16\pi, 16\pi)$ at (a) $Re = 1800$, (b) $Re = 1600$, (c) $Re = 1400$, (d) $Re = 1200$, (e) $Re = 1100$, (f) $Re = 1050$, (g) $Re = 1000$.

Gomé et al. [2020] computed the probabilities distributions for turbulent-laminar band decay, $P(\Delta t^d)$, where Δt^d is the time until decay. A key insight is that the probability distributions of turbulent band decay mimics a memoryless Poisson process,

$$P(\Delta t^d) = \exp(-\Delta t^d/\tau^d(Re)), \quad (1.12)$$

where $\tau^d(Re)$ refers to the mean lifetime for decay as a function of Re . Similarly, the band splitting process also follow a Poisson process

$$P(\Delta t^s) = \exp(-\Delta t^s/\tau^s(Re)), \quad (1.13)$$

white $\tau^s(Re)$ the mean splitting lifetime. Both τ^d and τ^s exhibit superexponential dependence on Re ,

$$\tau^{d,s} = \exp(\exp(Re)), \quad (1.14)$$

This is shown in figure 1.9, with a crossover point at $Re_{cross} \approx 965$, where both decay and splitting becomes equally probable. This crossover point is considered as the critical Reynolds number for the onset of turbulent bands.

While there has been progress made towards our understanding of infinitely periodic turbulent-laminar bands in MBUs, recent studies of isolated (non-periodic) turbulent bands (ITBs) reveal different behaviour. Notably, ITBs persist at Reynolds number below Re_{cross} at $Re = 700$ for durations exceeding $t = 10000$, exceeding the mean decay lifetime in figure 1.9. The ITBs are characterised by

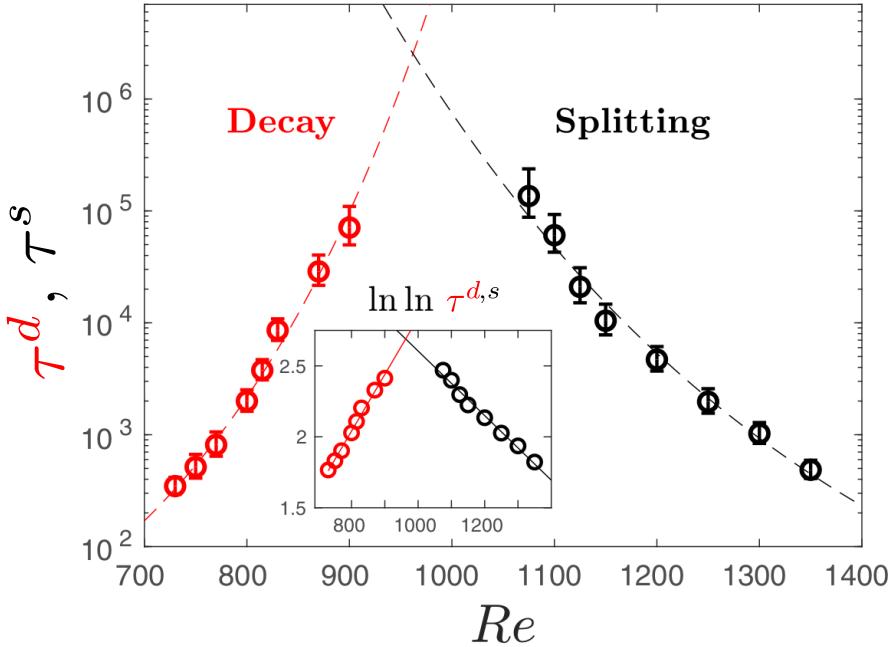


Figure 1.9: The mean decay times (red), τ^d , and mean splitting times (black), τ^s , as a function of Reynolds number, leading to a crossover point at $Re_{cross} \approx 965$, adapted from [Gomé et al., 2020].

streak generating head and a diffusive upstream tail. [Xiong et al., 2015, Tao et al., 2018, Shimizu and Manneville, 2019, Xiao and Song, 2020]. We conclude our discussion on transitional wall-bounded shear flows.

1.3 Rayleigh-Bénard convection

Rayleigh-Bénard convection (RBC) is a paradigmatic fluid configuration describing the motion of the fluid confined between two infinite-parallel plates heated from below and cooled from the top. As the bottom plate is heated, the bottom layer fluid becomes more buoyant and tends to rise, while the colder top fluid layer becomes relatively less buoyant and tends to sink, leading to an overturning of layers. Viscous forces between neighbouring fluid parcels act to resist the motion. As buoyancy overcomes these viscous forces, the fluid layers overturn, resulting in the initiation of buoyancy-driven convection, the physical mechanism underpinning RBC.

One of the earliest experimental studies dedicated to buoyancy-driven convection was conducted by Henri Bénard [Bénard, 1901], who observed the formation of hexagonal convection cells above a certain temperature threshold ΔT . These hexagonal patterns are referred to as Bénard cells are illustrated in figure 1.10(a) (adapted from [Koschmieder and Pallas, 1974]). Subsequently, Rayleigh [1916] carried out one of first linear stability analyses of buoyancy-driven convection, predicting the onset of convection at a critical Rayleigh number of $Ra_c = 657.5$. However, Rayleigh's analysis assumed an idealised free-free boundary conditions, which differed from the rigid-free setup of Bénard's experiment. The linear stability analysis for rigid-free configuration was later performed by Jeffreys [1928] yielding a higher critical Rayleigh number of $Ra_c = 1058$. In the rigid-rigid configuration, the critical Rayleigh number increases further to $Ra_c = 1708$ [Pellew and Southwell,

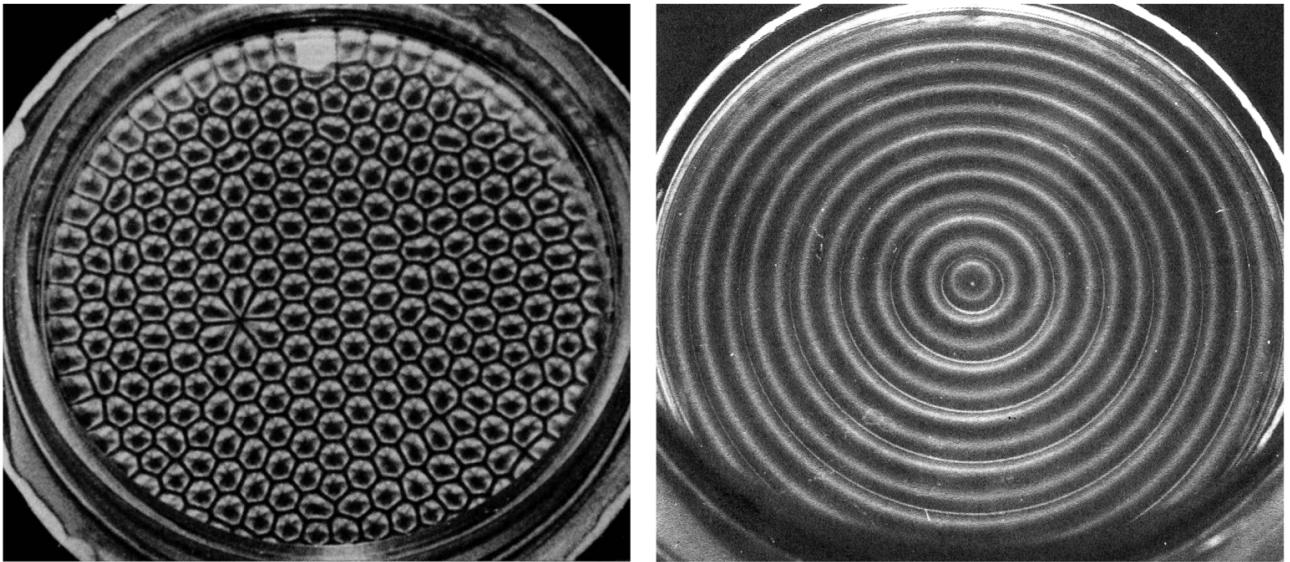


Figure 1.10: (a) Surface tension driven convection leading to the onset of hexagonal Bénard cells in a thin layer of silicone oil, heated from below and cooled by ambient air. A diamond defect appears, likely caused by plate imperfections. (b) Buoyancy driven convection in rigid plates, resulting to concentric convection rolls at 2.9 times the critical Rayleigh number. Both experiments were performed by Koschmieder and Pallas [1974], and the convection patterns were illuminated by aluminum powder, where the dark and bright regions refer to vertical and horizontal motions respectively. These higher resolution images were taken from [Van Dyke and Van Dyke, 1982].

1940]. The Rayleigh number in Bénard's original experiment contradicted results from linear stability analysis as it was found to be 300 to 1500 smaller than Ra_c for the free-free and rigid-free cases respectively [Wesfreid, 2017]. This contradiction, not recognised by Bénard at the time, lies in the significant role of surface tension in thin fluid layers exposed to air, now known as Bénard-Maragoni (BM) convection [Block, 1956, Cloot and Lebon, 1984, Manneville, 2006, Wesfreid, 2017]. In BM convection, fluid motion is primarily driven by surface tension gradients due to variations of temperature, forming hexagonal cells, as in figure 1.10(a). The preference for hexagonal cells in BM convection was later confirmed based on weakly nonlinear stability analysis [Cloot and Lebon, 1984]. As the fluid layer becomes thicker, surface-tension effects diminish and buoyancy-driven convection becomes dominant. Similarly, placing a rigid lid on top of a thin fluid layer suppresses surface-tension effects, resulting in buoyancy-driven convection. The preferred convection patterns based on weakly nonlinear stability analysis are the two-dimensional parallel rolls, now referred to as ideal straight rolls (ISRs) [Schlüter et al., 1965, Bodenschatz et al., 2000]. In circular containers, the ISRs conform to the geometry of the boundaries, forming concentric convection rolls illustrated in figure 1.10(b). Interestingly, hexagonal cells have been observed in buoyancy-driven flows of non-Boussinesq fluids [Hoard et al., 1970, Bodenschatz et al., 2000]. In this thesis, I will consider the RBP setup (and RBC in chapter 4) with rigid-rigid boundary conditions with for which the critical Rayleigh number is $Ra_c = 1708$. Notably, the corresponding critical wavelength is $q_c = 3.12/d$ (or $\lambda_c \approx 2d$), suggesting that distance separating the plates, d , dictates the length of a single roll, $l_{roll} = \lambda_c/2 \approx d$.

As mentioned earlier, stationary ISRs near q_c emerge just above Ra_c , based on weakly nonlinear

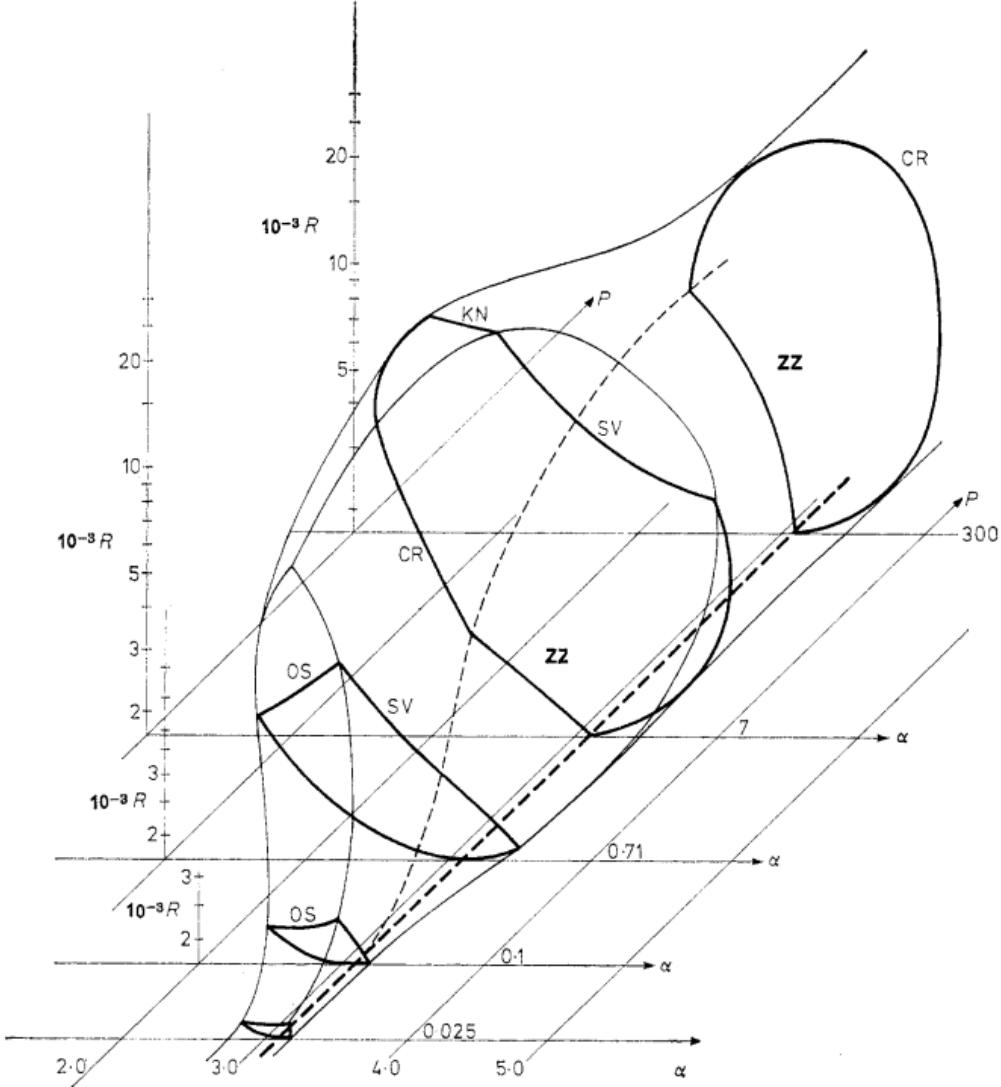


Figure 1.11: The Busse balloon describes the stability boundaries of ISRs in a $\varepsilon - q$ space. For larger wavenumbers, the instability mechanism is described by the skewed-varicose (SV) instability. For smaller wavenumbers, the instability mechanism is described by the Eckhaus instability. For large ε , the instability is described by the onset of oscillatory instability. Busse balloon digitised from [Plapp, 1997] for $Pr \approx 1$.

stability analysis. [Eckhaus, 1965, Schlüter et al., 1965]. However, this prediction contradicted by the emergence of time-dependent oscillatory ISRs in experiments [Rossby, 1969, Willis and Deardorff, 1970] at $Ra = 9200$ (or roughly five times Ra_c), where weakly nonlinear stability becomes inapplicable far from threshold. To address this, a direct secondary stability analysis was employed to study the stability of ISRs further from Ra_c , based on Galerkin truncation [Busse, 1972]. One of the key results from this analysis is the Busse balloon, which describes the stability boundaries of ISRs as a function of Ra and Pr , and roll wavenumber, α , shown figure 1.11 [Busse, 1978]. The boundaries of the Busse balloon are described by a range of secondary instabilities, each arising from different physical mechanisms [Busse, 1978]. At large Prandtl numbers, $Pr = O(10^2)$, the zig-zag (ZZ) and cross-roll (CR) instabilities delimits the balloon for small and large roll wavenumbers. The zig-zag instabilities cause zig-zag undulations while the CR instabilities generates rolls orthogonal to the underlying ISR

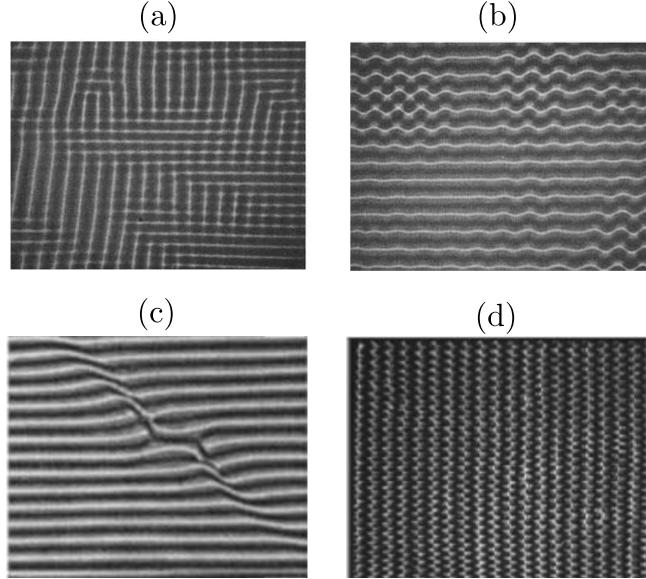


Figure 1.12: ISRs experiencing (a) cross-roll instability at $Ra = 3000, Pr = 100$ and (b) zig-zag instability at $Ra = 3600, Pr = 100$ [Busse and Whitehead, 1971]. (c) Skew-varicosed instability at $Ra = 5568, Pr = 1$ [Plapp, 1997], and (d) oscillatory instability at $Ra = 10384, Pr = 1$ [Cakmur et al., 1997a].

structure, effectively increasing or decreasing the roll wavenumber respectively [Busse and Whitehead, 1971]. Examples of these instabilities at $Pr = 100$ are illustrated in figure 1.12(a,b).

