STRUCTURES, BOUNDARY LAYERS AND PLUMES
IN
TURBULENT RAYLEIGH-BÉNARD CONVECTION

ERWIN P. VAN DER POEL

Structures, boundary layers and plumes in turbulent Rayleigh-Bénard convection

Erwin P. van der Poel

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Cover: Three-dimensional visualization of the temperature field in Rayleigh-Bénard convection at $Ra = 10^8$, $Pr = 1$ and $\Gamma = 0.71$. The plates are no-slip and impermeable, while there is lateral periodicity. The mean temperatures are transparent; only the extremes are visible.

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STRUCTURES, BOUNDARY LAYERS AND PLUMES IN TURBULENT RAYLEIGH-BÉNARD CONVECTION

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Introduction

The significance of Rayleigh-Bénard (RB) convection is best illustrated using natural convection. Natural convection is the motion of a fluid resulting from density differences. It is one of the most common sources of flow in the universe, if not the most common, and it can be found in small scale applications such as the cooling of computer chips [1] and in large-scale systems like stars [2, 3]. In between, natural convection can be found in industrial applications like the cooling of turbo-machinery [4] and the climate control inside houses and other buildings [5, 6]. As the name suggests, natural convection is even more present in nature. On our planet, fluid dynamics in the mantle [7], the atmosphere [8–10] and the ocean [11–13] are largely governed by it. It is even studied in the context of other planets [14].

The most common source of the temperature differences are either a concentration or a temperature heterogeneity, which results in forcing due to a gravity potential. A simple experiment can be designed using temperature; by heating water on a stove one can already observe natural convection. A similar setting was used for the pioneering experiments by Bénard [15] and the seminal linear stability analysis of Lord Rayleigh [16]. These works caused Avsec [17] to coin the term *Rayleigh-Bénard convection* for the heating of a fluid from below and cooling it at the top. Stability analysis shows [18] that from a critical temperature difference onwards, symmetry is broken and convection starts. Below that threshold there is only diffusion and heat transport is low. In the convective state coherent structure can be distinguished. These are the large-scale circulation (LSC) and the thermal plumes, where the LSC consists of one or more system-sized rolls that are driven by thermal plumes. The plumes are the main source of the heat transport, carrying large amounts of thermal energy from one plate to the other.

Governing equations

As defined, Rayleigh-Bénard convection is a fluid that is forced through a temperature field in a gravity potential. The temperature field itself, is in turn advected by the flow. Using these ingredients the so-called *Boussinesq equations* [19, 20] can be formulated. In Einstein notation the equations are

$$\partial_t u_i + u_j \partial_j u_i = -\rho^{-1} \partial_i p + \nu \partial_j^2 u_i + g \beta \theta \delta_{i3}, \quad (1)$$

$$\partial_t \theta + u_j \partial_j \theta = \kappa \partial_j^2 \theta, \quad (2)$$

$$\partial_i u_i = 0. \quad (3)$$

Here, u_i are the velocity components, θ the temperature, ρ the density, p the pressure, β isobaric the thermal expansion coefficient, g the gravitational acceleration, $\delta_{i,j}$ the Kronecker delta and ν and κ the kinematic viscosity and the thermal diffusivity, respectively. Equation 1 (with equation 3) can be seen as the incompressible Navier-Stokes equation with a vertical forcing proportional to the temperature and equation 2 is the convection-diffusion equation for temperature without a source or sink. In order to obtain these equations, the Boussinesq approximation is applied. This assumes that the properties of the fluid are constant, i.e. not a function of the temperature. However, some dependence is essential, as the fluid is driven by the variation of the density with the temperature. Which is why this restriction is relaxed, exclusively in the buoyancy (or forcing) term in the momentum equation (equation 1). In addition, heating by viscous dissipation is neglected and the flow is considered to be incompressible.

Using the Boussinesq equations with boundary conditions, several scales can be defined. The distance between the top cooling plate and the bottom heating plate, i.e. the vertical extent of the system, gives a length scale L . The difference in temperature between these plates gives a temperature scale Δ . The velocity is non-dimensionalized using the free-fall velocity $\sqrt{g\beta\Delta L}$, which additionally provides a time scale in the form of the free-fall time $\sqrt{L/(g\beta\Delta)}$. Using these scales the non-dimensional Boussinesq equations become

$$\partial_t u_i + u_j \partial_j u_i = -\partial_i p + \sqrt{\frac{\text{Pr}}{\text{Ra}}} \partial_j^2 u_i + \theta \delta_{i3}, \quad (4)$$

$$\partial_t \theta + u_j \partial_j \theta = \frac{1}{\sqrt{\text{RaPr}}} \partial_j^2 \theta, \quad (5)$$

$$\partial_i u_i = 0. \quad (6)$$

The dynamics are fully characterized by two control parameters only. These are the Rayleigh number $\text{Ra} = \beta g \Delta L^3 / (\kappa \nu)$ and the Prandtl number $\text{Pr} = \nu / \kappa$. In case there is a finite horizontal extent, the aspect ratio $\Gamma = d/L$ is another control parameter. Here, d is the width of the system. The Rayleigh number Ra can be conceptually seen as the driving of the system while the Prandtl number Pr is a property of the fluid. Examples of low Pr fluids are liquid metals and plasmas. Low Pr RB convection is characterized by strong dynamics but low heat flux [21, 22]. In the opposite

side of the spectrum, high Pr fluids can be found in the mantle of the Earth and in experiments glycerol is commonly used. Mantle dynamics can be approximated using the infinite Prandtl number limit [23–25]. High Pr flows are plume-dominated and contain weak large-scale flows. Increasing Ra, progressively makes the flow more complex. Increasing the temperature difference, the flow transitions from laminar to turbulence and it is the turbulent state where this thesis focuses on. Turbulence increases mixing, which is an essential property. However, it complicates analysis due to the large separation in scales in the flow. Intrinsic to turbulent flows, the correlation lengths (and times) are very short, resulting in a large separation in length scales. The small scale in the flow is substantially smaller than the largest scale, which in RB convection is the size of the system. This property is what makes numerical simulations of turbulent flows notoriously demanding.

Integral quantities

The response of the system is commonly quantified by the heat transfer and the kinetic energy, which we indicate with the Nusselt number Nu and the Reynolds number Re based on the root-mean-square vertical velocity $\text{Re} = u_3^{\text{RMS}} L / \nu$, respectively. Of these, the Nusselt number Nu has received most attention in the scientific effort on RB convection. It is the amount of heat transported by convection relative to the heat transport in the static state by conduction alone. It quantifies the increase in heat transport due to the motion of the fluid and is an important quantity in both industrial and geo- and astro-physical applications of RB convection. In this thesis, the thermal boundary conditions on the horizontal plates are exclusively isothermal. This allows the use of a single definition for Nu throughout, namely

$$\text{Nu} = \sqrt{\text{RaPr}} \langle u_z \theta \rangle_{A,t} - \langle \partial_z \theta \rangle_{A,t}, \quad (7)$$

where x and y are the horizontal coordinates and z the vertical coordinate. In addition, $\langle \cdot \rangle_A$ indicates the average over any horizontal area in three-dimensional (3D) systems and over any horizontal line in two-dimensional (2D) systems. Similarly, $\langle \cdot \rangle_V$ indicates the average over the complete volume in 3D systems and over the complete area in 2D systems. This chevron notation is used throughout the thesis to indicate the average. Nu is a time average and one could denote it as $\langle \text{Nu} \rangle_t$ and remove the time average from its definition, however Nu is used conform to RB literature. For the instantaneous Nu, the notation $\text{Nu}(t)$ is used. Nu can be additionally calculated as both a volume average of the convective term

$$\text{Nu} = \sqrt{\text{RaPr}} \langle u_z \rangle_{V,t} + 1, \quad (8)$$

and an area average on either of the horizontal plates of the diffusive term

$$\text{Nu} = -\langle \partial_z \theta |_{z=0,L} \rangle_{A,t}. \quad (9)$$

Since the RB is closed, Nu can additionally be calculated through the kinetic and thermal dissipation rates [26, 27], which can be used for verification in numerical studies (see §3).

$$\text{Nu} = \text{Pr} \langle (\partial_i u_j)^2 \rangle_{V,t} + 1, \quad (10)$$

$$\text{Nu} = \langle (\partial_i \theta)^2 \rangle_{V,t}. \quad (11)$$

A discrepancy between any of the altogether five different ways of calculating Nu indicates either insufficient statistical convergence or an under-resolved simulation and so comparing these is a useful test. In addition, it is common that resolution checks, in which simulations are redundantly run using an increased resolution, are used to prove sufficient resolution for some cases. Equations can be used conceptually. As Nu is proportional to the energy dissipation in the system, it becomes clear that Nu is directly related to the energy input required to keep the system in the (far from equilibrium) state that it is.

Rayleigh-Bénard convection

The scientific effort since the beginning of the 20th century on Rayleigh-Bénard convection can roughly be classified in three regions. These are the following, stability analysis [16, 18] around the critical Rayleigh number at which convection starts, small-scale properties [28] of velocity and temperature and large-scale heat flux and boundary layer scaling. Contemporary studies on RB convection are predominantly on the large-scale properties in a turbulent flow. This is no different for this thesis, since our research is driven by the curiosity for systems that are inaccessible to numerical and experimental studies. Less abstract, this is the study of RB convection at accessible Rayleigh numbers to estimate the properties of systems at very high Ra. For instance, the Ra in experiments reaches up to 10^{17} [29, 30] and in numerics up to 10^{12} [31, 32], while geo- and astrophysical systems are at Rayleigh numbers higher than 10^{20} [33].

The quantity that is most studied is the heat flux Nu. The dependence of Nu on Ra and Pr is one of the main objectives of theoretical studies. Early studies provided $\text{Nu} \sim \text{Ra}^\gamma$ scaling laws with a single exponent γ [26, 27, 34]. However, experimental results in local Ra ranges at various Pr reported a wide variety in exponents, prompting a unifying theory by Grossman-Lohse (GL) [35] that consists of different regimes with different exponents. The theory is based on the decomposition of the total dissipation rates into a contribution by the bulk and by the boundary layers and the different regimes are delimited by either of these contributions being dominant. It is fitted to experimental results, providing fitting coefficients that allow a $\text{Nu}(\text{Ra}, \text{Pr})$ prediction over the full parameter space in the so-called *classical* regime, which is the regime where the boundary layer is approximately laminar. Recently, the theory

is slightly updated and the coefficients are refitted to new, more accurate, data in §1. The assumption of a laminar boundary is expected to break down at a transitional Ra , where the boundary layer becomes turbulent. This transition inspires novel experimental and numerical studies on RB convection to make more accurate $Nu(Ra, Pr)$ predictions that can additionally be extrapolated to arbitrary Ra and Pr .

It is progressively becoming more common in science to obtain data from numerical simulations as well as experiments. The rise of numerics is apparent in most scientific areas and this is no different in RB convection, in particular in turbulent RB convection. However, this is complicated by the fact that the computational work is $\mathcal{O}(Re^3)$ for a turbulent Navier-Stokes simulation, taking into account the degrees of freedom and time advancing. Overhead from parallelization results in even more computational intensity. The most simple system to study turbulence in, is the three-dimensional periodic box used for homogeneous isotropic turbulence (HIT). Theoretically, in this system the largest scale separation can be achieved using the least amount of computational effort. A state-of-the-art study was on a grid of 12288^3 [36] and used hundreds of thousands of processors. It is computationally optimal due to the inherent three-dimensional symmetry of the domain, which unfortunately is not present in RB convection. This is caused by the horizontal plates, intrinsic to the RB system. These plates result in boundary layers that are required to be sufficiently resolved. In the most optimal case where there are no sidewalls, this entails that the grid in one dimension is non-uniform. In general, the grid in the other two directions can be uniform. Several options exist to simulate RB convection in this bounded domain. The scientific community has used amongst others second-order finite difference [37], fourth-order finite difference [38], fourth-order finite volume [39], fourth-order compact [40], pseudo-spectral [41], lattice-Boltzmann [42] and spectral-element [43] schemes. Each of these methods are a compromise between accuracy, performance and versatility and there is no consensus on which method is best. Nevertheless, one feature of a numerical scheme is becoming increasingly important, which is the scalability on distributed memory high performance computer clusters. To utilize the modern PetaFLOP machines, numerical codes are required to scale towards tens of thousands of processors. In this thesis, a novel parallelization scheme based on a second-order finite difference code [37] is presented. It uses the locality of explicit integration and finite-difference schemes in combination with the symmetry of the domain, to obtain scalability of up to at least 64K processors.

High Pr number flows contain, by definition, sharper gradients in the temperature field than in the velocity field [44](§3). Sharp gradients require higher resolution and in case the velocity and temperature have equal resolution, the velocity field will be overresolved. This is wasteful computationally, since imposing continuity on the velocity is the most computationally expensive step in most numerical codes. For high Pr simulations it is immediately apparent that solving the velocity and temperature

on different grids, with different resolutions, will result in an increase in computational efficiency. However, it has been shown in this thesis that even for Pr is unity RB convection, the gradients of the temperature field are sharper. This means that even for generic RB convection simulations with $Pr = 1$, computational savings can be realized by using multiple resolutions. This is the reason for a new scheme with multiple grids, which is implemented and tested in this thesis.