At moderate Prandtl numbers, $Pr = O(1)$, the Busse balloon is bounded by the skewed varicosed (SV) for high roll wavenumbers and the oscillatory (OS) instability at large Ra . The skewed-varicosed (SV) instability leads to roll-pinchig where pinched rolls merged into a single roll, reducing roll wavenumber while the oscillatory instability leads to the onset of an oscillatory ISRs. Examples of the respective instabilities at $Pr = 1$ are shown in figure 1.12(c,d). At higher wavenumbers, the skewed varicose (SV) instability becomes relevant at intermediate Prandlt numbers, characterised by roll pinching and merging that effectively reduces the roll wavenumber. Finally, the Eckhaus instability (not shown), related to the symmetry of the system, appears close to the Ra_c , leading a disturbance parallel to the underlying rolls which either creates or destroy rolls such that the resultant roll wavenumber adheres to the stability boundaries [Lowe and Gollub, 1985]. Near $Pr = 1$, the Eckhaus instability coincides with the crossroll instability (figure 6 from Bodenschatz et al. [2000], adapted from Plapp [1997].)

In this thesis, we focus on fluids with $Pr = 1$, where secondary instabilities such as skewed-varicose, Eckhaus and cross-roll instabilities typically arise. While the stability boundaries of the Busse balloon have been experimentally verified [Busse and Whitehead, 1971, Croquette, 1989a, Plapp, 1997], accurately predicting the wavenumber of ideal straight rolls (ISRs) remain difficult due to hysteresis and the existence of multiple stable ISRs of different roll wavenumbers. As Ra continuously increases, ISRs with wavenumbers outside the Busse Balloon undergo the secondary instabilities (described above) that drive their wavenumbers back to the stable boundaries. The hysteretic behaviour highlights that the roll wavenumber of the ISRs is strongly dependent on the system's history [Bodenschatz et al., 2000].

It is worth noting that the ISRs are the exception rather than the rule in RBC [Croquette, 1989b]. A range of non-ISR states, such as squares, travelling or stationary target patterns, giant rotating spirals, and oscillatory convection, have been observed over the years [Le Gal et al., 1985, Croquette, 1989a, Plapp, 1997, Hof et al., 1999, Rüdiger and Feudel, 2000, Borońska and Tuckerman, 2010a,b]. For example, Hof et al. [1999] identified eight stationary and two oscillatory state in cylindrical RBC with small aspect ratios at the same Rayleigh number. These results were later verified in numerical simulations and bifurcation analysis, reveal up to twelve stable branches near the onset ($Ra \leq 2500$) and the potential for hundreds more as Ra increases [Ma et al., 2006, Borońska and Tuckerman, 2010a,b].

In larger domains ($\Gamma \geq 28$), giant rotating spirals were found and have been investigated [Plapp and Bodenschatz, 1996, Plapp et al., 1998]. Experimental and numerical studies of RBC with varying sidewall boundary conditions (i.e. thermally insulating, conducting and no-slip) [Tuckerman and Barkley, 1988, Siggers, 2003, Paul et al., 2003, Bouillé et al., 2022], non-Boussinesq convection [Bodenschatz et al., 1992], and rotational effects [Hu et al., 1997] were investigated, where multiple states were also reported. In inclined RBC, Reetz and Schneider [2020], Reetz et al. [2020] identified up to sixteen stable and unstable invariant states, along with heteroclinic orbits connecting them. These findings indicate that RBC support a rich variety of coexisting stable states beyond ISRs, resulting to a system with multiple stable states above the critical Rayleigh number. To complicate matters further, RBC also exhibits spatiotemporal chaotic states.

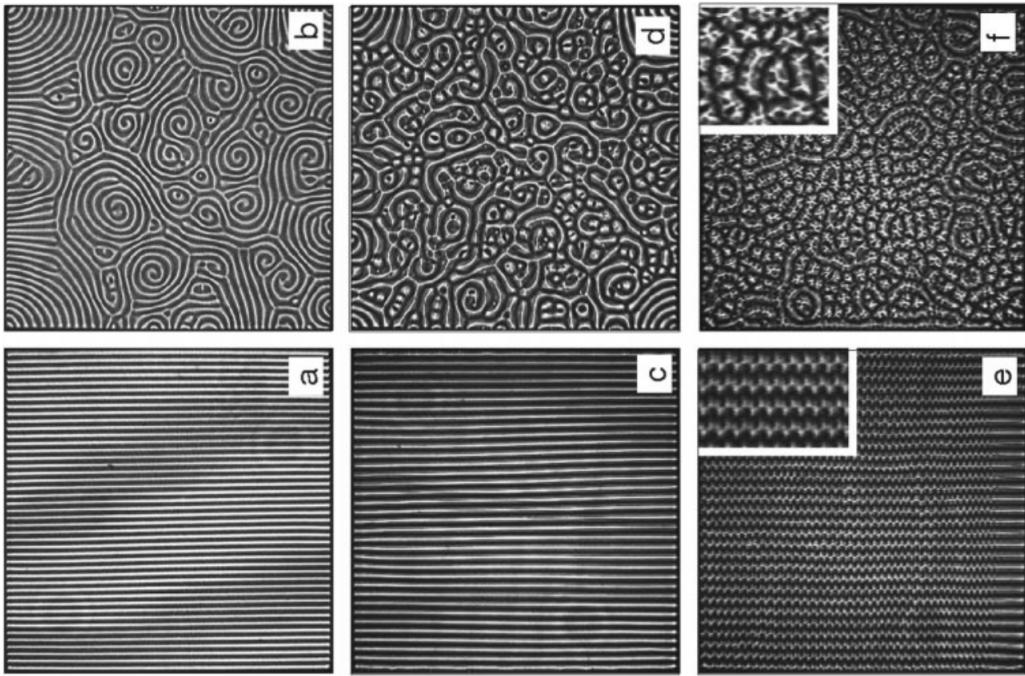


Figure 1.13: The coexistence of spiral defect chaos (SDC, top row) and ideal straight rolls (ISRs, bottom row) at (a,b) $Ra = 3279$, (c,d) $Ra = 6832$ and (e,f) $Ra = 10384$. The domain size is $\Gamma = 50$ and $Pr = 1$, adapted from Cakmur et al. [1997a].

In the late 1990s, convection rolls exhibiting spatio-temporal chaotic behaviour known as spiral defect chaos (SDC) were observed within the same stability boundaries where ISRs were expected [Morris et al., 1993, Hu et al., 1993, Decker et al., 1994, Hu et al., 1995, Morris et al., 1996, Cakmur

et al., 1997a, Ahlers, Egolf et al., 1998, 2000, Chiam et al., 2003, Vitral et al., 2020] Notably, ISRs emerge with carefully prepared initial conditions while uncontrolled initial conditions lead to SDC. It is now well established that SDC exists as intrinsic attractor of RBC, independent of sidewall conditions Morris et al. [1996], forming a bistable system with ISRs [Cakmur et al., 1997a] across a range of Ra at $Pr = 1$ illustrated in figure 1.13. However, this bistability appears to be Prandtl number dependent. At $Pr = 4$, the SDC appears to be transient decaying towards ISRs over long periods [Bajaj et al., 1997]. SDC has also been replicated in numerical simulations using two-dimensional Swift-Hohenberg equations [Swift and Hohenberg, 1977, Xi et al., 1993, Xi and Gunton, 1995, Schmitz et al., 2002, Karimi et al., 2011]. The critical Rayleigh number for the onset of SDC, Ra_s , depends on the domain's aspect ratio, and Prandtl number [Hu et al., 1995, Bajaj et al., 1997, Cakmur et al., 1997b, Bodenschatz et al., 2000]. SDC has been primarily reported in large aspect ratio domains ($\Gamma \gtrsim 20$), suggesting a minimal domain size for SDC to occur [Bodenschatz et al., 2000]. Furthermore, the leading Lyapunov exponents of SDC decreases as Γ [Egolf et al., 2000, Paul et al., 2007]. To better characterise SDC, several studies have investigated its spatial-temporal properties, such as the averaged roll-curvature Hu et al. [1995], probability distribution of spirals Ecke et al. [1995], Liu and Ahlers [1996] and correlation length-/time-scales [Morris et al., 1993, 1996, Cakmur et al., 1997b]. Specifically, the correlation length-scales were found to grow exponentially with [Morris et al., 1993, 1996, Cakmur et al., 1997b], suggesting that transition from ISRs to SDC resembles a phase transition. Similar spatiotemporal chaotic behaviour has been observed in other pattern-formation systems, including rotating RBC Hu et al. [1997], dielectric barrier discharge Dong et al. [2005] and advection diffusion reaction systems Affan and Friedrich [2014].

1.4 Rayleigh-Bénard Poiseuille (RBP) flows

This section describes the development of Rayleigh-Bénard Poiseuille (RBP) flows, integrating key findings from both plane Poiseuille flow (PPF) and Rayleigh-Bénard convection (RBC) systems discussed in §1.2 and §1.3 respectively. The neutral stability curves in the Rayleigh-Bénard Poiseuille (RBP) comprising of both plane Poisueuille flow (PPF) and Rayleigh-Béanrd convection (RBC) systems, are bounded by the onset of Tollmien-Schlichting waves at $Re_c = 5772.22$ [Orszag, 1971], and by the onset of convection rolls at $Ra_c = 1708$ [Pellew and Southwell, 1940], respectively. In RBP systems, the imposed mean Poiseuille flow in the RBP system breaks the rotational symmetry of the convection rolls, categorising them based on their orientation to the mean flow direction, namely: longitudinal, transverse and oblique rolls. These primary instabilities were first investigated by Gage and Reid [1968] in an infinitely extended layer. For longitudinal rolls, the linearised system reduces to the classical RBC problem. Thus, the critical Rayleigh number remains unchanged at $Ra_{\parallel} = Ra_c = 1708.8$ with a critical wavenumber, $\alpha_{\parallel} = \alpha_c = 3.13$, independent of Reynolds number Re and Prandtl number Pr [Pellew and Southwell, 1940, Kelly, 1994]. In contrast, the critical Rayleigh number for the onset of transverse rolls increases with Re , dependent on Pr [Gage and Reid, 1968, Müller et al., 1992, Nicolas et al., 1997]. The critical Rayleigh number for the onset of obliqued rolls can derived using by applying a Squire transformation [Squire, 1933] to transverse roll system. For a

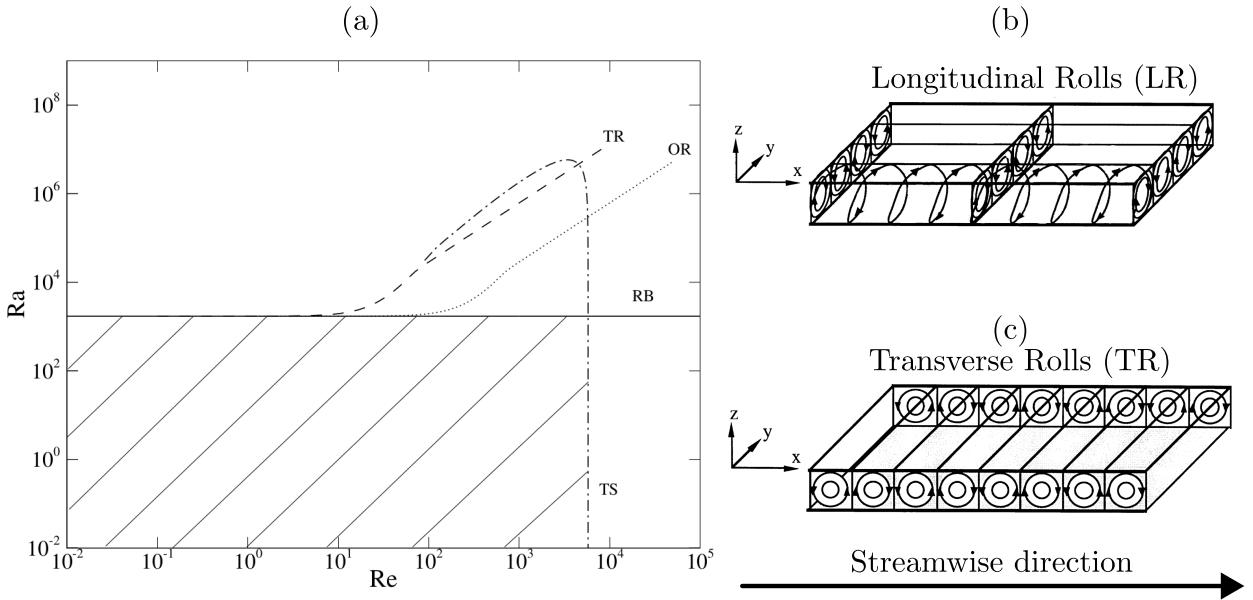


Figure 1.14: (a) Neutral stability curves of longitudinal rolls (LR), oblique rolls (OR), transverse rolls (TR) and Tollmien-Schlichting (TS) waves, adapted from [John Soundar Jerome et al. \[2012\]](#). The shaded area refers to damped perturbations. Sketch of (b) longitudinal and (c) transverse rolls, adapted from [Kelly \[1994\]](#).

given Ra , the corresponding critical Re for the onset of oblique rolls is higher than that for transverse rolls [[Gage and Reid, 1968](#)]. The neutral stability curves for the three different rolls are illustrated in figure 1.14.

Experimental studies in channels with large transverse aspect ratios (i.e. span-to-depth) showed the onset of longitudinal rolls [[Akiyama et al., 1971](#), [Ostrach and Kamotani, 1975](#), [Fukui et al., 1983](#)], while transverse rolls are more prevalent in narrower channels [[Luijkx et al., 1981](#), [Ouazzani et al., 1989, 1990](#)]. Linear stability analysis of longitudinal rolls for finite channels confirms that Ra_{\parallel} remains fairly independent for transverse aspect ratios greater than five, and increases quickly below that. Hence, for small Re , critical Rayleigh number of transverse rolls is smaller than that of longitudinal rolls, $Ra_{\perp} < Ra_{\parallel}$, giving rise to transverse rolls [[Nicolas et al., 2000](#)]. However, temporal linear stability analysis could not explain the observations by [Ouazzani et al. \[1990\]](#), where the laminar Poiseuille flow persisted in the same parameter space where transverse rolls were expected. This discrepancy was resolved by [Müller et al. \[1992\]](#), who showed that transverse rolls may be convectively or absolutely unstable, with the transition boundary aligning with the experimental data. Later, [Carrière and Monkewitz \[1999\]](#) showed that demonstrated that longitudinal rolls are always convectively unstable. Nonmodal stability analysis of subcritical RBP by [John Soundar Jerome et al. \[2012\]](#) revealed that the optimal transient growth is primarily dominated by streamwise rollers similar to those of PPF [[Reddy and Henningson, 1993](#)], with a spanwise wavenumber of $\beta_{opt} \approx 2.05$. The maximum amplification factor, G_{max} increases modestly with Ra , and the critical wavenumber approaches α_{\parallel} , indicative of longitudinal rolls.

For $Re > 0$ in infinite domains, the longitudinal rolls emerge as the dominant primary instability [[Gage and Reid, 1968](#)], and their secondary stability was analysed by [[Clever and Busse, 1991](#)].

They identified a time-dependent, wavy instability near $Re \sim 100$, giving rise to tertiary solutions in the form of wavy rolls. These wavy rolls have been observed experimentally and were found to be convectively unstable [Pabiou et al., 2003, 2005, Nicolas et al., 2010]. Clever and Busse [1991] also hypothesised that the wavy rolls are less efficient at transporting heating than longitudinal rolls for the same Ra , which was later confirmed numerically [Nicolas et al., 2012]. The influence of finite transverse aspect ratios on the onset of wavy rolls have also been studied [Xin et al., 2006, Nicolas et al., 2010], where the critical Ra was found to be approximately 1.5 times higher than in infinite domains Clever and Busse [1991]. Furthermore, the effect of external excitation has been explored, showing that increased excitation amplitude can reduce the development length required for wavy roll formation [Nicolas et al., 2010, 2012]. In the turbulent regime, shear driven turbulence has been shown to enhance heat transport in RBP flows [Scagliarini et al., 2014, 2015, Pirozzoli et al., 2017]. Extensions of the RBP configuration, such as flows over wavy walls or with sinusoidal thermal forcing have been investigated, potentially offering a reduction in drag and enhancing heat transport [Hossain et al., 2012, Hossain and Floryan, 2016, 2020]. For a comprehensive overview of RBP flows, the reader is referred to the reviews by Kelly [1994] and Nicolas [2002].

1.5 Thesis Outline

In this thesis, I am particularly focused on the transition behaviour of fluid flow in RBP systems by conducting direct numerical simulations and linear stability analysis. In particular, the onset of instabilities does not necessarily lead to turbulence, and are neither laminar nor turbulent, as we shall see later. For the sake of terminology, the transitional regimes can be loosely referred to as regimes that are neither laminar nor turbulent. There had been significant progress in our understanding of the instabilities of Rayleigh-Bénard convection and plane Poiseuille flows, their combined effects are not known. The motivation of this thesis is primarily academic, which explores the bridge between RBC and PPF.

The thesis is structured into the follows: §1 provides the background of this thesis, with relevant literature review. §2 presents the numerical methods, which includes the spectral/ hp element method, algorithms for solving the Navier-Stokes equations, linear stability analysis and edge tracking. §?? first presents a $Ra - Re$ phase space of the flow structures in RBP flows with a particular focus on the role of longitudinal rolls in sustaining turbulence as we introduce the *thermally-assisted sustaining process*. §3 presents the state space organisation of the bistability between spiral defect chaos and ideal straight rolls at $Ra = 2903$. We finally conclude this thesis, and present possible avenues of future work in §??.

Chapter 2

Numerical Methods

We will discuss the fundamentals of numerical methods relevant to solving the Navier-Stokes equations. We begin the discussion of the weighted of residuals (§2.1) and the spatial discretisation using spectral/*hp* element methods in one dimension (§2.3). This is followed by techniques for solving the Navier-Stokes equations (§2.4), introducing the velocity-correction scheme, enforcing a constant flow rate and the quasi-3D approach for semi-homogeneous domains. This chapter concludes with numerical techniques for the stability analysis of the Navier-Stokes equations (§2.5), including eigenvalue computation and edge tracking.

2.1 Method of weighted residuals

Spatial discretisation errors, or residuals, arises as one seeks an approximate solution to some partial differential equation (PDE). The method of weighted residual provides a generic mathematical framework in which constraints on the residual could be applied flexibly, defining the spatial discretisation scheme and its convergence properties. In summary, we approximate the solution of PDE by considering a finite expansion of a suitable basis, to which its coefficients are sought after by minimising the inner product between the PDE and a test (or weight) function. To demonstrate this, we consider a linear partial differential equation as,

$$\mathbf{L}[u(x)] = 0, \quad x \in \Omega, \tag{2.1}$$

where \mathbf{L} refers to a linear spatial differential operator subjected to some boundary conditions within the domain, Ω , while $u(x)$ refers to the exact solution of \mathbf{L} . Examples of PDEs with linear spatial differential operators include the Laplace equation, $\nabla^2 u = 0$, Poisson equation, $\nabla^2 u = f$, and the Helmholtz equation, $\nabla^2 u + \lambda u = f$. We suppose that the exact solution $u(x)$ can be approximated (discretised) by N finite number of basis (or expansion) functions, $\Phi(x)$.

$$u(x) \approx u^\delta(x) = \sum_{i=0}^{N-1} \hat{u}_i \Phi_i(x), \tag{2.2}$$

where $u^\delta(x)$ refers to the approximate solution of $u(x)$, consisting of a linear combination of the product between the i^{th} basis coefficient, \hat{u}_i , and the i^{th} global basis expansion, $\Phi_i(x)$, defined within Ω . Since $u^\delta(x)$ is an approximate solution of equation (2.5), we expect a residual (or ‘error’) between the exact solution, $u(x)$, and $u^\delta(x)$,

$$\mathbf{L}[u^\delta(x)] = R[u^\delta(x)], \quad (2.3)$$

where $R[u^\delta(x)]$ refers to the residual which depends on the approximate solution $u^\delta(x)$ and varying within Ω . In other words, equation (2.5) might not be satisfied everywhere in Ω . We need to place restrictions on the residual, such that it the residual approaches zero, $R \rightarrow 0$, and the approximate solution approaches the exact solution, $u^\delta(x) \rightarrow u(x)$. The method of residuals places a restriction on the residual by applying an inner product between the governing equation, and N test (or weight) functions, $v_j(x)$, and setting it to zero,

$$(v_j(x), R[u^\delta(x)]) = 0, \quad j = 0, \dots, N - 1. \quad (2.4)$$

Definition 2.1.1 (Inner product). The inner product between two functions $f(x)$ and $g(x)$ is,

$$(f, g) = \int_{\Omega} f(x)g(x)dx.$$

By setting equation (2.4) to zero, it becomes a system of N ordinary differential equations, where the N basis coefficients, \hat{u}_i . The choice of test function defines the projection methods, and examples of projection methods are shown in table 2.1. We emphasise that the method of weighted residuals merely describes the projection method, but does not specify the type of basis expansions, as we will discuss later in §2.3. The choice of projection method coupled with suitable basis expansions will have different solution convergence properties. A particular interest is on how quickly the residual vanishes as the number of basis expansions increases. For instance, by considering the Galerkin method coupled with Fourier expansions, one can expect exponential convergence, desirable for an efficient representation of turbulent dynamics.

Weight functions	Projection method
$v_j(x) = \delta(x - x_j)$	Collocation
$v_j(x) = \begin{cases} 1 & \text{if } x \in \Omega_j \\ 0 & \text{if } x \notin \Omega_j \end{cases}$	Finite-Volume
$v_j(x) = \phi_j$	Galerkin
$v_j(x) = \frac{\partial R}{\partial \hat{u}_j}$	Least-squares

Table 2.1: Examples of weight functions and projection methods

2.2 Galerkin Projection

The Galerkin projection remains a standard projection method in the context of the finite element method, where the test functions, $v(x)$, are chosen to be lie in the same functional space as the global basis functions, $\Phi(x)$. To demostrate the Galerkin projection method, we consider that the differential operator earlier in equation (2.1) as a 1D Helmholtz equation,

$$\mathbf{L}[u(x)] \equiv \frac{\partial^2 u(x)}{\partial x^2} - \lambda u(x) - f(x) = 0, \quad x \in \Omega := [0, l] \quad (2.5a)$$

$$u(0) = g_D, \quad \left. \frac{\partial u}{\partial x} \right|_{x=l} = g_N. \quad (2.5b)$$

where λ is a real positive constant, $f(x)$ is a forcing function, and Ω refers to the spatial domain bounded between 0 and l . To ensure that problem is well posed, Dirichlet and Neumann boundary conditions, g_D and g_N , are imposed at $x = 0$ and $x = l$ respectively. Equation 2.5 is commonly referred to as the strong or classical form.

The subsequent step in Galerkin projection methods is take the inner product of the equation (2.5) with a test function, $v(x)$, that satisfies the homogeneous Dirichlet boundary conditions by definition, i.e. $v(0) = 0$, and setting the inner product to zero,

$$(v(x), \mathbf{L}[u(x)]) = \int_0^l v \left[\frac{\partial^2 u(x)}{\partial x^2} - \lambda u(x) + f(x) \right] dx = 0. \quad (2.6)$$

This step is equivalent to applying the method of weighted residuals (§2.1), where $u(x)$ could refer to the approximate solution, $u^\delta(x)$. Next, we perform integration by parts,

$$\underbrace{\int_0^l \frac{\partial v}{\partial x} \frac{\partial u}{\partial x} dx}_{a(v,u)} + \underbrace{\int_0^l \lambda v u dx}_{f(v)} = \underbrace{\int_0^l v f dx}_{f(v)} + \left[v \frac{\partial u}{\partial x} \right]_0^l. \quad (2.7)$$

This equation is typically referred to as the weak ¹ form of equation (2.5). In compact notation, we define the bilinear and linear forms as,

$$a(v, u) = f(v), \quad (2.8a)$$

where $a(v, u)$ and $f(v)$ are typically referred to as the strain energy and forcing function in structural mechanics, required to remain finite. To ensure this, we restrict the choice of solutions $u(x)$ to lie in the solution space, \mathcal{U} , defined as

$$\mathcal{U} := \{u \mid u \in H^1(\Omega), u(0) = g_D\}, \quad (2.9)$$

¹The notions of the *weak* and *strong* are refers to the smoothness (regularity) required of admissible solutions. In the weak formulation, the highest derivative involved is up to first-order, so the solution space is H^1 . This space is generally larger than that of the strong formulation, which required $u \in H^2(\Omega)$. Since $H^2(\Omega) \subset H^1(\Omega)$ the weak formulation imposeds a ‘less stringent’ constraint of the solution space of admissible functions.

where $u \in H^1$ refers to functions of u belonging to Sobolev space of order 1, and satisfying the Dirichlet condition, $u(0) = g_D$, at $x = 0$.

Definition 2.2.1 (Sobolev space). We define Sobolev space of order $n \geq 1$ on Ω ,

$$H^n(\Omega) = \{u \mid u \in L_2(\Omega), D^\alpha u \in L_2(\Omega), \forall \alpha : \alpha \leq n\},$$

where $D^\alpha u$ refers to derivatives up to order α and $L_2(\Omega)$ refers to functions that are square integrable.

Definition 2.2.2 (L_2 space). The space $L_2(\Omega)$ refers to functions that are square integrable,

$$(u, u)_{L_2} = \int_{\Omega} |u(x)|^2 d\Omega < \infty. \quad (2.10)$$

We consider admissible functions up to the first derivatives, the highest order derivative in the weak formulation of equation (2.6). Similarly, the space of test functions, \mathcal{V} , is defined as,

$$\mathcal{V} := \{v \mid v \in H^1, v(0) = 0\}, \quad (2.11)$$

where $v \in H^1$ are refer to test functions belonging to the Sobolev the space of order 1, and is defined to be zero, $v(0) = 0$ on Dirichlet boundary condition, $x = 0$. The generalised weak form is therefore finding $u(x) \in \mathcal{U}$, such that

$$a(v, u) = f(v), \quad \forall v \in \mathcal{V}. \quad (2.12)$$

At this point, equation (2.12) is infinite dimension as the function spaces, \mathcal{U} and \mathcal{V} , contain infinitely many functions. To obtain an approximate solution, $u^\delta(x)$, we restrict ourselves to finite dimensional subspaces, $\mathcal{U}^\delta \subset \mathcal{U}$, and $\mathcal{V}^\delta \subset \mathcal{V}$. The problem is then to find $u^\delta \in \mathcal{U}^\delta$, such that

$$a(v^\delta, u^\delta) = f(v^\delta), \quad v^\delta \in \mathcal{V}^\delta. \quad (2.13)$$

Here, the subspaces $u^\delta \in \mathcal{U}^\delta$ and $v^\delta \in \mathcal{V}^\delta$ are not the same, compare equations (2.9) and (2.11), necessary for the standard Galerkin projection procedure where they should lie in the same subspace. To ensure that they belong to the same space, we lift the solution u^δ into two parts,

$$u^\delta = u^{\mathcal{H}} + u^{\mathcal{D}}. \quad (2.14)$$

where $u^{\mathcal{H}} \in \mathcal{V}^\delta$ satisfies the homogeneous Dirichlet condition (e.g. is zero on Dirichlet boundaries), belonging to the same subsapce as $v^\delta \in \mathcal{V}^\delta$, while $u^{\mathcal{D}} \in \mathcal{U}^\delta$ satisfies the Dirichlet boundary conditions $u^{\mathcal{D}}(0) = g_D$. Hence, the standard Galerkin projection method is to search for the homogeneous solution, $u^{\mathcal{H}} \in \mathcal{V}^\delta$, such that,

$$a(v^\delta, u^{\mathcal{H}}) = f(v^\delta) - a(v^\delta, u^{\mathcal{D}}). \quad (2.15)$$

This concludes the classical Galerkin formulation. Under certain assumptions of a , a solution is guaranteed under the Lax-Milgram theorem [Lax and Milgram, 1955].

2.3 Spectral/ hp element method

We have described the procedure for approximating a solution of a PDE using the classical Galerkin projection technique. However, the spatial discretisation scheme, related to the choice of basis (and test) functions, remains undiscussed. In this section, we discuss the spectral/ hp element method [Patera, 1984], where the solution is partitioned into a set of non-overlapping finite elements of size h , consisting of a linear combination of continuous orthogonal polynomial functions up to order P . It leverages the geometric flexibility of classical finite-element methods, allowing for the representation of complex engineering geometries, and the exponential (spectral) convergence properties of classical spectral methods, where the solution error decreases exponentially. Suppose we consider $P + 1$ linearly independent polynomials spanning the polynomial space of \mathcal{P}_P , the error of a smooth solution with element size of h and polynomial order P has the property of [Karniadakis and Sherwin, 2005],

$$\|u(x) - u^\delta(x)\| \leq Ch^P \|u(x)\| \approx O(h^P). \quad (2.16)$$

where C is some constant. Equation 2.16 implies that the error decreases linearly with h , and exponentially with P . This section is organised into domain partition, standard elements, assembly process, modal and nodal expansion functions, numerical integration and differentiation, concluding with an example in 1D.

2.3.1 Domain partition

The first step concerns the partitioning the domain into a set of (finite) elemental regions. We consider an example in one dimension within Ω , and partition it into a set of N_{el} elements, where Ω^e , refers to the elemental partitions with $1 \geq e \geq N_{el}$, such that they meet at their boundaries and do not overlap,

$$\Omega = \bigcup_{e=1}^{N_{el}} \Omega^e, \quad \text{where } \bigcap_{e=1}^{N_{el}} \Omega^e = \emptyset \quad (2.17)$$

where the e^{th} element is defined as,

$$\Omega^e = \{x \mid x_{e-1} \geq x \geq x_e\}. \quad (2.18)$$

Each element can be represented by a linear combination of orthogonal basis expansions. The basis expansions can be either modal or nodal expansions, as we shall see later.

2.3.2 Standard Elements

In general, we expect to work with non-uniform elements that may have arbitrarily shapes, making the definition of basis expansions potentially unwieldy. To simplify the formulation, it is convenient to define a *standard* element,

$$\Omega_{st} = \{\xi \mid -1 \geq \xi \geq 1\}, \quad (2.19)$$

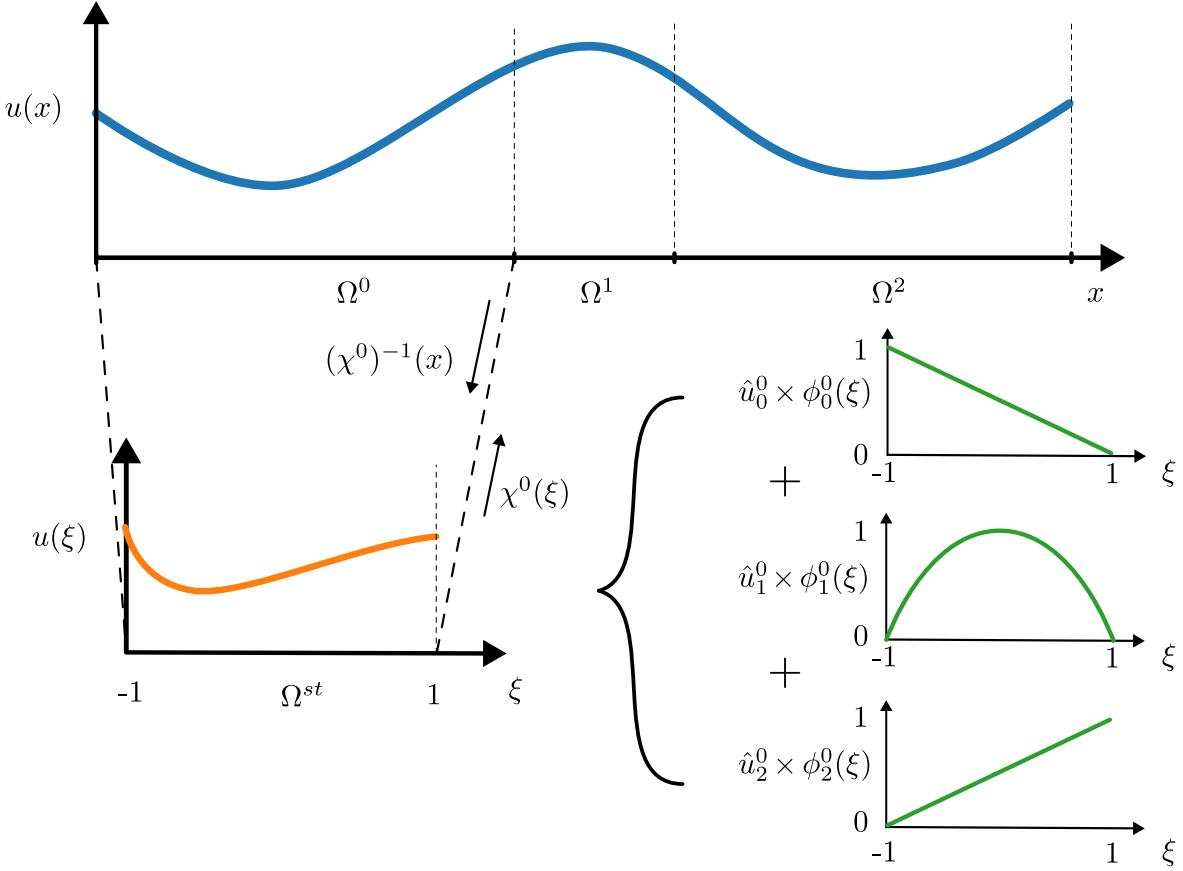


Figure 2.1: A spectral/ hp element representation of $u(x)$, consisting of three non-overlapping finite elements, each containing a linear combination of local expansion bases of up to $P = 2$.