The view on turbulent RB convection is largely based on Kolmogorov's view on homogeneous isotropic turbulence [45], where it is assumed that due to the large fluctuations, the full phase is explored. While this theory is still upheld for HIT, multiple states despite strong turbulence are recently found in various bounded inhomogeneous systems [46–50]. That transitions between different flow states in laminar flows has been well known and explored in the context of spatial-temporal chaos and pattern formation [51], but that they also occur between states in turbulent systems is surprising. The significance of this discovery is that the different states can have an effect on the global properties of the flow. In this thesis we show that this phenomenon can be studied in two-dimensional RB convection and that the heat flux depends on which roll state the flow is in. E.g., a system with two vertically stacked rolls has a different Nu than a system with three rolls. For certain control parameters, these multiple roll states can be stable. The two-dimensional domain is very convenient to study the connection between the roll states and the heat flux, as it is relatively inexpensive to simulate and easy to visualize.

These multiple states are up to now only seen in systems that are fully bounded. In RB convection, this entails that the system is not only bounded vertically by the heating and cooling plates, but also by sidewalls. The effect of temperature boundary conditions on the flow has been extensively studied and was found to be negligible [41]. However, the effect of the velocity boundary conditions, what an adiabatic sidewall essentially is, has not received much attention. It has been shown that in contrast to the temperature boundary conditions, the velocity boundary conditions have a profound effect on not only the heat flux but also the flow topology and the computational requirements. A striking example is the emergence of so-called *zonal* flows [52, 53] that appear at high Ra in two-dimensional flows with lateral periodicity and stress-free plate boundaries. Whereas the canonical roll-like flows have an increased heat flux, zonal flows can temporarily suppress heat flux completely. An exhaustive study on the effect of various velocity boundary conditions is presented in this thesis. In addition, a comparison is made between two-dimensional and three-dimensional bounded RB convection. Here, it can be seen that although 2D RB convection is very useful to understand 3D RB convection and an interesting problem with real-world applications by itself, large differences can be found, in particular at low Pr .

It is expected that there is an asymptotic regime of RB convection [3, 54, 55], named the *ultimate* regime, where the heat flux becomes independent on the molecu-

lar properties of the fluid. The basis of heat flux scaling arguments is the theoretical bound on the scaling of Nu with Ra , namely $Nu \lesssim Ra^{1/2}$ [56–58], subsequently attenuated with corrections for the heat flux through the turbulent boundary layer. This boundary layer is assumed to have a logarithmic velocity and temperature profile, analogous to the logarithmic boundary layer in turbulent pipe and channel flows [59]. The existence of this regime in Taylor-Couette flow has been confirmed [60], however, there is no such consensus in RB convection [61, 62]. The driving in TC is much more efficient than in RB, which is why the ultimate regime is relatively easily reached. The RB community consists of experimentalists that claim the observation of the transition towards the ultimate regime [29, 63], albeit at different Rayleigh numbers; experimentalist that do not observe a transition up to high Ra [30]; theoreticians that predict the existence of the ultimate regime on the basis of a shear Reynolds number [35] and theoreticians that are skeptical of the existence due to either the persistence of a viscosity dominated part of the boundary layer or the bounded nature of temperature in contrast to momentum. The numerical division stands on the sideline of this field of controversy, as current computational power prevents reaching the expected transitional Rayleigh numbers. Nevertheless, one can be suspicious of the fact that the experimental community has pushed their setups beyond their limits of validity, judging from the discrepancies between them and inconsistencies within them. Even though the required Ra cannot be reached, numerical studies are valuable in providing information on the ultimate regime.

A commonly used approach in theoretical RB convection is using horizontal averages. This approximates the RB system as a heated pipe flow, where the bulk velocity is taken as the large-scale wind velocity in RB. In line with this approximation, the boundary layer can transition to a turbulent boundary layer over the full horizontal extent simultaneously. However, evidences of a boundary layer that is locally turbulent have been found recently [64]. In this thesis we will show that, at least from a certain Ra onwards, the horizontal structure of the boundary layer has a rich variety of profiles and relate these profiles to various boundary layer regions. These regions are obscured when horizontal averages are used and can only become visible in the detailed studies such as those presented here.

Outline of the thesis

Many concepts in Rayleigh-Bénard convection are illustrated by the phenomenological Grossmann-Lohse theory [35]. The fitting coefficients used in the $Nu(Ra, Pr)$ prediction by the GL theory are recently updated and the underlying process is explained in §1. The data for two-dimensional simulations in §§4,5,8 are obtained using a fourth order finite difference code [38], while for the other chapters the second order scheme detailed in §2 is used. In §2, a new parallelization of this scheme

is described, with which high Reynolds (and Rayleigh) number wall-bounded flows can be simulated. This scheme is extended in §3 by decoupling the sizes of the grids used for the momentum and scalar fields. This provides savings to computational times even when the diffusivities of these fields are equal, but especially for cases where the scalar diffusivity is much higher. In §4 different flow states in two dimensions are connected to the heat flux, where it is shown that there is a strong dependence of the heat flux on the flow state. This is further studied as function of aspect ratio and Rayleigh number in §5. Here, also an efficient algorithm to store flow state information is presented. A more general study of the effect of the plate and sidewall velocity boundary conditions on the heat flux is described in §6. Logarithmic profiles are not only in the ultimate regime of RB convection, but also in the classical regime. Two-dimensional RB is a very suitable system to study these profiles, which is illustrated in §7. A comparison between two- and three-dimensional RB is detailed in §8. Using a numerical cylindrical system, interesting statistics of the emission of thermal plumes are extracted up to high Rayleigh numbers in §9.

The unifying theory of scaling in thermal convection: The updated prefactors*

The unifying theory of scaling in thermal convection [35] (henceforth the GL theory) suggests that there are no pure power laws for the Nusselt and Reynolds numbers as function of the Rayleigh and Prandtl numbers in the experimentally accessible parameter regime. In Grossmann and Lohse (2001) [66] the dimensionless parameters of the theory were fitted to 155 experimental data points by Ahlers and Xu (2001) [67] in the regime $3 \times 10^7 \leq Ra \leq 3 \times 10^9$ and $4 \leq Pr \leq 34$ and Grossmann and Lohse (2002) [68] used the experimental data point from Qui and Tong (2001) [69] and the fact that $Nu(Ra, Pr)$ is independent of the parameter a , which relates the dimensionless kinetic boundary thickness with the square root of the wind Reynolds number, to fix the Reynolds number dependence. Meanwhile the theory is on one hand well confirmed through various new experiments and numerical simulations. On the other hand these new data points provide the basis for an updated fit in a much larger parameter space. Here we pick four well established (and sufficiently distant) $Nu(Ra, Pr)$ data points and show that the resulting $Nu(Ra, Pr)$ function is in agreement with almost all established experimental and numerical data up to the ultimate regime of thermal convection, whose onset also follows from the theory. One extra $Re(Ra, Pr)$ data point is used to fix $Re(Ra, Pr)$. As Re can depend on the definition and the aspect ratio the transformation properties of the GL equations are discussed in order to show how the GL coefficients can easily be adapted to new Reynolds number data while keeping $Nu(Ra, Pr)$ unchanged.