where Ω_{st} refers to the standard element defined in local coordinates, $\xi \in [-1, 1]$. Within this standard element, the formulation of basis expansions, as well as differential and integration operations, can be carried out in the local coordinate system ξ , before mapping the solution back to the global domain, x . We can map the standard element into any arbitrary global coordinates based on a linear mapping $\chi^e : \Omega_{st} \rightarrow \Omega$,

$$x = \chi^e(\xi) = \frac{1 - \xi}{2}x_e + \frac{1 + \xi}{2}x_{e+1}, \quad \xi \in \Omega_{st} \quad (2.20)$$

which has an analytical inverse, $(\chi^e)^{-1}(x)$,

$$\xi = (\chi^e)^{-1}(x) = 2 \frac{x - x_{e-1}}{x_e - x_{e-1}} - 1, \quad x \in \Omega^e. \quad (2.21)$$

For illustration purposes, we consider that the standard element can be represented by three local basis expansions of polynomial order of up to $P = 2$,

$$\phi_0^e(\xi) = \frac{1 - \xi}{2}, \quad \phi_1^e(\xi) = (1 + \xi)(1 - \xi), \quad \phi_2^e(\xi) = \frac{1 + \xi}{2}, \quad (2.22)$$

where ϕ_0^e, ϕ_1^e and ϕ_2^e refers to the linear and quadratic local basis expansions of the e^{th} element. These local basis expansions is illustrated in figure 2.1. We note that the formulations of local basis

expansion here is merely an example. In practice, the local basis expansions are usually chosen to have orthogonality properties under a certain inner product. The approximate solution is now represented as,

$$u^\delta(x) = \sum_{e=0}^{N_{el}-1} \sum_{i=0}^P \hat{u}_i^e \phi_i^e(\chi^e(\xi)). \quad (2.23)$$

where \hat{u}_i^e refers to the local expansion basis coefficients. The approximate solution, $u^\delta(x)$, now lie within the solution space \mathcal{U}^δ defined as,

$$\mathcal{U}^\delta := \{u^\delta \mid u^\delta \in H^1, u^\delta(\chi^e(\xi)) \in \phi_i^e(\xi), \forall i : 0 \leq i \leq P, \forall e : 0 \leq e \leq N_{el}\} \quad (2.24)$$

2.3.3 Global assembly

In this section, we introduce the concept of global assembly (or direct stiffness summation) which relates the global basis expansions (equation (2.2)), $\Phi_i(x)$, to the local basis expansions (equation (2.23)), $\phi_i^e(x)$, where the solution can be approximated using either formulation,

$$u^\delta(x) = \sum_{i=0}^{N-1} \hat{u}_i \Phi_i(x) = \sum_{e=0}^{N_{el}-1} \sum_{i=0}^P \hat{u}_i^e \phi_i^e(\chi^e(\xi)). \quad (2.25)$$

In general, we can represent the global and local basis coefficients each as a column vector,

$$\hat{\mathbf{u}}_g = \begin{pmatrix} \hat{u}_0 \\ \vdots \\ \hat{u}_N \end{pmatrix}, \quad \hat{\mathbf{u}}_l = \begin{pmatrix} \hat{\mathbf{u}}^0 \\ \vdots \\ \hat{\mathbf{u}}^{N_{el}-1} \end{pmatrix}, \quad (2.26)$$

where $\hat{\mathbf{u}}^e = (\hat{u}_0^e, \dots, \hat{u}_P^e)^T$, $\hat{\mathbf{u}}_g \in \mathbb{R}^N$, $\hat{\mathbf{u}}_l \in \mathbb{R}^{N_{loc}}$ and $N_{loc} = N_{el}(P + 1)$. As there can be more global degrees of freedom than local degrees of freedom, $N > N_{loc}$, we need to impose some conditions on the local expansion coefficients. One of the common approach is to enforce C^0 continuity across elemental boundaries, referred to as the continuous Galerkin projection. Following the definition of local basis expansions in equation (2.22), this condition can be supplemented using,

$$\hat{u}_P^{e-1} = \hat{u}_0^e. \quad (2.27)$$

The graphical representation of this condition enforcing C^0 continuity between the element boundaries for three finite elements with $P = 2$ local basis expansions, and the relationship between global and local basis coefficients are shown in figure 2.2. We can relate the global and local basis coefficients with an assembly matrix, $\mathbf{A} \in \mathbb{R}^{N_{loc} \times N}$,

$$\hat{\mathbf{u}}_l = \mathbf{A} \hat{\mathbf{u}}_g. \quad (2.28)$$

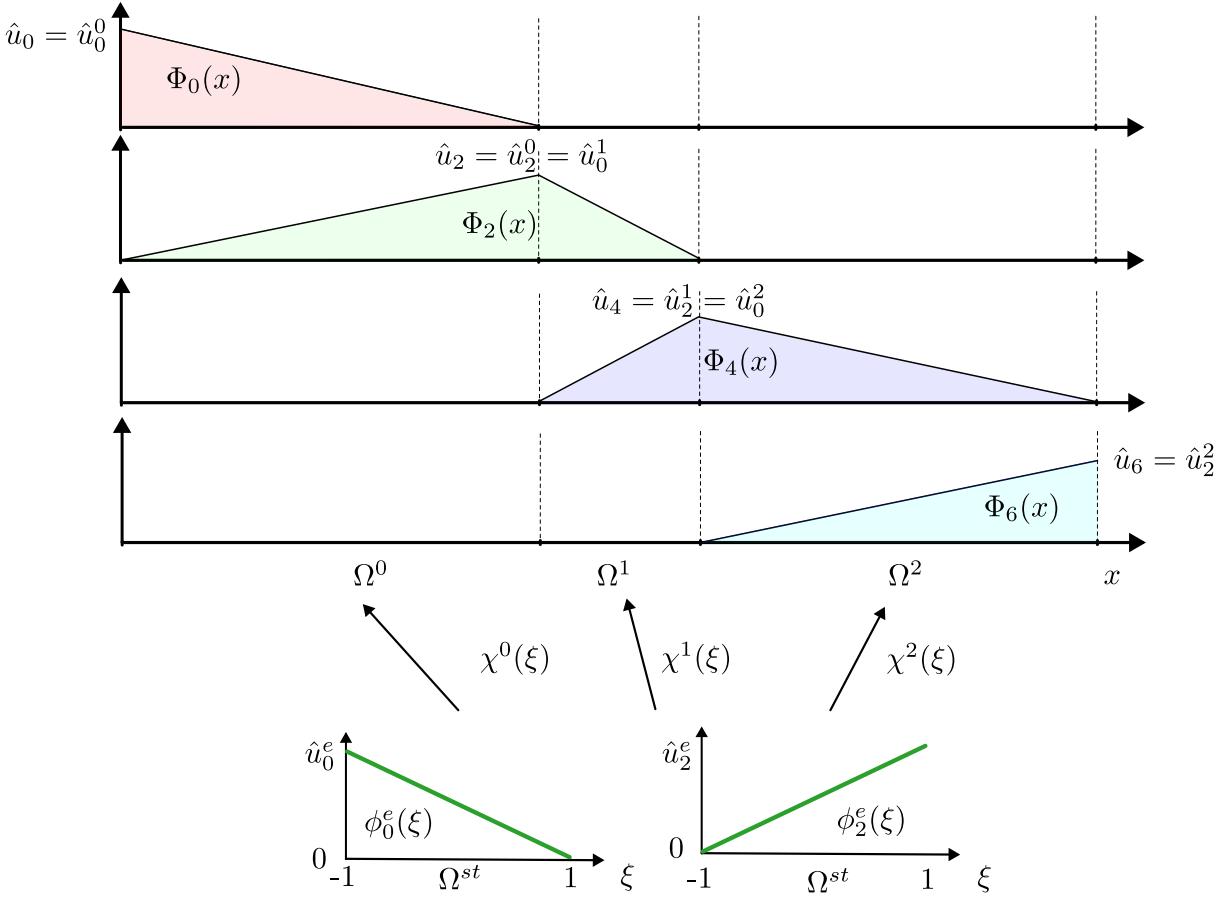


Figure 2.2: A graphical representation of C^0 across elemental boundaries and the relationship between local basis coefficients, u_0^e, u_2^e , and global basis expansions, u_i .

In the case for $P = 2$ and three finite elements as in the case of figures 2.1 and 2.2, the assembly matrix and the vectors of global and local basis coefficients are given as,

$$\hat{\mathbf{u}}_l = \begin{pmatrix} \hat{u}_0^0 \\ \hat{u}_1^0 \\ \hat{u}_2^0 \\ \hat{u}_0^1 \\ \hat{u}_1^1 \\ \hat{u}_2^1 \\ \hat{u}_0^2 \\ \hat{u}_1^2 \\ \hat{u}_2^2 \end{pmatrix}, \quad \mathbf{A} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}, \quad \hat{\mathbf{u}}_g = \begin{pmatrix} \hat{u}_0 \\ \hat{u}_1 \\ \hat{u}_3 \\ \hat{u}_4 \\ \hat{u}_5 \\ \hat{u}_6 \end{pmatrix}, \quad (2.29)$$

The assembly matrix \mathbf{A} ‘scatters’ the global degrees of freedom to local degrees of freedom, while the transpose of it, \mathbf{A}^T , performs the reverse, referred to as global assembly. For example, we wish to perform integration in the domain Ω ,

$$\mathbf{I}_g[j] = (\Phi_j(x), u^\delta(x)), \quad (2.30)$$

where $\mathbf{I}_g \in \mathbb{R}^N$ refers to a vector containing the integral between $\Phi_i(x)$ and $u^\delta(x)$. This is related to first performing integration using local expansion basis within standard elements, and then assembling using \mathbf{A}^T ,

$$\mathbf{I}_g = \mathbf{A}^T \mathbf{I}_l, \quad (2.31a)$$

where,

$$\mathbf{I}_g = \begin{bmatrix} \mathbf{I}_0 \\ \vdots \\ \mathbf{I}_{N_g-1} \end{bmatrix}, \quad \mathbf{I}_l = \begin{bmatrix} \mathbf{I}^0 \\ \vdots \\ \mathbf{I}^{N_{el}-1} \end{bmatrix}, \quad \text{with} \quad \mathbf{I}^e = \begin{bmatrix} \int_{-1}^1 \phi_0^e(\xi) u(\chi^e) \frac{d\chi^e}{d\xi} d\xi \\ \vdots \\ \int_{-1}^1 \phi_{P-1}^e(\xi) u(\chi^e) \frac{d\chi^e}{d\xi} d\xi \end{bmatrix}, \quad (2.31b)$$

and $\mathbf{I}_l \in \mathbb{R}^{N_{loc}}$ refer to the vector of integration operations performed within a standard element. In the spectral/ hp element approach, we perform integration and differentiation using local basis expansions within a standard element. After doing so, we assemble the local operations from the standard element to the global domain by using \mathbf{A}^T , as we shall show later using a 1D example. We note that the structure of assembly matrix is generally sparse, where the entries either contain 0, 1 or -1 in multidimensional formulation. Therefore, the assembly matrix is not constructed in practice, and a mapping array is used instead.

2.3.4 Local basis expansions

The choice of local basis expansions, $\phi_i^e(\xi)$, concerns the representation of the solution, and the convergence properties of the numerical solver, in particular, the condition number of the mass and laplacian matrices. In general, the local basis expansions can be classified into two groups, either *modal* or *nodal* expansions.

Modal expansions

Modal expansions, or hierarchical expansions, describes a set of expansion basis where an expansion set (\mathcal{X}_{P-1}^δ) of order $P - 1$, is contained within a set (\mathcal{X}_P^δ) of order P , e.g. $\mathcal{X}_{P-1}^\delta \subset \mathcal{X}_P^\delta$. An example of modal expansions are the Jacobi polynomials, $P_p^{\alpha,\beta}(x)$, representing a family of solutions to the Sturm-Liouville problem within, $x \in [-1, 1]$. The Jacobi polynomials become symmetric for $\alpha = \beta$, referred to ultraspheric polynomials. Special cases of ultraspheric polynomials are the Legendre polynomials, $\alpha = \beta = 1$, and the Chebyshev polynomials, $\alpha = \beta = 1/2$. Within the Nektar++ framework, we utilise the *modified* basis, constructed using on the Jacobi polynomials and modified (hence its name) by linear expansions given as,

$$\phi_p(\xi) \rightarrow \psi_p(\xi) = \begin{cases} \frac{1-\xi}{2} & \text{for } p = 0 \\ \left(\frac{1-\xi}{2}\right) \left(\frac{1+\xi}{2}\right) P_{p-1}^{1,1}(\xi) & \text{for } 0 < p < P \\ \frac{1+\xi}{2} & \text{for } p = P, \end{cases} \quad (2.32)$$

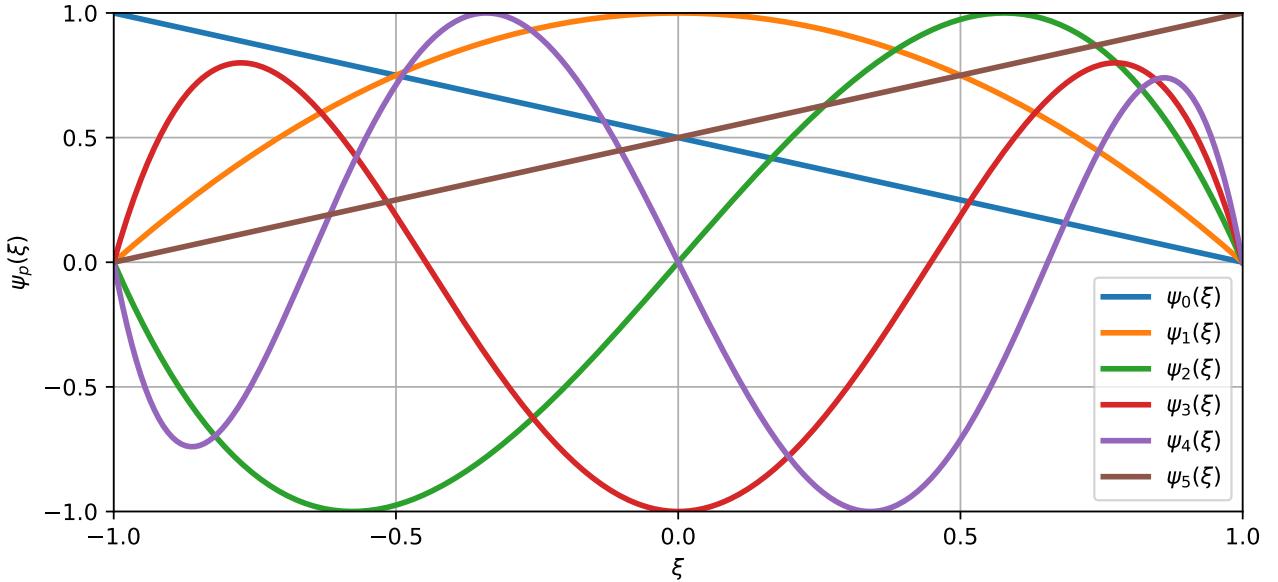


Figure 2.3: The modified basis for up to $P = 5$ normalised to $-1 \leq \psi_p \leq 1$.

We note that $\phi_p(\xi)$ refers to a general local expansion basis while $\psi_p(\xi)$ to definition of the modified basis. The one-dimensional expansion modes of the modified basis of up to $P = 5$ is shown in figure 2.3. The linear modes, corresponding to $p = 0$ and $p = P$, are the only expansions which has a magnitude of at the boundaries, referred to as boundary modes. The modified basis for $0 < p < P$, are clearly hierarchical, and have non-zero values except at the boundaries, referred to as interior/bubble modes.

Nodal expansions

Nodal expansions are basis expansions that are non-hierarchical, $\mathcal{X}_{P-1}^\delta \not\subset \mathcal{X}_P^\delta$. An example of nodal expansions are the Lagrange polynomials,

$$\phi_p(\xi) \rightarrow h_p(\xi) = \frac{\prod_{q=0, q \neq p}^P (\xi - \xi_q)}{\prod_{q=0, q \neq p}^P (\xi_p - \xi_q)} \quad (2.33)$$

The Lagrange polynomials, $h_p(\xi)$, are particular attractive as it has a unit value at discrete nodal values, ξ_q , and zero everywhere else, $h_p(\xi_q) = \delta_{pq}$, which implies that

$$u^\delta(\xi_q) = \sum_{p=0}^P \hat{u}_p h_p(\xi_q) = \sum_{p=0}^P \hat{u}_p \delta_{pq} = \hat{u}_q, \quad (2.34)$$

where the Lagrange coefficient \hat{u}_q is the same as the value evaluated at the node ξ_q . The nodal values, ξ_q , are based on the Gauss-Lobatto-Legendre (GLL) points which will be defined later in §2.3.5. Figure 2.4 presents Lagrange expansions evaluated along the GLL points.

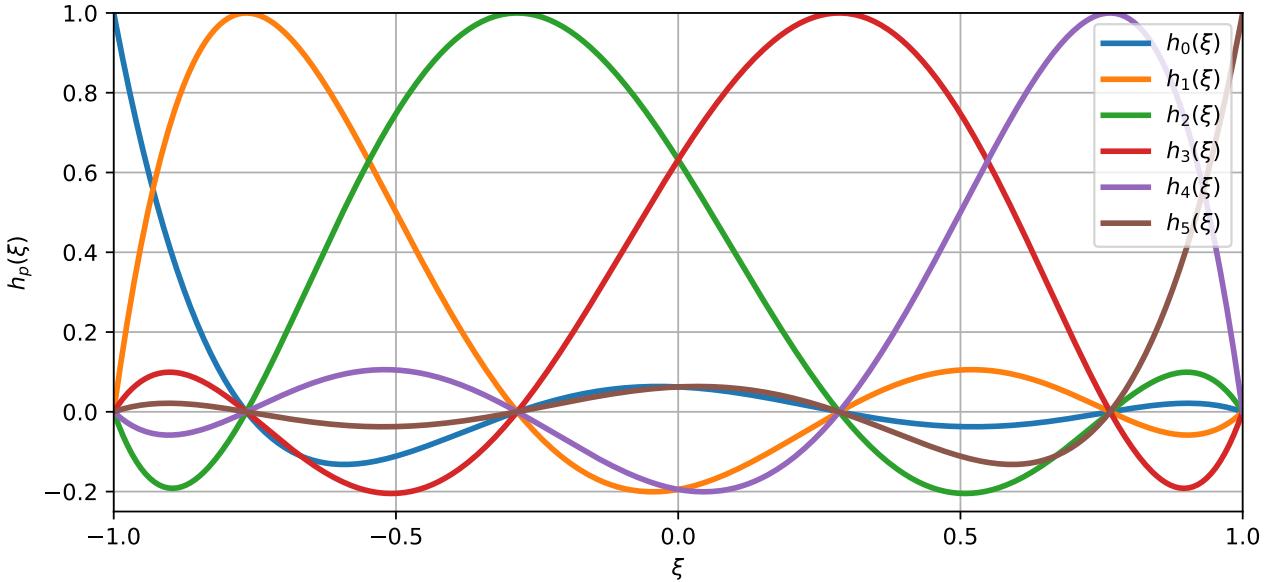


Figure 2.4: Lagrange polynomials for $P = 5$ with nodal values along GLL points.

Multi-dimensional expansions

We have introduced modal and nodal expansions in one dimension, and its extension to multi-dimensions bases can be generalised using a tensorial expansion of the local expansion bases. The standard element in a two dimensional quadrilateral, \mathcal{Q}^2 , and a three dimensional hexahedral \mathcal{H}^3 , are given as,

$$\mathcal{Q}^2 = \{-1 \leq \xi_1, \xi_2 \leq 1\}, \quad \mathcal{H}^3 = \{-1 \leq \xi_1, \xi_2, \xi_3 \leq 1\} \quad (2.35)$$

where ξ_1, ξ_2, ξ_3 refers to the local coordinates in multi-dimensions. Thus, the multi-dimensional expansion bases for quadrilaterals and hexadrals using modified bases are simply a tensor product of the one dimensional modified bases,

$$\phi_{pq}(\xi_1, \xi_2) = \psi_q(\xi_1)\psi_q(\xi_2), \quad \text{and} \quad \phi_{pqr}(\xi_1, \xi_2, \xi_3) = \psi_q(\xi_1)\psi_q(\xi_2)\psi_r(\xi_3). \quad (2.36)$$

An example of the modal tensorial bases, for $p = q = 4$ in a standard quadrilateral element is shown in figure 2.5. While we have discussed the tensorial the expansions for regular domains such as the standard quadrilateral and hexahedral elements, the extensions for simplex domains such as triangles, tetrahedrals, prisms and pyramids commonly used to represent complex geometries, are less straightforward. The challenge for simplexes is that the local coordinates, ξ_1, ξ_2, ξ_3 , become dependent where a direct tensorial expansion becomes unwieldy. Instead, a collapsed coordinate system is introduced, providing a transformation from a standard simplex element to a standard regular element. In this thesis, we utilise quadrilateral elements. The reader is referred to [Karniadakis and Sherwin \[2005\]](#) for more details about the multi-dimensional formulation of regular and simplex elements.

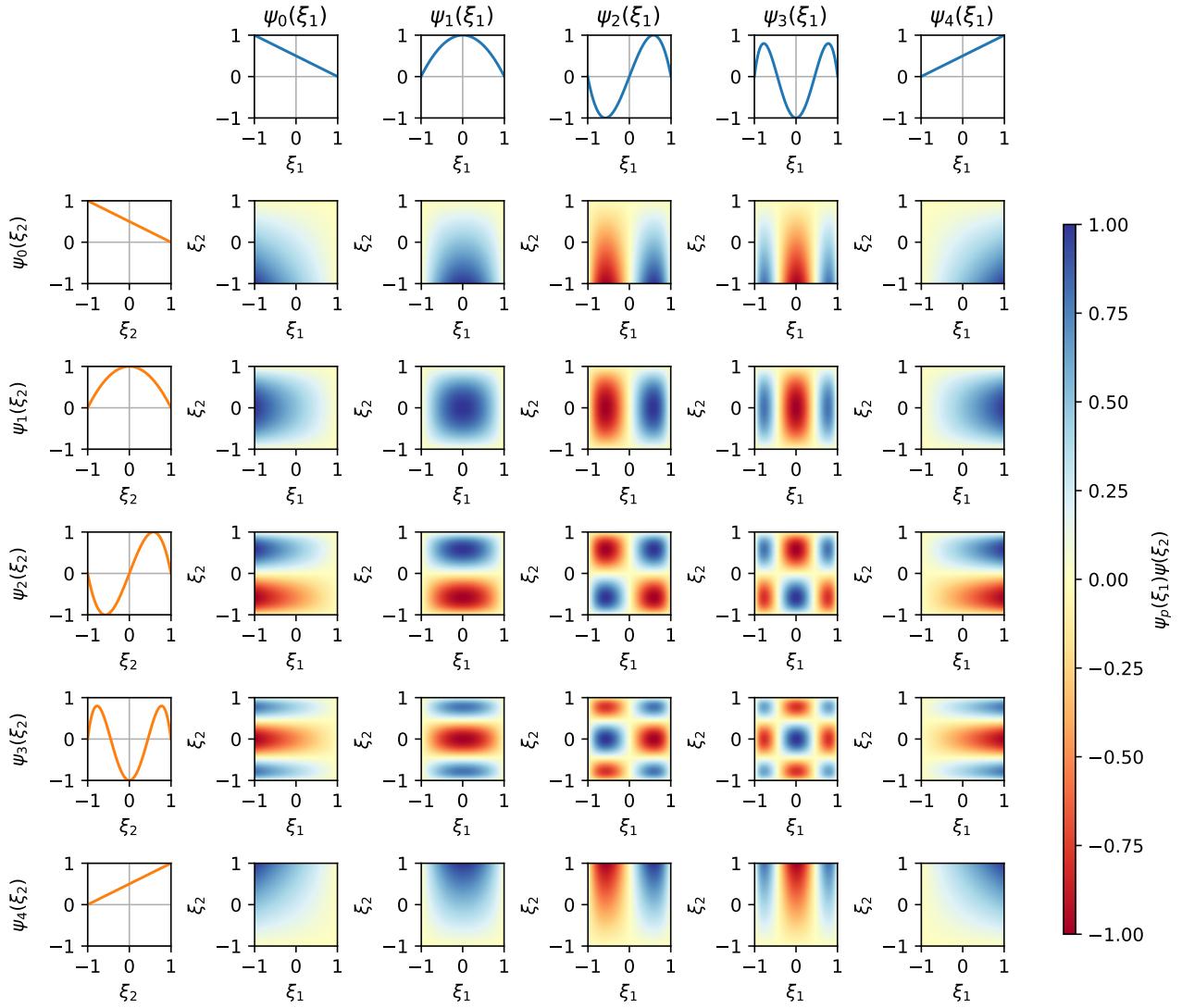


Figure 2.5: Two dimensional modified basis with $p = q = 4$ in a standard quadrilateral, $-1 \leq \xi_1, \xi_2 \leq 1$. The modified bases are normalised to $-1 \leq \phi_{pq} \leq 1$.

2.3.5 Gaussian quadrature

In the Galerkin formulation, we perform integration between basis functions routinely, and an efficient numerical technique is sought after. Suppose we want to approximate the integral of a function, $u(\xi)$, in a standard element numerically given as,

$$\int_{-1}^1 u(\xi) \, d\xi = \sum_{i=0}^{Q-1} w_i u(\xi_i) + R(u). \quad (2.37)$$

The premise is determine the optimal number of quadrature points, Q , integration weights, w_i , and zeros, ξ_i , in which the integral error, $R(u)$, can be minimised. If $u(\xi)$ is of polynomial order of P , we may expect that we require at least $P + 1$ equispaced points to represent $u(\xi)$ sufficiently. Using Gaussian quadrature rules, we can approximate an integral of a function of order P , with far fewer than $P + 1$ points with specific integration weights and zeros. In general, Gaussian quadrature rules

can be grouped into three categories: Gauss, Gauss-Radau and Gauss-Lobatto quadrature. The main difference between the three categories are on the inclusion of the end points. Gauss quadrature rule evaluates the integral without the end points $\xi = \pm 1$. Gauss-Radau quadrature rule either select one of the end points, typically at $\xi = -1$. Gauss-Lobatto quadrature rule consider both end points. We will only focus on describing the Gauss-Lobatto quadrature rules and the zeros of Jacobi polynomials known as the Gauss-Lobatto-Jacobi quadrature rules given as,

$$\xi_i^{\alpha,\beta} = \begin{cases} -1 & i = 0, \\ \xi_{i-1,Q-2}^{\alpha+1,\beta+1} & i = 1, \dots, Q-2, \\ 1, & i = Q-1, \end{cases} \quad (2.38a)$$

$$w_i^{\alpha,\beta} = \begin{cases} (\beta + 1)C_{0,Q-2}^{\alpha,\beta}, & i = 0, \\ C_{i,Q-2}^{\alpha,\beta}, & i = 1, \dots, Q-2, \\ (\alpha + 1)C_{Q-1,Q-2}^{\alpha,\beta}, & i = Q-1, \end{cases} \quad (2.38b)$$

$$C_{i,Q-2}^{\alpha,\beta} = \frac{2^{\alpha+\beta+1}\Gamma(\alpha+Q)\Gamma(\beta+Q)}{(Q-1)(Q-1)!\Gamma(\alpha+\beta+Q+1)[P_{Q-1}^{\alpha,\beta}(\xi_i)]^2} \quad (2.38c)$$

where $w_i^{\alpha,\beta}$, $\xi_i^{\alpha,\beta}$ are the zeros (or sometimes referred to as quadrature points) and weights of the Gauss-Lobatto-Jacobi quadrature rules, and Γ refers to the Gamma function. For $\alpha = \beta = 0$, the quadrature points is known as the Gauss-Lobatto-Legendre (GLL) points, typically employed for Lagrange polynomials. By evaluating the integral using the zeros and integrations weights defined above, we can obtain an exact integral of the function $u(\xi)$, of polynomial order P , with at least $Q \geq (P+3)/2$ quadrature points.

2.3.6 Numerical differentiation

In the same fashion as Gaussian quadrature rules, we want to evaluate the derivative of a function, $u^\delta(\xi)$ numerically. Suppose that we want to differentiate in x using local coordinates given as,

$$\frac{du^\delta(\xi)}{dx} = \frac{du^\delta(\xi)}{d\xi} \frac{d\xi}{dx} = \sum_{p=0}^P \hat{u}_p \frac{d\phi_p(\xi)}{d\xi} \frac{d\xi}{dx}, \quad (2.39)$$

where $d\xi/dx$ is the jacobian. The main step in involves evaluating the derivative of the local expansion bases, $d\phi_p(\xi)/d\xi$, referred to as collocation differentiation as differentiation is performed in physical space. Suppose that we express the solution of polynomial order P with modified polynomials, $\phi_p(\xi) \rightarrow \psi_p(\xi)$, through a set of $Q \geq P+1$ quadrature points, the derivative in discrete local coordinates is expressed as,

$$\left. \frac{du^\delta(\xi)}{d\xi} \right|_{\xi=\xi_i} = \sum_{j=0}^{Q-1} \hat{u}_j \left. \frac{d\psi_j(\xi)}{d\xi} \right|_{\xi=\xi_i} = \sum_{j=0}^{Q-1} D_{ij} \hat{u}_j, \quad (2.40)$$

where D_{ij} refers to the differential matrix containing values of the derivative of the basis at discrete quadrature points given as,

$$D_{ij} = \frac{dh_j(\xi)}{d\xi} \Big|_{\xi=\xi_i}, \quad (2.41)$$

which is often pre-computed. To differentiate a function, $u(\xi)$, we typically need to construct the differential matrices, and the general representation of the differential matrix is,

$$D_{ij} = \begin{cases} \frac{p'_Q(\xi_i)}{p'_Q(\xi_j)} \frac{1}{\xi_i - \xi_j}, & i \neq j, \\ \frac{p''_Q(\xi_i)}{2p'_Q(\xi_i)}, & i = j. \end{cases} \quad (2.42)$$

where $p'_Q(\xi_i), p''_Q(\xi_i)$ refers to the first and second differentiative of Jacobi polynomials evaluated at the quadrature points ξ_i .

2.3.7 Example in 1D

We have outlined the basic formulation of spectral/ hp element methods in a single dimension. To conclude the section on spectral/ hp element methods, we will describe its solution procedure, converting the weak form of the Helmholtz equation into a system of linear equations, and introduce the mass and laplacian matrices. Starting from the weak form,

$$\underbrace{\lambda \int_{-1}^1 v^\delta u^H d\xi}_{\mathbf{M}^e \hat{\mathbf{u}}^e} + \underbrace{\int_{-1}^1 \frac{\partial v^\delta}{\partial \xi} \frac{\partial u^H}{\partial \xi} d\xi}_{\mathbf{L}^e \hat{\mathbf{u}}^e} = \underbrace{\int_{-1}^1 v^\delta f d\xi}_{\hat{\mathbf{f}}^e} - \underbrace{\int_{-1}^1 \frac{\partial v^\delta}{\partial \xi} \frac{\partial u^D}{\partial \xi} d\xi}_{\mathbf{L}^0} + v(l)g_N, \quad (2.43)$$

we wish to seek the solution $u^H(\xi)$. Recall that the solution space of $u^H(\xi)$ and $v^\delta(\xi)$ are the same, following the standard Galerkin projection procedure. Suppose they can be discretised by spectral/ hp elements with e elements and local basis expansions of up to polynomial order P ,

$$u^H(\xi) = \sum_{i=0}^P \hat{u}_i^e \phi_i^e(\xi), \quad v^\delta(\xi) = \sum_{i=0}^P \hat{v}_i^e \phi_i^e(\xi). \quad (2.44)$$

Substituting into equation (2.43) and evaluating the first term on the left hand side through a set of Q quadrature points.

$$\begin{aligned} \int_{-1}^1 \sum_{i=0}^P \hat{v}_i^e \phi_i^e(\xi) \sum_{i=0}^P \hat{u}_i^e \phi_i^e(\xi) d\xi &= \sum_{q=0}^{Q-1} \left[\sum_{i=0}^P \hat{v}_i^e \phi_i^e(\xi_q) \sum_{i=0}^P \hat{u}_i^e \phi_i^e(\xi_q) \right] w_q^e \\ &= (\hat{\mathbf{v}}^e)^T (\mathbf{B}^e)^T \mathbf{W}^e \mathbf{B}^e \hat{\mathbf{u}}^e \\ &= \hat{\mathbf{v}}^T \mathbf{M}^e \hat{\mathbf{u}}^e \end{aligned} \quad (2.45)$$

where $\mathbf{M}^e = (\mathbf{B}^e)^T \mathbf{W} \mathbf{B}^e \in \mathbb{R}^{(P+1) \times (P+1)}$ refers to the elemental mass matrix, while $\mathbf{B}^e \in \mathbb{R}^{Q \times (P+1)}$ refers to the elemental basis matrix, and $\mathbf{W}^e \in \mathbb{R}^{Q \times Q}$, the elemental weight matrix, a diagonal matrix

consisting of discrete integration weights along Q quadrature points.

$$\mathbf{B}^e = \begin{bmatrix} \phi_0(\xi_0) & \cdots & \phi_P(\xi_0) \\ \vdots & \ddots & \vdots \\ \phi_0(\xi_Q) & \cdots & \phi_P(\xi_Q) \end{bmatrix}, \quad \mathbf{W}^e = \begin{bmatrix} w_0^e & & 0 \\ & \ddots & \\ 0 & & w_{Q-1}^e \end{bmatrix} \quad (2.46)$$