*Based on: R.J.A.M. Stevens, E.P. van der Poel, S. Grossmann, D. Lohse, *The unifying theory of scaling in thermal convection: The updated prefactors*, J. Fluid. Mech. **736** 177–194 (2013) [65]

1.1 Introduction

A commonly used perspective for the heat flux scaling in RB convection is the Grossmann-Lohse (GL) theory [35, 66, 68, 70]. The basis for this theory of scaling in RB convection are exact global balances for the energy and thermal dissipation rates derived from the Boussinesq equations and the decomposition of the flow in boundary layer (BL) and bulk contributions. The scaling of the dissipation rates in the BLs is assumed to obey Prandtl-Blasius-Pohlhausen scaling [71], which is justified as long as the shear-Reynolds numbers of the BLs are not too large, and the scaling relations in the bulk are estimated based on Kolmogorov-type arguments for homogeneous isotropic turbulence. While the theory gives the different *scaling relations* for the individual contributions to the energy dissipation rates in the bulk and in the BL, namely $\epsilon_{u,bulk}$ and $\epsilon_{u,BL}$, and to the thermal dissipation rates in the bulk (background) and in the BLs (plus the plumes [70]), namely $\epsilon_{\theta,bulk}$ and $\epsilon_{\theta,BL}$, the *absolute sizes* of these four relative contributions are not given by the theory. They are expressed in four dimensionless prefactors c_i , $i = 1, 2, 3, 4$ for $\epsilon_{u,BL}$, $\epsilon_{u,bulk}$, $\epsilon_{\theta,BL}$, and $\epsilon_{\theta,bulk}$, respectively, which have to be obtained from experimental or numerical data for $Nu(Ra, Pr)$.

When the theory was developed early this century, such data were scarce and often contradicting each other, due to sidewall and plate effects, insufficient knowledge of the material properties of the fluid, lack of numerical resolution and other problems. [66] used 155 data points for $Nu(Ra, Pr)$ in the parameter range $3 \times 10^7 \leq Ra \leq 3 \times 10^9$ and $4 \leq Pr \leq 34$ obtained by [67], which was the most extensive data set at that time. This fixed $Nu(Ra, Pr)$ for *all* Ra and Pr , considered as valid up to the ultimate regime of thermal convection, where the Prandtl-Blasius type BL becomes unstable. $Re(Ra, Pr)$ was fixed [68] with one extra adoption of the prefactor a , i.e. the amplitude parameter of the Prandtl BL thickness, in the Prandtl-Blasius scaling relation $\lambda_u = aL/\sqrt{Re}$, to the experimental data of [69], where λ_u is the mean thickness of the kinetic BL and L the height of the sample.

Although the data to which we adopted the four prefactors c_i and a were relatively *local* in parameter space, the theory was rather successful in describing the *global* behavior $Nu(Ra, Pr)$ and also $Re(Ra, Pr)$, as described in detail in [87]. This included the prediction that for $Pr \approx 1$ the onset to the ultimate regime should take place when Ra is of the order of 10^{14} . This prediction was based on an assumed onset of a sheared BL instability at a shear Reynolds number $Re_s \approx 420$, which is the value given in [88]. Indeed, very recently a transition that might be that of the ultimate regime is observed around this Rayleigh number [89]. Thanks to joint efforts of the community the experimental and numerical data situation for $Nu(Ra, Pr)$ has considerably improved in the last decade. Measurements have been extended to a much larger domain in the Ra - Pr parameter space, see the updated phase diagrams in figure 1.1 and figure 1.8, and plate- and sidewall corrections are much better under-

Figure 1.1: Phase diagram in Ra - Pr plane for RB convection according to the GL-model [35, 66, 68, 70] in a $\Gamma = 1$ sample with no-slip boundary conditions. The upper solid line means $Re = 1$; the lower nearly parallel solid line corresponds to $\epsilon_{u,BL} = \epsilon_{u,bulk}$; the curved solid and dashed line is $\epsilon_{\theta,BL} = \epsilon_{\theta,bulk}$; and along the long-dashed line $\lambda_u = \lambda_\theta$, i.e., $2aNu = \sqrt{Re}$. The dash-dotted line indicates where the laminar kinetic BL is expected to become turbulent, based on a critical shear Reynolds number $Re_s^* = 1014$ of the kinetic BL, see text. The data are from [67, 72–86]. Note that for the Stevens et al. data, points from different papers have been combined in the graph. The four large red open squares indicate the location of the four $Nu(Ra, Pr)$ points and the large red open circle the $Re(Ra, Pr)$ point that have been used for the new GL-fit.

stood and taken into account [77, 87, 90–93]. One notices that for $\Gamma = 1/2$ higher Ra number values have been obtained than for $\Gamma = 1$, while the Pr number dependence is much more explored for $\Gamma = 1$ than for $\Gamma = 1/2$. Furthermore, due to the increasing computational power and better codes the numerical data are now well converged, confirming and complementing the experimental data. Meanwhile [31, 94] achieved $Ra = 2 \cdot 10^{12}$ at $Pr = 0.7$ in a $\Gamma = 1/2$ sample and obtained a good agreement with the experimental data of [89] and [30].

This situation calls for a *refit* of the four prefactors c_i and a of the GL theory, in spite of the success of the theory with the coefficients of [66]: It is clear that the surface $Nu(Ra, Pr)$ above the Ra-Pr parameter space will be much more stable and "wobble" less if we put it on four distant and trustable "legs" $Nu_i(Ra_i, Pr_i)$, $i = 1, 2, 3, 4$, rather than putting it on four "legs" somewhere in the center but close to each other. As we will see $Nu(Ra, Pr)$ is only determined by the choice of these four $Nu(Ra, Pr)$ data points from experiments. The accuracy of the GL-fit is verified by comparing it with several data sets over a wide parameter regime and by making a second fit that reveals in which regimes there is some uncertainty. Including more data points in the fitting procedure does not lead to better fits since data tend to be clustered in the phase space. Therefore including more data points increases the weight of some data without actually adding additional physical information. An additional Reynolds number measurement is necessary to fix a and the relation between a and Re_L , which is the Reynolds number for which no bulk is left and the whole flow consists of laminar boundary layer as will be explained below. The shortcoming of the old set of c_i , a , and Re_L was particularly obvious for small Pr, say $Pr \leq 1$ (see figure 1.5), because at the days of [66] no reliable information was available in that parameter regime and therefore no Nusselt data of that regime had been included into the fit.