Next, we move onto the second term on the left hand side,

$$\begin{aligned} \int_{-1}^1 \sum_{i=0}^P \hat{v}_i^e \frac{d\phi_i^e}{d\xi} \sum_{i=0}^P \hat{u}_i^e \frac{d\phi_i^e}{d\xi} d\xi &= \sum_{q=0}^Q \left[\sum_{i=0}^P \hat{v}_i^e D_{qi}^e \phi_i^e(\xi_q) \sum_{i=0}^P \hat{u}_i^e D_{qi}^e \phi_i^e(\xi_q) \right] w_q^e \\ &= \hat{\mathbf{v}}^T (\mathbf{B}^e)^T (\mathbf{D}^e)^T \mathbf{W}^e \mathbf{D}^e \mathbf{B}^e \hat{\mathbf{u}}^e \\ &= \hat{\mathbf{v}}^T \mathbf{L}^e \hat{\mathbf{u}}^e \end{aligned} \quad (2.47)$$

where $\mathbf{L}^e = (\mathbf{B}^e)^T (\mathbf{D}^e)^T \mathbf{W}^e \mathbf{D}^e \mathbf{B}^e \in \mathbb{R}^{(P+1) \times (P+1)}$ refers to the elemental Laplacian matrix while $\mathbf{D}^e \in \mathbb{R}^{Q \times (P+1)}$ refers to the differential matrix defined in equation (2.42). Moving onto the first term on the right hand side,

$$\begin{aligned} \int_{-1}^1 \sum_{i=0}^P \hat{v}_i^e \phi_i^e(\xi) f^e(\xi) d\xi &= \sum_{q=0}^P \sum_{i=0}^P \hat{v}_i^e \phi_i^e(\xi_q) f^e(\xi_q) w_q^e, \\ &= \hat{\mathbf{v}}^T (\mathbf{B}^e)^T \mathbf{W}^e \mathbf{f}^e \\ &= \hat{\mathbf{v}}^T \hat{\mathbf{f}}^e, \end{aligned} \quad (2.48)$$

where $\hat{\mathbf{f}}^e$, is referred to the elemental forcing vector. As we bolt the elemental laplacian, mass matrices, and forcing vector, the system of linear equations within a standard element is given as,

$$[\lambda \mathbf{M}^e + \mathbf{L}^e] \hat{\mathbf{u}}^e = \hat{\mathbf{f}}^e. \quad (2.49)$$

We note that the boundary conditions have been omitted. To include the boundary conditions, we consider the full system of linear of equations consisting of e number of elements,

$$\lambda \underbrace{\begin{bmatrix} \mathbf{M}^0 + \mathbf{L}^0 & \mathbf{0} \\ \mathbf{0} & \ddots \\ \mathbf{0} & \mathbf{M}^{N_{el}-1} + \mathbf{L}^{N_{el}-1} \end{bmatrix}}_{\mathbf{M}_l + \mathbf{L}_l} \underbrace{\begin{bmatrix} \hat{\mathbf{u}}^0 \\ \vdots \\ \hat{\mathbf{u}}^{N_{el}-1} \end{bmatrix}}_{\hat{\mathbf{u}}_l} = \underbrace{\begin{bmatrix} \hat{\mathbf{f}}^0 \\ \vdots \\ \hat{\mathbf{f}}^{N_{el}-1} \end{bmatrix}}_{\hat{\mathbf{f}}_l} + \underbrace{\begin{bmatrix} \mathbf{L}^0 g_D \\ \vdots \\ \mathbf{0} \end{bmatrix}}_{\mathbf{g}_D} + \underbrace{\begin{bmatrix} \mathbf{0} \\ \vdots \\ g_N \end{bmatrix}}_{\mathbf{g}_N}, \quad (2.50)$$

where $\mathbf{M}_l \in \mathbb{R}^{N_{el}(P+1) \times N_{el}(P+1)}$, $\mathbf{L}_l \in \mathbb{R}^{N_{el}(P+1) \times N_{el}(P+1)}$, $\hat{\mathbf{u}}_l \in \mathbb{R}^{N_{el}(P+1)}$ refers to the local mass matrix, local laplacian matrix and the vector of local expansion coefficients. On the right hand side, $\hat{\mathbf{f}}_l \in \mathbb{R}^{N_{el}(P+1)}$, $\mathbf{g}_D^{N_{el}(P+1)}$, $\mathbf{g}_N^{N_{el}(P+1)}$ refers local forcing vector, Dirichlet and Neumann boundary conditions in vector form. Lastly, to ensure that the solution remains C^0 continuous across the elemental

boundaries, we perform the assembly process by using the assemble matrices (see §2.3.3),

$$\lambda \mathbf{A}^T (\mathbf{M}_l + \mathbf{L}_l) \mathbf{A} \hat{\mathbf{u}}_g = \mathbf{A}^T (\hat{\mathbf{f}}^l + \mathbf{g}_D + \mathbf{g}_N), \quad (2.51)$$

and obtain the solution for $\hat{\mathbf{u}}_g$.

2.4 Numerical techniques for solving the Navier-Stokes equations

2.4.1 Velocity Correction Scheme

The spatial discretisation of the Helmholtz operator and its numerical solution procedure has been discussed using the spectral/ hp element methods. Here, we describe the numerical methods that is used to solve the Navier-Stokes equations given as,

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\nabla p + \nu \nabla^2 \mathbf{u} + \mathbf{f} \quad (2.52a)$$

$$\nabla \cdot \mathbf{u} = 0, \quad (2.52b)$$

with boundary conditions,

$$\mathbf{u} = 0, \quad \text{on } \partial\Omega. \quad (2.52c)$$

Here, the primitive variables are velocity and pressure (\mathbf{u}, p) and we assumed unit density, $\rho = 1$, with the kinematic viscosity appearing as the control parameter. The time evolution of velocity is explicit expressed in equation (2.52a), but does not appear for the pressure, which is coupled to the velocity field, enforcing the incompressibility condition. Several strategies exist for addressing the coupled velocity-pressure fields by

1. Solving the coupled system such as the Uzawa algorithm,
2. Splitting methods,
3. Change of coordinates (e.g. vorticity-streamfunction approach).

We adopt splitting methods, which solves the of the Navier-Stokes equation by splitting them into ‘subequations’, and solving them sequentially. These methods, belonging to the broader family of projection methods introduced by Chorin [1967] and Témam [1969], and can be further classified into pressure-correction or velocity-correction schemes. This thesis employs the use of the high-order velocity-correction scheme introduced by Karniadakis et al. [1991]. We rewrite the incompressible Navier-Stokes equations in semi-discrete form with using linear and nonlinear operators as,

$$\frac{\partial \mathbf{u}}{\partial t} = \mathbf{N}(\mathbf{u}) - \nabla p + \nu \mathbf{L}(\mathbf{u}), \quad (2.53a)$$

$$\nabla \cdot \mathbf{u} = 0, \quad (2.53b)$$

with boundary conditions,

$$\mathbf{u}|_{\Omega} = 0, \quad \mathbf{u}(t = 0) = \mathbf{u}_0. \quad (2.53c)$$

The nonlinear, \mathbf{N} , linear, \mathbf{L} , operators are obtained from a suitable spatial-discretisation method such as the spectral/ hp element method. The nonlinear and linear operators are defined as,

$$\mathbf{N}(\mathbf{u}) \equiv -(\mathbf{u} \cdot \nabla)\mathbf{u} = -\frac{1}{2}[(\mathbf{u} \cdot \nabla)\mathbf{u} + \nabla \cdot (\mathbf{u}\mathbf{u})], \quad \mathbf{L}(\mathbf{u}) \equiv \nabla^2\mathbf{u}, \quad (2.54)$$

We note that the nonlinear terms are written in the skew-symmetric to minimise aliasing errors [Karniadakis et al., 1991]. To advance the velocity at time step, \mathbf{u}^n , to the next time step, \mathbf{u}^{n+1} , we integrate equation (2.53) over a time step Δt ,

$$\mathbf{u}^{n+1} - \mathbf{u}^n = \underbrace{\int_{t_n}^{t_{n+1}} \mathbf{N}(\mathbf{u}) dt}_{\Delta t \sum_{q=0}^{J_e-1} \beta_q \mathbf{N}(\mathbf{u}^{n-q})} - \underbrace{\int_{t_n}^{t_{n+1}} \nabla p dt}_{\Delta t \nabla \bar{p}^{n+1}} + \nu \underbrace{\int_{t_n}^{t_{n+1}} \mathbf{L}(\mathbf{u}) dt}_{\Delta t \sum_{q=0}^{J_i-1} \gamma_q \mathbf{L}(\mathbf{u}^{n+1-q})}. \quad (2.55)$$

The velocity correction scheme evaluates the underbraced terms in three successive independently from left to right independently, effectively ‘splitting’ equation (2.53) from this point onwards. The first step we perform is to extrapolate the advection velocities, by approximating the nonlinear terms using an explicit scheme such as the Adams-Bashforth family of J_e order,

$$\frac{\hat{\mathbf{u}} - \sum_{q=0}^{J_e-1} \alpha_q \mathbf{u}^{n-q}}{\Delta t} = \sum_{q=0}^{J_e-1} \beta_q \mathbf{N}(\mathbf{u}^{n-q}), \quad (2.56)$$

where $\hat{\mathbf{u}}$ is denotes the primary intermediate velocity field desired and α_e, β_e refers to the time integration coefficients for a prescribe J_e -th order, described later. After evaluting $\hat{\mathbf{u}}$, we move onto the second term in equation (2.55), which defines the pressure at time step $n + 1$ as,

$$\frac{\hat{\mathbf{u}} - \hat{\mathbf{u}}}{\Delta t} = -\nabla p^{n+1}. \quad (2.57)$$

$\hat{\mathbf{u}}$ denotes as the secondary intermediate velocity. In this single equation, we seek to obtain two unknown solutions, $\hat{\mathbf{u}}$ and p^{n+1} , which is ill-posed, and seek to impose certain restrictions. The splitting method assumes that the secondary intermediate velocity is divergence free, $\nabla \cdot \hat{\mathbf{u}} = 0$, and satisfies the Dirichlet boundary conditions normal to the boundary, $\hat{\mathbf{u}} \cdot \mathbf{n} = \mathbf{u}|_{\Omega} \cdot \mathbf{n}$. By considering the assumptions above and the divergence of equation (2.57), we obtain the pressure Poisson equation with the primary intermediate velocity acting as the forcing term,

$$\nabla^2 p^{n+1} = \nabla \cdot \left(\frac{\hat{\mathbf{u}}}{\Delta t} \right) \quad (2.58a)$$

and boundary conditions,

$$\frac{\partial p^{n+1}}{\partial n} = \mathbf{n} \cdot \left(\frac{\hat{\mathbf{u}} - \hat{\mathbf{u}}}{\Delta t} \right). \quad (2.58b)$$

While the pressure boundary condition (2.58b) is straightforward to evaluate, it is sensitive to large splitting errors [Karniadakis et al., 1991]. To overcome this, we consider a high-order boundary condition of pressure, obtained by taking the normal dot product of equation (2.53),

$$\frac{\partial p^{n+1}}{\partial t} = - \sum_{q=0}^{J_e-1} \beta_q \left[\frac{1}{\Delta t} \mathbf{u}^{n-q} + \nu [\nabla \times (\nabla \times \mathbf{u}^{n-q})] + (\mathbf{u}^{n-q} \cdot \nabla) \mathbf{u}^{n-q} \right] \cdot \mathbf{n}. \quad (2.59)$$

Notably, the linear operator is expressed as $\mathbf{L}(\mathbf{u}) = \nabla(\nabla \cdot \mathbf{u}) - \nabla \times (\nabla \times \mathbf{u})$, favouring numerical stability [Orszag et al., 1986, Karniadakis et al., 1991]. J_e is the order the explicit scheme as in equation (2.56). After solving for the pressure Poisson equation, the secondary intermediate velocity could be subsequently obtained using equation (2.57). After which, we can move onto the final substep in equation (2.55), by solving a Helmholtz equation for \mathbf{u}^{n+1} ,

$$\frac{\gamma_0 \mathbf{u}^{n+1} - \hat{\mathbf{u}}}{\Delta t} = \nu \sum_{q=0}^{J_i-1} \gamma_q \mathbf{L}(\mathbf{u}^{n+1-q}), \quad (2.60)$$

where the linear terms are treated based similar to the family of Adams-Moulton implicit scheme and J_i, γ_q denotes the order of the scheme and time integration coefficients, completing the velocity correction scheme. The time integration coefficients are determined from stiffly stable schemes shown in table 2.2, an improvement from the Adams-family schemes [Karniadakis et al., 1991]. The high

Coefficients	1^{st} order	2^{nd} order	3^{rd} order
γ_0	1	3/2	11/6
α_0	1	2	3
α_1	0	-1/2	-3/2
α_2	0	0	1/3
β_0	1	2	3
β_1	0	-1	-3
β_2	0	0	1

Table 2.2: Integration coefficient of stiffly stable schemes from Karniadakis et al. [1991].

order velocity correction scheme and be summarised in a three step process of the following,

$$\mathbf{u}^n \xrightarrow{\mathbf{N}(\mathbf{u}^n)} \hat{\mathbf{u}} \xrightarrow{\nabla^2 p} \hat{\mathbf{u}} \xrightarrow{\mathbf{L}(\hat{\mathbf{u}})} \mathbf{u}^{n+1},$$

evolving the velocity fields at time step n to $n + 1$.

2.4.2 Fourier spectral/ hp modes

Fourier-Chebyshev-Fourier type discretisation have been recognised as preferred method for performing direct numerical simulations (DNS) of transitional or turbulent channel flows [Kim et al., 1987] owing to its efficient representation of the inhomogeneous wall-normal directions and the homogeneous streamwise and spanwise directions, using Chebyshev and Fourier expansions respectively.

The Fourier spectral/ hp element method draws on this approach, where the homogeneous and

the inhomogeneous directions are represented by the Fourier expansions and spectral/ hp elements respectively. This approach has been commonly referred to as the Quasi-3D or (2.5D) approach, allowing for the representation of two inhomogeneous directions. For example, in the turbulent channel flows with riblets, the Fourier expansions are used to represent the periodic streamwise, while the spectral/ hp elements are used to discretise the wall-normal direction. In the analysis of three-dimensional wakes of cylinders where the Fourier expansions are treated in the spanwise directions. In this thesis, we routinely use the the Quasi-3D approach, consisting of the 2D spectral/ hp elements with 1D Fourier expansions are used to discretise the cross stream plane and streamwise flow respectively. The velocity and pressure in the spectral/ hp plane is described by two dimensional modified bases with Fourier expansions,

$$\begin{bmatrix} \mathbf{u}^\delta(x, y, z, t) \\ p^\delta(x, y, z, t) \end{bmatrix} = \sum_{k=0}^{N_z-1} \sum_{p=0}^P \sum_{q=0}^P \psi_p(x) \psi_q(y) e^{ik\beta z} \begin{bmatrix} \hat{\mathbf{u}}_{p,q,k}(t) \\ \hat{p}_{p,q,k}(t) \end{bmatrix} = \sum_{k=0}^{N_z-1} e^{ik\beta z} \begin{bmatrix} \tilde{\mathbf{u}}_k(x, y, t) \\ \tilde{p}_k(x, y, t) \end{bmatrix} \quad (2.61)$$

where $\beta = \frac{2\pi}{L_z}$ is the spanwise wavenumber, L_z the spanwise length, N_z the number of Fourier expansions. Substituting equation 2.61 into the Navier-Stokes equations and taking the Fourier transform (equivalently to the Galerkin projection with respect to Fourier expansion as a test function) yields a system of N_z decoupled equations, amenable for parallel processing,

$$\frac{\partial \tilde{\mathbf{u}}_k}{\partial t} = -\tilde{\nabla}_k \tilde{p}_k + \nu(\nabla_{x,y}^2 - k^2 \beta^2) \tilde{\mathbf{u}}_k - [\widehat{(\mathbf{u} \cdot \nabla) \mathbf{u}}]_k \quad (2.62a)$$

$$-k\beta \tilde{\nabla} \cdot \tilde{\mathbf{u}}_k = 0, \quad k = 0, \dots, N_z - 1 \quad (2.62b)$$

where, $\tilde{\nabla}_k = (\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, ik\beta)$, $\nabla_{x,y}^2 = (\frac{\partial^2}{\partial x^2}, \frac{\partial^2}{\partial y^2})$ and $[(\widehat{\mathbf{u} \cdot \nabla}) \mathbf{u}]_k$ refers to the Fourier-transformed of the k^{th} nonlinear term.

2.4.3 Maintaining fluid flow through a channel

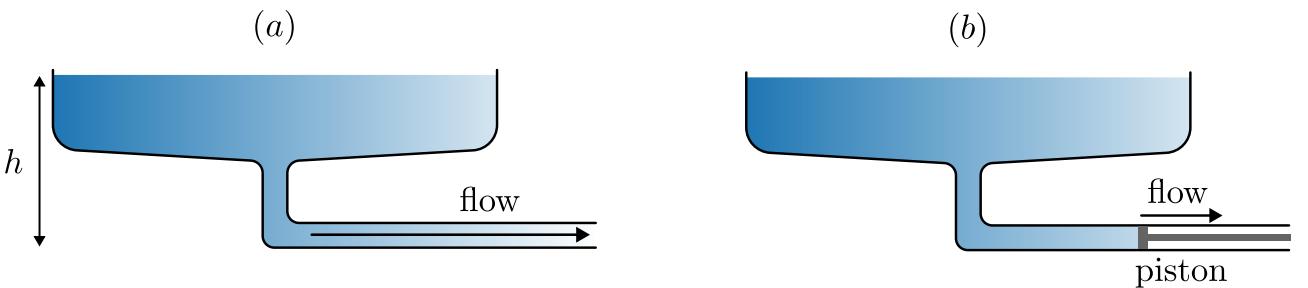


Figure 2.6: (a) Flow rate driven by a pressure gradient from an reservoir elevated by h . (b) Flow driven by a piston at a constant flow rate.

In general, there are two approaches to drive a fluid flow through a channel, either by maintaining a constant pressure drop, or a constant volumetric flux (flow rate). This difference is illustrated in figure 2.6, whereby the flow through the channel is driven by a constant pressure drop from an elevated

reservoir of constant height h in figure 2.6(a), while a piston moves at a constant speed rightwards, drawing fluid through the channel at a constant volumetric flux in figure 2.6(b).

Constant pressure via body-forcing

As we prescribe the homogeneous direction along the streamwise directions, a pressure drop cannot be prescribe directly. Instead, we substitute the constant pressure drop with a constant body force $\mathbf{f} = f_x \hat{\mathbf{e}}_x$ in the streamwise direction,

$$\frac{\partial u}{\partial t} + (u \cdot \nabla)u = -\nabla p + \nu \nabla^2 u + f_x, \quad (2.63)$$

The central question now becomes what is the magnitude of body force required a laminar or turbulent flow. To begin this discussion, we assume that we can decompose our flow variables into a mean and a fluctuating component,

$$u(x, y, t) = U(y) + u'(x, y, t), \quad (2.64)$$

where $U(y) = \langle u \rangle$ refers to the averaged velocity and $\langle \cdot \rangle = \frac{1}{TL_x L_z} \int \cdot dz dx dt$ refers to the temporal and span-averaged operator. The fluctuating component is defined with an average of 0, i.e. $\langle u' \rangle = 0$. Next, we substitute this decomposition into equation (2.63), and perform the averaging operation,

$$\begin{aligned} & \left\langle \frac{\partial(U + u')}{\partial t} + (U + u') \frac{\partial(U + u')}{\partial x} + (V + v') \frac{\partial(V + v')}{\partial y} \right. \\ & \left. = -\frac{\partial(P + p')}{\partial x} + \nu \nabla^2(U + u') + F_x + f'_x \right\rangle. \end{aligned} \quad (2.65)$$

For a statistically stationary turbulent (or laminar) channel flow with periodic streamwise boundary conditions, we can make the following assumptions:

1. stationary flow $\frac{\partial U}{\partial t} = 0$,
2. fully-developed in x , $\frac{\partial}{\partial x} \rightarrow 0$,
3. $\frac{\partial V}{\partial y} = 0$, as a consequence of continuity and the no-slip boundary condition.
4. $\langle u', v', w', p' \rangle = 0$, based on the definition of fluctuations,
5. $\frac{\partial p}{\partial x} = 0$ due to the enforced periodicity in x .

Applying the assumptions above, the mean momentum equations simplify into,

$$\langle F_x \rangle = \left\langle \frac{\partial(u'v')}{\partial y} \right\rangle - \nu \frac{\partial U^2}{\partial y^2}, \quad (2.66)$$

where the body force on the left-hand side balances the sum of Reynolds stresses and viscous diffusion on the right-hand side. Next, we integrate the expression from $y \in [-1, 1]$,

$$2F_x = [\langle u'v' \rangle]_{y=-1}^{y=1} + \nu \left[\frac{\partial U}{\partial y} \Big|_{y=1} - \frac{\partial U}{\partial y} \Big|_{y=-1} \right]. \quad (2.67)$$

The wall shear stress is defined by $\tau_w = \nu \frac{\partial U}{\partial y} \Big|_{y=1}$ (ρ is assumed to be 1), and it is antisymmetric about the channel centreline, $\nu \frac{\partial U}{\partial y} \Big|_{y=1} = -\nu \frac{\partial U}{\partial y} \Big|_{y=-1}$. Due to the no-slip condition, the Reynolds shear stresses is zero, i.e. $[u'v'] \Big|_{y=-1,1} = 0$. Hence, the expression above simplifies to,

$$\tau_w = F_x. \quad (2.68)$$

In other words, the body force F_x is balanced by the wall shear stress (drag), τ_w , along the channel walls. In the case of laminar flow, τ_w can be determined analytically, and the body force required for sustaining a laminar flow for a velocity profile of $u(y) = 1 - y^2$, is $F_x = -2\nu$. However, to determine the wall shear stress (and hence the magnitude of body force) is not as straightforward task for transitional or turbulent channel flow as there isn't an analytical expression for τ_w and its dependence on Reynolds number. Instead, we can only rely on empirical relations of turbulent channel flow between the skin friction coefficient, $c_f = \tau_w / \frac{1}{2}\rho U_c^2$ and Reynolds number Re_c from [Dean \[1978\]](#).

$$c_f = 0.00302 Re_c^{-1/4}, \quad (2.69)$$

where Re_c is the Reynolds number based on the laminar centerline velocity. Similarly, the skin

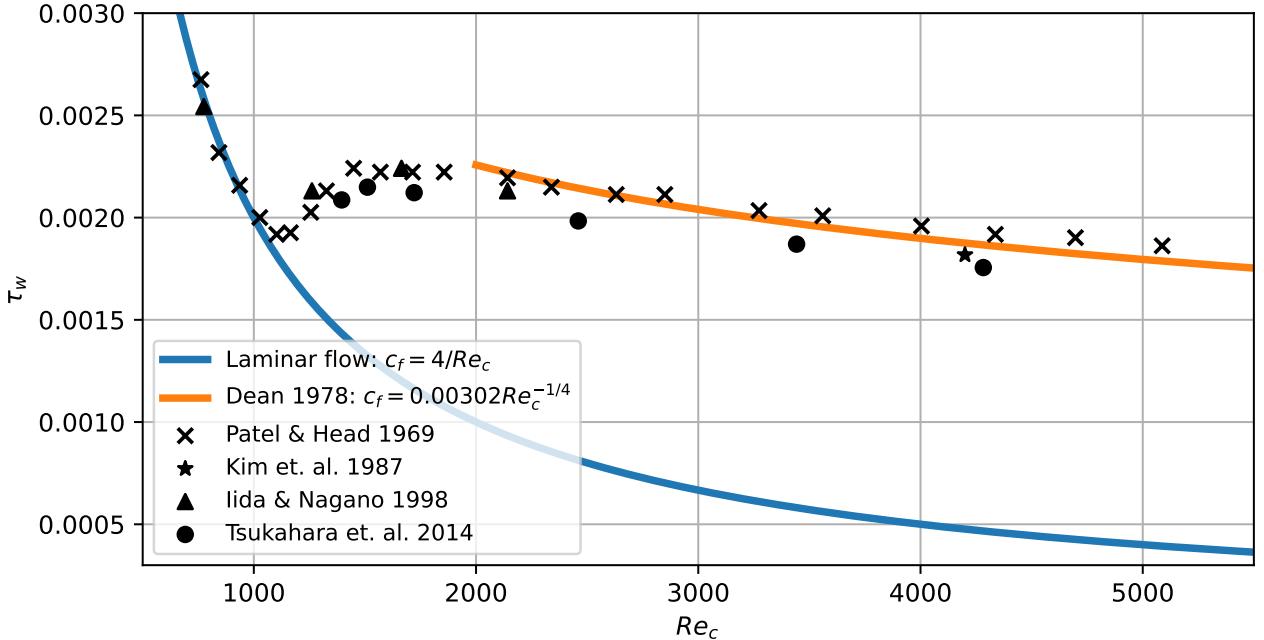


Figure 2.7: τ_w against Re_c using skin friction coefficients from [Dean \[1978\]](#) with $\rho = U_c = 1$. Experimental scatter points from [[Patel and Head, 1969](#), [Kim et al., 1987](#), [Iida and Nagano, 1998](#), [Tsukahara et al., 2014a](#)].

friction coefficient for the case of laminar flow is $c_f = 4/Re_c$ [Dean, 1978]. Figure 2.7 illustrates the relationship between τ_w and Re_c of channel flow using empirical relationship from Dean [1978] (here $\rho = U_c = 1$) and experimental data from Patel and Head [1969], Kim et al. [1987], Iida and Nagano [1998], Tsukahara et al. [2014a]. While the empirical relation for laminar flow, $Re_c \lesssim 1000$ and turbulent flow $Re_c \gtrsim 2000$ appears reasonably robust, the wall shear stress in the transitional region is lacking therefore, the body forcing approach is not preferred.

Constant volumetric flux

An alternative approach is to enforce a constant volumetric flux, illustrated using the piston method in figure 2.6(b). We employ the efficient Green's function approach introduced by Chu and Karniadakis [1993], and outline its solution procedure. The volumetric flux is defined as,

$$Q(\mathbf{u}) = \frac{1}{2\mu(R)} \int_R \mathbf{u} \cdot d\mathbf{s}, \quad (2.70)$$

where $Q(\cdot)$ refer to the flow rate operator through the surface R with surface area of $\mu(R)$. The idea is to append a correction velocity, \mathbf{u}_{corr} , to the velocity field at time step n , \mathbf{u}^n , such that the corrected solution, $\bar{\mathbf{u}}^n = \mathbf{u}^n + \mathbf{u}_{corr}$, has the desired volumetric flux $\bar{Q} = Q(\bar{\mathbf{u}}^n)$. While adding two solutions together is straightforward, the resultant velocity field may not directly satisfy the Navier-Stokes equations. Fortunately, we can leverage the velocity correction scheme which (in general) evaluates the nonlinear advection terms followed by a linear terms (pressure and dissipation). This process is summarised as,

$$\begin{cases} \frac{\partial \mathbf{u}}{\partial t} = \mathbf{N}(\mathbf{u}) \\ \mathbf{u}(\mathbf{x}, 0) = \mathbf{u}^n \end{cases} \xrightarrow{\hat{\mathbf{u}}(\mathbf{x}, \Delta t)} \begin{cases} \frac{\partial \mathbf{u}}{\partial t} = -\nabla p + \nu \mathbf{L}(\mathbf{u}) \\ \mathbf{u}(\mathbf{x}, 0) = \hat{\mathbf{u}}(\mathbf{x}, \Delta t), \end{cases} \quad (2.71)$$

where $\mathbf{u}(\mathbf{x}, 0) = \mathbf{u}^n$ and $\hat{\mathbf{u}}(\mathbf{x}, \Delta t)$ refer to the initial condition for the nonlinear advection terms, and the intermediate velocity, the initial condition for the linear terms, respectively. Since the second step correspond to solving the linear Stokes equation, any solution of the linear Stokes (such as \mathbf{u}_{corr}) added to the final solution will still satisfy the linear Stokes equations - a property of linear differential equations. We consider the linear Stokes equation governing the evolution of the correction velocity,

$$\frac{\partial \mathbf{u}_{corr}}{\partial t} = -\nabla p_{corr} + \nu \mathbf{L}(\mathbf{u}_{corr}) + \alpha^n \hat{\mathbf{e}}_x, \quad (2.72)$$

where α^n is the undetermined magnitude of body force at time step n in the streamwise direction, $\hat{\mathbf{e}}_x$, required to maintain the desired flow rate $\bar{Q} = Q(\mathbf{u}^n) + Q(\mathbf{u}_{corr})$. Since \mathbf{u}_{corr} is appended to \mathbf{u}^n , the initial condition for \mathbf{u}_{corr} must be $\mathbf{u}_{corr}(\mathbf{x}, 0) = 0$, so that \mathbf{u}^n remains compatible with the initial conditions in equation (2.71). Since α^n is undetermined, we normalise the equation with respect to α^n , yielding the linear Stokes equations with unit forcing,

$$\frac{\partial \mathbf{v}}{\partial t} = -\nabla \hat{p} + \nu \mathbf{L}(\mathbf{v}) + \hat{\mathbf{e}}_x, \quad \mathbf{v}(\mathbf{x}, 0) = \mathbf{0}, \quad (2.73)$$

where $\mathbf{v} = \mathbf{u}_{corr}/\alpha^n$ and $\hat{p} = p_{corr}/\alpha^n$. The corrected velocity field becomes

$$\bar{\mathbf{u}} = \mathbf{u} + \alpha^n \mathbf{v}^1, \quad (2.74)$$

where \mathbf{v}^1 is solution field obtained by solving equation (2.73) in the first time step. To match the target volumetric flux, \bar{Q} , we need to scale α^n such that,

$$\bar{Q} = Q(\bar{\mathbf{u}}^n) = Q(\mathbf{u}^n) + Q(\alpha^n \mathbf{v}^1). \quad (2.75)$$

which gives,

$$\alpha^n = \frac{\bar{Q} - Q(\mathbf{u}^n)}{Q(\mathbf{v}^1)}, \quad (2.76)$$

evaluated at every time step n . The Green's function approach is computationally efficient as we only need to compute \mathbf{v}^1 and $Q(\mathbf{v}^1)$ once during the first time step and reuse it for subsequent time steps. The process of adding the correction velocity at the end of velocity correction scheme can be summarised in the procedure as follows,

$$\mathbf{u}^n \xrightarrow{\mathbf{N}(\mathbf{u}^n)} \hat{\mathbf{u}} \xrightarrow{\nabla^2 p} \hat{\mathbf{u}} \xrightarrow{\mathbf{L}(\hat{\mathbf{u}})} \mathbf{u}^{n+1} \xrightarrow{\alpha^{n+1} \mathbf{v}^1} \bar{\mathbf{u}}^{n+1}.$$

2.5 Stability analysis of the Navier-Stokes equations

2.5.1 Algorithms for linear stability analysis

In this section, we present a general overview of the numerical procedure for linear stability analysis. Linear stability analysis examines the stability of a base flow by considering the evolution of infinitesimal perturbations. These perturbations in general, may either grow or decay exponentially, indicating whether the base flow is linearly unstable or stable respectively. In §1.2, we introduced linear stability analysis in the context of wall-bounded shear flows leading to the Orr-Sommerfeld equations, where the base flows depend on a single inhomogeneous and two homogeneous directions, commonly referred to as local² stability analysis. For example, the laminar Poiseuille flow, $U(y) = 1 - y^2$ and the laminar Couette flow $U(y) = y$, $y \in [-1, 1]$. For some flows such as boundary layers, wakes and jets, their base flows are not strictly parallel. By considering a weak dependence on the stream and spanwise directions, their stability are described by the parabolised stability equations [Herbert, 1997]. When the base flow depends on two spatially inhomogeneous directions, $U(x, y)$, or three spatially inhomogeneous directions, $U(x, y, z)$, the analysis of such states are commonly referred to as biglobal or triglobal stability analysis, respectively [Theofilis, 2003]. If the base flow is time-dependent, such as in the secondary instability of cylinder flows, we use Floquet stability analysis [Henderson and Barkley, 1996].

In this section, we consider a time-independent base flow and consider a generic decomposition

²Referring to being spatially local in the context of ‘real’ flows which are typically inhomogeneous in all directions

of the velocity field in three spatial dimensions,

$$\mathbf{u}(\mathbf{x}, t) = \mathbf{U}(\mathbf{x}) + \mathbf{u}'(\mathbf{x}, t), \quad (2.77)$$

where $\mathbf{U}(\mathbf{x})$, $\mathbf{u}'(\mathbf{x}, t)$ refers to the base flow and perturbations. Substituting this into the Navier-Stokes equations and linearising,

$$\frac{\partial \mathbf{u}'}{\partial t} = -(\mathbf{U} \cdot \nabla) \mathbf{u}' - (\mathbf{u}' \cdot \nabla) \mathbf{U} - \nabla p' + \frac{1}{Re} \nabla^2 \mathbf{u}', \quad (2.78a)$$

$$\nabla \cdot \mathbf{u}' = 0. \quad (2.78b)$$

This can be rewritten in as,

$$\frac{\partial}{\partial t} \mathbf{q}' = \mathcal{L} \mathbf{q}', \quad \mathcal{L} = \begin{bmatrix} -(\mathbf{U} \cdot \nabla) - (\nabla \mathbf{U}) + \frac{1}{Re} \nabla^2 & -\nabla \\ \nabla \cdot & 0 \end{bmatrix}, \quad (2.79)$$

where \mathcal{L} refer to the linearised operator and, $\mathbf{q}' = (\mathbf{u}', p')^T$. Assuming an initial perturbation, $\mathbf{q}'(\mathbf{x}, t = 0) = \mathbf{q}_0$, its evolution to time T is given by,

$$\mathbf{q}(\mathbf{x}', T) = \mathcal{A}(T, Re) \mathbf{q}_0, \quad \text{where } \mathcal{A}(T, Re) = \exp(\mathcal{L}T). \quad (2.80)$$

We assume that the perturbations can be represented as a normal mode,

$$\mathbf{q}'(\mathbf{x}, t) = \tilde{\mathbf{q}}(\mathbf{x}) \exp(\lambda t) + \text{c.c} \quad (2.81)$$

where $\lambda_j, \tilde{\mathbf{q}}_j(x)$ refer to the j^{th} eigenvalue and eigenmode, and c.c refers to the complex conjugate. Substituting the normal mode into equation (2.80), we obtain an eigenvalue problem,

$$\mathcal{A}(T, Re) \tilde{\mathbf{q}}_j = \mu_j \tilde{\mathbf{q}}_j, \quad \mu_j = \exp(\lambda_j T). \quad (2.82)$$

where μ_j refers to the eigenvalue of $\mathcal{A} = \exp(\mathcal{L}T)$, and we typically set $T = 1$ [Barkley et al., 2008]. The real component of the eigenvalues determine the stability of the base flow, which can be either,

1. Unstable: $\Re(\lambda) > 0$,
2. Stable: $\Re(\lambda) < 0$,
3. Neutral: $\Re(\lambda) = 0$.

This concludes the mathematical overview of linear stabiltiy analysis, and the challenge lies in the computing the eigenpairs of \mathcal{A} efficiently. For large matrices, $\mathcal{A} \in \mathbb{R}^{M \times M}$ (assuming it is real here for simplicity), direct eigenvalue solvers such as the QR algorithm costing $O(M^3)$ might be computationally infeasible. Another concern is that we are typically only interested in the most dangerous (leading) eigenvalues of largest real parts, and not the full spectrum. Lastly, we do not have access to \mathcal{A} in a time stepping based code.