The structure of the chapter is as follows: In section 2 we will provide the refit of the GL theory for an aspect ratio $\Gamma = 1$, leading to $Nu(Ra, Pr)$ in the whole parameter space up to the ultimate state. In section 3 we discuss the robustness of the fit. In section 4 we will show that this fit also describes the available data for $\Gamma = 1/2$ and will in particular discuss the onset of the ultimate regime. Section 5 gives conclusions and an outlook on the new challenges.

Figure 1.2: Compensated three-dimensional visualization of a) $Nu(Ra,Pr)$ and b) $Re(Ra,Pr)$. The four $Nu(Ra,Pr)$ points and the $Re(Ra,Pr)$ point used to fit the GL parameters $c_1 = 8.05$, $c_2 = 1.38$, $c_3 = 0.487$, $c_4 = 0.0252$ have been indicated by the black points in the $Nu(Ra,Pr)$ and $Re(Ra,Pr)$ graph, respectively.

1.2 Refit of the GL theory for $\Gamma = 1$

The GL theory describes $Nu(Ra,Pr)$ and $Re(Ra,Pr)$ with the following two coupled equations [87],

$$(Nu - 1)RaPr^{-2} = c_1 \frac{Re^2}{g(\sqrt{Re_L/Re})} + c_2 Re^3, \quad (1.1)$$

$$Nu - 1 = c_3 Re^{1/2} Pr^{1/2} \left\{ f \left[\frac{2aNu}{\sqrt{Re_L}} g \left(\sqrt{\frac{Re_L}{Re}} \right) \right] \right\}^{1/2} + c_4 Pr Re f \left[\frac{2aNu}{\sqrt{Re_L}} g \left(\sqrt{\frac{Re_L}{Re}} \right) \right], \quad (1.2)$$

where the crossover functions f and g model the crossover from the thermal boundary layer nested in the kinetic one towards the inverse situation and that for which $\lambda_u \sim L$ loses its scaling with Re since λ_u extends to sample half-height $L/2$ and cannot increase further with decreasing Re ; for details see [66]. As described by [68] the prefactor a has to be determined from experimental data. Whereas the definition of the Nusselt number is very clear there are various reasonable ways to define a Reynolds number. We decided to use one experimental data point of [69] to determine the value of a and from figure 1 of [68] we read $Ra = 4.2 \cdot 10^9$, $Pr = 5.5$, $Re = 2.1 \cdot 10^3$. In addition we demand for the Reynolds number Re_L that $\lambda_u = aL/\sqrt{Re_L} = L/2$, meaning that $Re_L = (2a)^2$ is fixed for given a .

In order to get accurate values for the four dimensionless prefactors c_i , it is necessary to choose four data points with as much information on the richness of the RB

Figure 1.3: Comparison of the Ra-scaling of the original GL-fit from [66] (a) with the new fit (b) for water, i.e. $Pr = 4.38$ unless mentioned otherwise, in a $\Gamma = 1$ sample. The circles [79] and squares [95] indicate experimental results. Open symbols indicate the uncorrected data and solid symbols the data after correction for the finite plate conductivity. The diamonds [96] ($Pr = 5.4$), right pointing triangles [97], and left pointing triangles [39] indicate results from numerical simulations. The solid (black) line indicate the GL fit of section 1.2 and the dashed (blue) line the GL fit in section 1.3.

Figure 1.4: Comparison of the Ra-scaling of the original GL-fit from [66] (a) with the new fit (b) in a $\Gamma = 1/2$ sample and varying Pr , see phase diagram in figure 1.8. The right pointing triangles are the experimental data from [98] with wall corrections [80], left pointing triangles [74], upward pointing triangles [76], downward pointing triangles [99], diamonds [30], crosses [100], hexagons [80], circles [89, 101], and plusses [102, 103] indicate experimental data and the squares results from numerical simulations [31, 94]. The solid (black) line indicate the GL fit of section 1.2 and the dashed (blue) line the GL fit in section 1.3.

Figure 1.5: Comparison of the Pr-scaling of the original GL-fit from [66] (a) with the new fit (b) for different Ra. The right pointing triangle [72], left pointing triangle [21], and the upward pointing triangle [104] indicate experimental results. The circles [86] and squares [105] indicate numerical results obtained in a cylinder with aspect ratio $\Gamma = 1$. The plusses [106] indicate numerical results obtained in a periodic domain and the diamonds [107] and crosses [108] numerical results obtained in a box with free slip boundary condition at the sidewall. The colors black, purple, magenta, red, and blue (from bottom to top) corresponds to the Ra numbers 5×10^5 , 10^6 , 5×10^6 , 10^7 , and 10^8 . The solid lines indicate the GL fit of section 1.2 and the dashed lines the GL fit in section 1.3.

system as possible, which means that data points from different regimes should be selected. Therefore we determined the c_i from the data points of [79] at $Ra = 1.8 \times 10^7$ and $Ra = 2.25 \times 10^{10}$, both with $Pr = 4.38$, the data point from [75] with $Pr = 818$ at $Ra = 2.04 \times 10^8$, and the data point from [72] at $Ra = 1 \times 10^7$ with $Pr = 0.025$. The location of these data points in the RB phase diagram is indicated by the large red squares in figure 1.1 and by the black dots in the corresponding three-dimensional $Nu(Ra, Pr)$ visualization in figure 1.2a. Figure 1.1 shows that these data are indeed within different regimes. The reason for choosing these specific data points is two-fold. First of all we consider these four data points to be reliable. And apart from the data point by [75], which is the only experiment in that large Pr regime, all data points agree very well with experimental or numerical data from other groups, see figures 1.3 and 1.5. In addition, these four data points are relatively far apart in the Ra-Pr parameter space to ensure that they provide the theory with as much information on the richness of the RB physics as possible. To provide information on the Ra-scaling we selected the measurements of [79] at $Ra = 1.8 \times 10^7$ and $Ra = 2.25 \times 10^{10}$ with $Pr = 4.38$. In order to include information on the transition between the 'upper' and 'lower' regimes, which is modeled by the crossover functions f and g , it is necessary to include data points in the low, intermediate, and high Pr number regime. We do this selecting next to the intermediate Pr number data from [79], the low $Pr = 0.025$ num-

ber measurement by [72] at $Ra = 1 \times 10^7$ and the high $Pr = 818$ measurement by [75] at $Ra = 2.04 \times 10^8$. Altogether the four data points provide information from three different Pr numbers and four different Ra numbers. From these four data points, and an initial guess for a , we determine the c_i with a fourth order Newton-Raphson root finding method or by using a trust-region-reflective optimization algorithm, which both gave the same result. Subsequently, the $Re(Ra, Pr)$ point of [69] is used to find the appropriate value of a with the transformation property of the GL model [68], which is described below in detail. Due to this transformation property of the GL equations the four $Nu(Ra, Pr)$ data points determine the Nusselt number dependence, while the Re number data point of [69] fixes the absolute value of the Reynolds number throughout the phase space. This results in the following five GL parameters $c_1 = 8.05$, $c_2 = 1.38$, $c_3 = 0.487$, $c_4 = 0.0252$, and $a = 0.922$. The difference in significant number is due to the fact that some coefficients are less sensitive to uncertainty than others.

It was pointed out by [68] that $Nu(Ra, Pr)$ is invariant and thus independent of the parameter a under the following transformation

$$Re \rightarrow \alpha Re, \quad (1.3)$$

$$a \rightarrow \alpha^{1/2} a, \quad (1.4)$$

$$c_1 \rightarrow c_1 / \alpha^2, \quad (1.5)$$

$$c_2 \rightarrow c_2 / \alpha^3, \quad (1.6)$$

$$c_3 \rightarrow c_3 / \alpha^{1/2}, \quad (1.7)$$

$$c_4 \rightarrow c_4 / \alpha, \quad (1.8)$$

$$Re_L \rightarrow \alpha Re_L. \quad (1.9)$$

We note that the above transformation is consistent with the relation $Re_L = (2a)^2$ used above and allows for the transformation of the above set of coefficients to different Reynolds number definitions or aspect ratios. Such a new set of coefficients is obtained by first determining α . Here α is determined as $Re_1(Ra, Pr)/Re_2(Ra, Pr)$, where Re_1 is the Reynolds number value of a measurement point in the data set at a given Ra and Pr and Re_2 is the Reynolds number value obtained from the GL model with the coefficients mentioned above. Subsequently, equations (1.4) to (1.9) can be used to calculate the new coefficients.

In figures 1.3 to 1.5 we compare the original GL-fit from [66] with this new GL-fit. These figures clearly reveal that the new GL-fit is much closer to the data in the low Pr number regime, while maintaining the similar excellent agreement for the high Pr number data as before. We emphasize that this excellent agreement with all other presently available data from experiments and simulations confirms that the c_i and a values we calculated describes $Nu(Ra, Pr)$ well in the regime that is nowadays covered by state of the art experiments and simulations. It is also noteworthy that

figure 1.3 and 1.4 show that the Nu number scaling with Ra is well predicted by the GL-theory for Ra values that are decades higher than the highest Ra number point that is used to determine the c_i values, namely $Ra = 2.25 \times 10^{10}$, thus showing the predictive power of the GL-theory.

1.3 Robustness

To illustrate the robustness of the fit presented above, we made a second fit to four other data points, i.e. the data points from [79] at $Ra = 2.96 \times 10^7$ and $Ra = 1.92 \times 10^{10}$ with $Pr = 4.38$, the one from [75] at $Ra = 2.24 \times 10^8$ with $Pr = 554$ and finally the data point by [107] at $Ra = 10^7$ with $Pr = 0.07$. Three out of these four data points lie relatively close to the original four data points, but the low $Pr = 0.07$ point from [107] substantially differs from the original $Pr = 0.025$. The reason that three of the four points are close to the original four points in the $Ra - Pr$ parameter space is that one can only select "reliable legs" in regimes where many measurements have been done and these regimes only cover a limited part of the parameter space.

The resulting GL coefficients are $c_1 = 11.8$, $c_2 = 1.33$, $c_3 = 0.528$, $c_4 = 0.0222$, and $a = 0.843$ compared to $c_1 = 8.05$, $c_2 = 1.38$, $c_3 = 0.487$, $c_4 = 0.0252$, and $a = 0.922$ of the fit described above. In order to compare the two fits we show both fits together with experimental and numerical data from several experiments in figures 1.3, 1.4, 1.5, and 1.7. In addition we give the relative difference in $Nu(Ra, Pr)$ calculated in the fit described in the previous section and Nu calculated from this additional fit in the parts of the parameter space where the GL fit is valid in figure 1.6. A comparison between both fits shows that the difference is very minor in the regimes IV_u , II_u , and I_u , and that the differences increase in the regimes II_l , IV_l , and III_u , which are very far away from the region in the parameter space where reliable data points are available. The reason is that a very small variation in the measurements point can lead to significant differences if the implied information is extrapolated over many decades in Ra and Pr using the GL-theory. For the fits compared here the differences increase up to about 10%. We find that the differences are mainly caused by the uncertainty in the [75] data, which is reflected by the two different data points we took from this data set. In figure 1.7 we compare the [75] measurements with the original GL-fit from [66], and the two fits presented in this work. Panels a, b and c show that the measured $Nu/Ra^{1/3}$ decreases faster with increasing Ra than predicted by the GL model. A comparison of the [75] data with other data obtained at $Pr = 4.38$ shows that the measurements in the lower Ra number regime collapse very well with other measurements, while for the higher Ra the measured Nusselt number seems a little lower in the [75] experiments than in other experiments. Figure 1.7d compares the [75] measurements between $Ra \approx 2 \times 10^8$ and $Ra \approx 2.4 \cdot 10^8$ with the different GL-fits and shows that the fit presented in section 1.2 uses a high Pr number point

Figure 1.6: Relative difference between Nu calculated from the original fit and Nu calculated from the additional fit. The color scale ranges from black to white, indicating agreement mostly up to $\approx 4\%$. Only in two small ranges, III_u and IV_l , it goes up to 10%.

that aligns with the reliable $Pr = 4.38$ data point, while the second fit uses a high Pr number point of the lower branch. In this way the uncertainty of these measurements is reflected by the two fits and as is shown in figure 1.6 this difference is mostly visible near regime I_∞ and III_∞ .

1.4 GL theory for $\Gamma = 1/2$ and ultimate regime

In principle, the c_i depend on the aspect ratio Γ . However, it is well known that only small differences in Nu are observed between $\Gamma = 1/2$ and $\Gamma = 1$ [87]. This weak aspect ratio dependence is confirmed by figure 1.4, which shows that the Ra number scaling for $Pr = 0.7$ in a $\Gamma = 1/2$ sample is captured very accurately by the new fit for $\Gamma = 1$, and in the low Ra number regime the new fit is even much better than the original GL-fit from [66].