Power Iteration Method

A simple method in computing the dominant eigenpair is the power iteration method,

Definition 2.5.1 (Power iteration). Given a diagonalisable matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$ and a non-zero vector \mathbf{x}_0 , the sequence of matrix vector products between them (we neglect normalisation here),

$$\mathbf{Ax}_0, \mathbf{A}^2\mathbf{x}_0, \mathbf{A}^3\mathbf{x}_0, \dots, \mathbf{A}^k\mathbf{x}_0. \quad (2.83)$$

approaches the eigenvector of \mathbf{A} with the largest magnitude. i.e. $\tilde{\mathbf{x}}_1 = \lim_{k \rightarrow \infty} \mathbf{A}^k \mathbf{x}_0$. The dominant eigenvalue, λ_1 , can be computed using the Rayleigh quotient, $\lambda_1 = \frac{\tilde{\mathbf{x}}_1^T \mathbf{A} \tilde{\mathbf{x}}_1}{\tilde{\mathbf{x}}_1^T \tilde{\mathbf{x}}_1}$.

Arnoldi Method

We typically require two to four eigenpairs with the largest real parts. To compute more than one eigenpair, we utilise the Arnoldi method [Arnoldi, 1951], belonging to a class of Krylov subspace iterative methods, for performing a Hessenberg reduction.

Definition 2.5.2 (Krylov Subspaces). Given a matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$ and a non-zero vector $\mathbf{x}_0 \in \mathbb{R}^n$, the k^{th} -Krylov subspace, $\mathcal{K}_n(\mathbf{A}, \mathbf{x}_0, k)$ is defined by,

$$\mathcal{K}_n(\mathbf{A}, \mathbf{x}_0, k) = \text{span}\{\mathbf{x}_0, \mathbf{Ax}_0, \mathbf{A}^2\mathbf{x}_0, \mathbf{A}^3\mathbf{x}_0, \dots, \mathbf{A}^{k-1}\mathbf{x}_0\}. \quad (2.84)$$

Definition 2.5.3 (Hessenberg reduction). The Hessenberg reduction is a matrix decomposition technique commonly used for the computing eigenpairs of matrices. Given a unsymmetric matrix $\mathbf{A} \in \mathbb{R}^{N \times N}$ (we assume that \mathbf{A} is real for simplicity), we seek a decomposition of the form,

$$\mathbf{A} = \mathbf{Q} \mathbf{H} \mathbf{Q}^T, \quad (2.85)$$

where,

- $\mathbf{H} \in \mathbb{R}^{N \times N}$ is an upper Hessenberg matrix (i.e. $a_{i,j} = 0$ for $i > j + 1$)
- $\mathbf{Q} \in \mathbb{R}^{N \times N}$ is an orthonormal matrix (i.e. $\mathbf{Q}^{-1} = \mathbf{Q}^T$), whose columns $\mathbf{q}_1, \dots, \mathbf{q}_N$, form an orthonormal basis.

The Hessenberg reduction shows that \mathbf{A} and \mathbf{H} are similar matrices, which have the same eigenvalues. If $\mathbf{Ax} = \lambda \mathbf{x}$, using $\mathbf{Q}^T = \mathbf{Q}^{-1}$ and multiplying (2.85) by \mathbf{x} ,

$$\mathbf{Ax} = \mathbf{Q} \mathbf{H} \mathbf{Q}^{-1} \mathbf{x} \Rightarrow \lambda \mathbf{x} = \mathbf{Q} \mathbf{H} \mathbf{Q}^{-1} \mathbf{x} \Rightarrow \lambda \mathbf{Q}^{-1} \mathbf{x} = \mathbf{H} \mathbf{Q}^{-1} \mathbf{x} \Rightarrow \lambda \mathbf{y} = \mathbf{H} \mathbf{y}. \quad (2.86)$$

Hence, $\lambda(\mathbf{A}) = \lambda(\mathbf{H})$, and their eigenvectors are related by $\mathbf{x} = \mathbf{Q} \mathbf{y}$.

The Arnoldi method generates a sequences of vectors $[\mathbf{u}_0, \mathbf{Au}_0, \dots, \mathbf{A}^{k-1}\mathbf{u}_0]$ that spans the k -dimensional Krylov subspace. These vectors, are known as Arnoldi vectors [Golub and Van Loan, 2013], and are used to construct an orthogonal matrix via the Gram-Schmidt process, $\mathbf{Q} = [\mathbf{q}_1, \mathbf{q}_2, \dots, \mathbf{q}_k] \in$

$\mathbb{R}^{M \times K}$. This is equivalent to performing a partial Hessenberg reduction of $\mathcal{A} = \mathbf{Q}\mathbf{H}\mathbf{Q}^T$, where the eigenvalues of $\mathcal{A} \in \mathbb{R}^{N \times N}$ can be approximated by a smaller Hessenberg matrix $\mathbf{H} \in \mathbb{R}^{k \times k}$, suitable for a direct eigenvalue computation using the QR algorithm. The k -step Arnoldi factorisation of \mathcal{A} gives,

$$\mathcal{A}\mathbf{Q}_k = \mathbf{Q}_k\mathbf{H}_k + \mathbf{r}_k\mathbf{e}_k^T, \quad (2.87)$$

where $\mathbf{H} \in \mathbb{R}^{k \times k}$ refers to the upper Hessenberg matrix, $\mathbf{e}_k = [0, \dots, 0, 1] \in \mathbb{R}^k$, and $\mathbf{r}_k \in \mathbb{R}^N$ is a residual vector. If $\mathbf{x} = \mathbf{Q}_k\mathbf{y}$, and $\mathbf{H}\mathbf{y} = \lambda\mathbf{y}$ then,

$$(\mathcal{A} - \mathbf{I}\lambda)\mathbf{x} = (\mathbf{e}_k^T\mathbf{y})\mathbf{r}_k. \quad (2.88)$$

In other words, the residual vector difference between the approximation of $\lambda(\mathcal{A})$, using $\lambda(\mathbf{H})$. If $\|\mathbf{r}_k\| = 0$, then $\lambda(\mathbf{H}) \subseteq \lambda(\mathcal{A})$.

We now present the Arnoldi method by generating k Arnoldi vectors,

$$\mathbf{T}_k = [\mathbf{u}_0, \mathbf{u}_1, \dots, \mathbf{u}_{k-1}] = \left[\mathbf{u}_0, \frac{\mathcal{A}(T, Re)\mathbf{u}_0}{\alpha_1}, \frac{\mathcal{A}(T, Re)\mathbf{u}_1}{\alpha_2}, \dots, \frac{\mathcal{A}(T, Re)\mathbf{u}_{k-1}}{\alpha_k} \right], \quad (2.89)$$

where α_j is scaled such that $\|\mathbf{u}_j\| = 1$. Following [Barkley et al., 2008], the projection of \mathcal{A} onto the Krylov subspace is given as,

$$\mathcal{A}\mathbf{T}_k = \mathbf{T}_{k+1}D_k^{(k+1)}, \quad (2.90)$$

where $D_k^{(k+1)} \in \mathbb{R}^{(k+1) \times k}$ is a shifted diagonal matrix with entries $D_{ij} = \alpha_i \delta_{i,j+1}$. We assume that \mathbf{T}_k and \mathbf{T}_{k+1} admit QR decompositions,

$$\mathcal{A}\mathbf{Q}_k\mathbf{R}_k = \mathbf{Q}_{k+1}\mathbf{R}_{k+1}\mathbf{D}_k^{(k+1)}, \quad (2.91)$$

where $\mathbf{Q}_k \in \mathbb{R}^{N \times k}$, $\mathbf{R}_k \in \mathbb{R}^{k \times k}$ and $\mathbf{Q}_{k+1}, \mathbf{R}_{k+1}$ are similarly defined. The upper Hessenberg matrix $\mathbf{H}_k^{(k+1)} \in \mathbb{R}^{(k+1) \times k}$ is defined as,

$$\mathbf{H}_k^{(k+1)} = \mathbf{R}_{k+1}\mathbf{D}_k^{(k+1)}\mathbf{R}_k^{-1}, \quad (2.92)$$

in which the last row of $\mathbf{H}_k^{(k+1)}$ only contains a single non-zero entry, $h^* = h_{k,k-1}$. By substituting the definition of the upper Hessenberg matrix and separating the last row of $\mathbf{H}_k^{(k+1)}$ we obtain,

$$\mathcal{A}\mathbf{Q}_k = \mathbf{Q}_k\mathbf{H}_k + h^*\mathbf{q}_k\mathbf{e}_k^T. \quad (2.93)$$

Equation (2.93) describes the projection of \mathcal{A} onto the Krylov subspace spanned by orthonormal bases \mathbf{Q}_k , yielding a smaller \mathbf{H}_k matrix. The accuracy of this approximation is dictated by the magnitude of the residual term, $h^*\mathbf{q}_k\mathbf{e}_k^T$. Assuming that \mathbf{H}_k is diagonalisable as $\mathbf{H}_k = \Psi_k \Lambda_k \Psi_k^{-1}$, we multiply equation (2.93) by Ψ_k ,

$$\mathcal{A}\mathbf{Q}_k\Psi_k = \mathbf{Q}_k\Psi_k\Psi_k^{-1}\mathbf{H}_k\Psi_k + h^*\mathbf{q}_k\mathbf{e}_k^T\Psi_k. \quad (2.94)$$

Simplifying the expression above we get,

$$\mathcal{A}\mathbf{V}_k = \mathbf{V}_k\Lambda_k + h^*\mathbf{q}_k\mathbf{e}_k^T\boldsymbol{\Psi}_k, \quad (2.95)$$

where Λ_k contains the k eigenvalues and $\mathbf{V}_k = \mathbf{Q}_k\boldsymbol{\Psi}_k$ the eigenvectors of \mathcal{A} . The error in approximating the j^{th} eigenpair is given by,

$$\varepsilon_j = \|\mathcal{A}\mathbf{v}_j - \lambda_j\mathbf{v}_j\| = \|h^*\mathbf{q}_k\mathbf{e}_k^T\psi_j\| = |h^*|\mathbf{v}_j[k-1]|, \quad (2.96)$$

where $\mathbf{v}_j[k-1]$ is the last component of the eigenvector \mathbf{v}_j .

Lastly, we are generally interested in obtaining the eigenpairs with the the largest real part. We introduce exponential power method [Tuckerman and Barkley, 2000], which is naturally considered by time stepping an initial perturbation \mathbf{q}'_0 from $t = 0$ to T ,

$$\mathbf{q}'(T) = \exp(\mathcal{L}T)\mathbf{q}'_0 = \mathcal{A}(T)\mathbf{q}'_0. \quad (2.97)$$

The dominant eigenvalues, μ , of \mathcal{A} obtained from the Arnoldi method described above, which correspond to the eigenvalue of the largest real part λ , of \mathcal{L} by $\mu = \exp(\lambda T)$, where T is typically set to 1. For further details on this algorithm, the reader is referred to Barkley et al. [2008] for more details.

In summary, the algorithm described above have been implemented in Nektar++, referred to as the ‘modified’ Arnoldi algorithm, which modifies the existing time-stepper code with a wrapper function that generates Arnoldi vectors and solves the Hessenberg matrix using the subroutine dgeev from LAPACK (Linear Algebra PACKage, [Anderson et al., 1999]). The modified Arnoldi algorithm has been verified against using a separate implementation based on the third-party package ARPACK (ARnoldi PACKage [Lehoucq et al., 1998]) [Rocco, 2014].

2.5.2 Edge tracking

In the section, we consider the dynamical system interpretation of transition, where the laminar state is separated by the turbulent state by an edge, referred to the edge of chaos. Along this edge, there could be attractors, sometimes in the form of travelling-waves, tori, and high-order invariant sets, known as the edge states. For the edge tracking, we use the bisection method [Skufca et al., 2006, Schneider et al., 2007, Khapko et al., 2016], with an initial condition given by

$$\mathbf{x}_0 = \chi\mathbf{x}_L + (1-\chi)\mathbf{x}_T \quad (2.98)$$

where \mathbf{x}_0 refers to an initial condition consisting of a weighted sum, $\chi \in [0, 1]$, between a laminar state, \mathbf{x}_L , and a turbulent state, \mathbf{x}_T . Since the laminar and turbulent state forms a bistable system, there could be (at least) one critical value of $\chi \in [0, 1]$, where the trajectory walks along the ‘edge’ between the turbulent and laminar state without decaying to either states. To find this χ_c , we perform n successive bisections between χ_L^n, χ_T^n , the upper and lower bounds such that the trajectory relaminaris or become turbulent respectively, where χ^n is updated by $\chi^n = \frac{1}{2}(\chi_L^n + \chi_T^n)$ At every n^{th} bisection,

it involves a stopping criteria, a tolerance based on the deviation of an observable (e.g. wall shear stresses) away from the initial condition. Then, a direct numerical simulation is reinitialised with an initial condition given by equation (2.98) For every successive bisection, the difference between two trajectories, $\Delta\chi^n = \chi_L^n - \chi_T^n$, decays like $\Delta\chi^n \sim 0.5^n$, and is related to the Lyapunov exponent of the edge

$$\Delta\chi \approx C \exp(\mu_e t) \quad (2.99)$$

where μ_e, C refers to the Lyapunov exponent of the edge and a constant. In practice, we consider $n = 10, 20$ and for $n = 10$, the solution along the edge is converged. After we determine the critical χ_c , we repeat the bisections step by replacing the laminar state, \mathbf{x}_L , and the turbulent state \mathbf{x}_T , which the solution trajectory with χ_L and χ_T , that has been terminated after exceeded the threshold. We refer this repetition as the number of ‘outer’ bisections, while the bisection for χ^n is referred to ‘inner bisections’ After a certain number of ‘outer’ bisections, the trajectory may converge towards an attractor, which may exist in a form of travelling-waves, periodic orbits or a chaotic attractor. This attractor sits along the edge is referred to as the edge state, a saddle acting as a separatrix between the turbulent and laminar attractor. We describe the algorithm of edge tracking in algorithm 2.5.2

Algorithm 1 Algorithm for edge tracking between a turbulent and laminar state

```
1: Initialise maxInBisects, maxOutBisects           ▷ Maximum inner and outer bisections
2: Initialise tol                                     ▷ Tolerance for stopping criteria (e.g., wall-shear stress)
3: outBisects ← 0
4: while outBisects < maxOutBisects do
5:   if outBisects == 0 then
6:      $\mathbf{x}_L, \mathbf{x}_T \leftarrow \text{input}()$                   ▷ Initial laminar and turbulent states
7:   end if
8:    $\chi_L \leftarrow 0, \chi_T \leftarrow 1, \chi \leftarrow \frac{1}{2}(\chi_L + \chi_T)$     ▷ Initialise bisection coefficients
9:    $\mathbf{x}_0 \leftarrow \chi \mathbf{x}_T + (1 - \chi) \mathbf{x}_L$                       ▷ Initialise initial condition
10:  inBisects ← 0
11:  while inBisects < maxInBisects do
12:    k ← 0,  $\Delta \leftarrow 10^6$ 
13:    while  $\Delta > \text{tol}$  do
14:       $\mathbf{x}_{k+1} \leftarrow \text{TimeIntegrate}(\mathbf{x}_k)$ 
15:       $\Delta \leftarrow |\mathbf{x}_{k+1} - \mathbf{x}_0|$                          ▷ Deviation from initial condition
16:      k ← k + 1
17:    end while
18:    if isTurbulent( $\mathbf{x}_k$ ) then                                ▷ Check if terminal state is turbulent
19:       $\chi_L \leftarrow \chi$                                          ▷  $\mathbf{x}_L$  gets larger weight
20:      if inBisects == maxInBisects - 1 then
21:         $\mathbf{x}_T \leftarrow \mathbf{x}_k$                                ▷ Save turbulent-leaning initial condition
22:        break
23:      end if
24:    else
25:       $\chi_T \leftarrow \chi$ 
26:      if inBisects == maxInBisects - 1 then
27:         $\mathbf{x}_L \leftarrow \mathbf{x}_k$                                ▷ Save laminar-leaning initial condition
28:        break
29:      end if
30:    end if
31:     $\chi \leftarrow \frac{1}{2}(\chi_L + \chi_T)$ 
32:     $\mathbf{x}_0 \leftarrow \chi \mathbf{x}_L + (1 - \chi) \mathbf{x}_T$           ▷ Update initial conditions
33:    inBisects++
34:  end while
35:  outBisects++
36: end while
```

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