The location in Ra-Pr space of the various regimes of the GL theory is based on the coefficients c_i and a . The updated lines that encompass the regimes are plotted in the phase diagrams shown in figures 1.1 and 1.8. The line that indicates the onset of the ultimate regime, where the kinetic boundary layer has become turbulent, is now based on the new coefficients, the transition at $Ra = 5 \cdot 10^{14}$, observed by [89] for $Pr = 0.86$, and the Re number measurements by [69]. This gives $Re_s^* = 1039$ ($a = 0.922$) and for the second fit we made, see section 1.3, we get $Re_s^* = 954$ ($a = 0.843$). In a $\Gamma = 1/2$ sample [89] found experimentally that $Re = 0.252Ra^{0.434}Pr^{0.750}$ using a recently developed and tested elliptic approximation [89, 109–112], which defines Re unambiguously, based on properties of correlation functions. Using this relation at $Ra = 10^{13}$ and $Pr = 0.86$ this gives $Re_s^* = 572$ with $a = 0.684$ for the first fit, see section 1.2, and $Re_s^* = 521$ with $a = 0.623$ for the second fit we made, see section

Figure 1.7: Panel a, b, and c show the Nusselt number measurements of [75] versus Ra in comparison to the original GL-fit from [66] (panel a), the GL fit presented in section 1.2 (panel b), and the second fit discussed in section 1.3. Panel d shows the Pr number dependence of the [75] experiments for $Ra \approx 2 \times 10^8$ compared to the three different GL fits mentioned above.

1.3. These Re_s^* values are different from the previously used $\text{Re}_s^* = 420$ with $a = 1.72$ taken from pipe flow [88]. From the transformation property of the GL equations one gets that Re_s^* increases by a factor of α when Re increases by a factor α , while a increases by a factor $\sqrt{\alpha}$. The a values found here are significantly different from $a = 0.482$, which was found by [68]. Calculating the Re_s^* values equivalent to $a = 0.482$ from the a and Re_s combinations mentioned above, i.e. $a = 0.843$ with $\text{Re}_s^* = 954$, $a = 0.922$ with $\text{Re}_s^* = 1039$, $a = 0.684$ with $\text{Re}_s^* = 572$, and $a = 0.623$ with $\text{Re}_s^* = 521$, gives $\text{Re}_s^* = 298 \pm 15$ for the new coefficients, so we see that the notification of Re_s^* alone, without a is not sufficient.

The phase diagram in figure 1.8 shows that the measurements of [89] up to $\text{Ra} \approx 10^{15}$ at $\text{Pr} = 0.86$ are up to now the only experiments that likely have reached the expected ultimate regime. They observe a transition that could be the onset of the ultimate regime at $\text{Ra} = 5 \cdot 10^{14}$ and a transition region for $10^{13} \leq \text{Ra} \leq 5 \cdot 10^{14}$. The experiments by [89] are the only room temperature experiments for $\text{Ra} \gtrsim 10^{12}$, while all other experiments that have reached these Ra numbers are low temperature experiments with Helium close to the critical point [30, 63, 80, 99, 102, 103, 113, 114]. In these low temperature experiments it is difficult to reach the ultimate regime because the Pr number increases with increasing Ra , see figure 1.8. Nevertheless the low temperature experiments by [30] seem to come very close to the ultimate regime and one may wonder why the transition region observed by [89] was not observed in the [30] experiments. As discussed in detail by [101], presumably the scatter of the [30] data at this highest Ra (which seems to be due primarily to the uncertainties in the fluid properties) as well as the fact that the transition is smooth are the reasons for this. Figure 1.4 shows that the magnitude of the scatter in the [30] data is similar to the observed increase in the compensated Nusselt number in the transition regime by [89]. The phase diagram also shows that other low temperature experiments by [63, 99], [80], and [102, 103] do not reach the transition to the ultimate regime based on a critical shear Reynolds number and therefore no transition due to a boundary layer shear instability is expected in these experiments.

1.5 Conclusions and outlook

In this chapter we have used the availability of new experimental and numerical data, and our increased understanding of the physics of the Rayleigh-Bénard system to determine the prefactors of the unifying theory for scaling in thermal convection, i.e. the GL theory, much more accurately. The resulting $\text{Nu}(\text{Ra}, \text{Pr})$ function is in very good agreement with almost all established experimental and numerical data up to the ultimate regime of thermal convection, and has significantly improved the predictions. In figure 1.4 one can notice an onset of what might be the ultimate regime in the $\text{Nu}(\text{Ra})$ scaling of the measurements of [89]. Extensions of the GL theory to

◀ Castaing et al. (1989)	■ Ahlers and Xu (2001)	▲ Roche et al. (2010)
▶ Chavanne et al. (1997)	◆ Chaumat et al. (2002)	▼ Stevens et al. (2010–2011)
▲ Glazier et al. (1999)	▶ Burnishev et al. (2010)	■ Urban et al. (2011–2012)
▼ Niemela et al. (2000)	▶ Ahlers et al. (2009)	● He et al. (2012)

Figure 1.8: Phase diagram in Ra-Pr plane for RB convection in a $\Gamma = 1/2$ sample with no-slip boundary conditions. The lines are the same as in figure 1.1. The data are from [30, 31, 63, 67, 73, 76, 80, 81, 87, 89, 94, 98, 102, 103].

the ultimate regime by [55] are able to explain the observed Reynolds number scaling in that regime as well as the origin of the log-profiles observed in the claimed ultimate regime by [64].

In line with [66], we have determined the prefactors from experimental measurements. This has great value as it shows that the information of only five data-points is sufficient to accurately predict $Nu(Ra, Pr)$ and $Re(Ra, Pr)$ up to the ultimate regime. All is based on the GL theory, which builds on exact global balances for the energy and thermal dissipation rates, derived from the Boussinesq equations, and the decomposition of the flow in boundary layer and bulk contributions. A finding with further implications is that the value a , i.e. the amplitude parameter of the Prandtl BL thickness, is higher than found by [68]. This a value is for example used by [44] to determine the number of grid points that should be placed in the boundary layers. [44] compared the theoretical predictions with results from simulations in $\Gamma = 1/2$ samples. For this aspect ratio the newly found value of a ($a = 0.684$ for fit of section 1.2 and $a = 0.623$ of section 1.3) is higher, but still relatively close to the previously used $a = 0.482$. However, it looks like that for $\Gamma = 1$ case a is even higher ($a = 0.922$ for the fit of section 1.2 and $a = 0.843$ for the fit of section 1.3), which could have implications for the resolution that should be used in simulations. This finding confirms the conclusions of [94] who pointed out that the only way to really confirm that the used numerical resolution is sufficient is to obtain the same Nusselt number with different grids resolutions as there is namely always some uncertainty in estimates of the required grid resolution.

A further challenge we want to pursue is to calculate the c_i and a directly from the fluid equations, without the input of any experimental or numerical data, or at least quantitatively relate their values to important fluid concepts like Prandtl-Blasius-Pohlhausen theory, the von Karman-Prandtl theory, etc. in order to get an even deeper understanding of the GL theory.

A pencil distributed code for strongly turbulent wall-bounded flows*

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

*Based on: E. P. van der Poel, R. Ostilla-Mónico, J. Donners and R. Verzicco, *A pencil distributed code for strongly turbulent wall-bounded flows*, Comp. Fluids, **116** 10–16 (2015) [115]. Parallelization and initial coding by van der Poel. Implementation of Poisson solver and new time-marching scheme by Ostilla-Mónico. Donners provided later help with optimizing the code. Writing and discussion done by everybody.

2.1 Introduction

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

The seminal works on homogeneous isotropic turbulence by Orszag & Patterson [116] and on pressure-driven flow between two parallel plates (also known as channel flow) by Kim, Moin and Moser [117], while difficult back then, could be performed easily on contemporary smartphones. Computational resources grow exponentially, and the scale of DNS has also grown, both in memory and floating point operations (FLOPS). In approximately 2005, the clock speed of processors stopped increasing, and the focus shifted to increasing the number of processors used in parallel. This presents new challenges for DNS, and efficient code parallelization is now essential to obtaining scientific results.

Efficient parallelization is deeply tied to the underlying numerical scheme. A wide variety of these schemes exist; for trivial geometries, i.e. domains periodic in all dimensions, spectral methods are the most commonly used [118]. However, for the recent DNS of wall-bounded flows, a larger variation of schemes is used. For example, in the present year, two channel flow DNSs at similar Reynolds numbers detailed DNSs were performed using both a finite-difference schemes (FDS) in the case of Ref. [119] or a more complex spectral methods in the case of Ref. [120]. FDS also present several advantages, they are very flexible, allowing for complex boundary conditions and/or structures interacting through the immersed boundary method with relative ease [121]. A commonly asserted disadvantage of low-order FDS is the higher truncation error relative to higher order schemes and spectral methods. However, this is only true in the asymptotic limit where the grid spacing becomes sufficiently fine, i.e. $\Delta x \rightarrow 0$, that is commonly not reached. Additionally, aliasing errors are much smaller for lower order schemes [122, 123]. Lower-order schemes have been shown to produce adequate first- and second-order statistics, but require higher resolution when compared to spectral methods for high order statistics [124–126]. Because lower-order schemes are computationally very cheap the grid resolution can in general be larger for the same computational cost compared to higher order schemes, although one has to consider the higher memory bandwidth over FLOPS ratio.

In this chapter, we will detail the parallelization of a second-order FDS based on the approach by Verzicco & Orlandi [37] to two wall bounded systems, Rayleigh-

Bénard (RB) convection, the flow in a fluid layer between two parallel plates; one heated from below and cooled from above and Taylor-Couette (TC) flow, the flow between two coaxial independently rotating cylinders; although our code can easily be extended to any flow that is wall-bounded in one dimension. This FDS scheme has already been used in pure Navier-Stokes simulations [37], Navier-Stokes simulations combined with immersed boundary methods [127], for Rayleigh-Bénard convection [86, 128–133] and for Taylor-Couette flow [60, 134]. The numerical results have been validated against experimental data numerous times. We will exploit several advantages of the large Re regime and the boundary conditions to heavily reduce communication cost; opening the possibility to achieve much higher drivings.

The chapter is organized as follows: §2.2 describes TC and RB in more detail. In §2.3 the numerical scheme which is used to advance the equations in time is detailed. In §2.4 we show that in thermal convection, the Courant-Friedrichs-Lewy (CFL) [135] stability constraints on the time-step due to the viscous terms become less strict than those due to the nonlinear terms at high Rayleigh (Reynolds) numbers. In §2.5 we detail a pencil decomposition to take advantage of the new time integration scheme and the choice of data arrangement in the pencil decomposition. Finally, in §2.6 we compare the computational cost of the existing and the new approach and present an outlook of what further work can be done to combine this approach with other techniques.

2.2 Rayleigh-Bénard convection and Taylor-Couette flow

RB and TC are paradigmatic models for convective and shear flows, respectively. They are very popular systems because they are mathematically well defined, experimentally accessible and reproduce many of the interesting phenomena observed in applications. A volume rendering of the systems can be seen in figure 2.1. The Reynolds numbers in the common astro- and geophysical applications are much higher than what can be reached currently in a laboratory. Therefore it is necessary to extrapolate available experimental results to the large driving present in stars and galaxies. This extrapolation becomes meaningless when transitions in scaling behavior are present, and it is expected that once the Rayleigh number, i.e. the nondimensional temperature difference, becomes large enough, the boundary layers transition to turbulence. This transition would most likely affect the scaling of interesting quantities. However, experiments disagree on exactly where this transition takes place [29, 80]. DNS can be used to understand the discrepancies amongst experiments. However, to reach the high Rayleigh numbers (Ra) of experiments new strategies are required. DNS must resolve all scales in the flow, and the scale separation between the smallest scale and the largest scale grows with Reynolds number. This means larger grids are needed, and the amount of computational work W scales

Figure 2.1: Left: RB flow for $Ra = 10^8$, $Pr = 1$ and $\Gamma = 2$ in Cartesian coordinates. The horizontal directions are periodic and the plates are subjected to a no-slip and isothermal boundary condition. Red/yellow indicates hot fluid, while (light) blue indicates cold fluid. The small heat carrying structures known as thermal plumes as well as a large-scale circulation can be seen in the visualization, highlighting the scale separation in the flow. Right: TC flow with an inner cylinder Reynolds number $Re = 10^5$, a stationary outer cylinder, and a radius ratio $\eta = r_i/r_o = 0.714$. Green fluid has a high angular velocity while blue fluid has a low angular velocity. The smallness of the structures responsible for torque transport, and thus the need for fine meshes, can be appreciated clearly.

approximately as $W \sim Re^4$ [136].

Simulations of RB commonly imitate the cylindrical geometry most used in experiments. Recently, a DNS with aspect ratio $\Gamma = D/L = 1/3$, where D is the diameter of the plates and L the height of the cell, reached $Ra = 10^{12}$ using 1.6 Billion points with a total cost of 2 Million CPU hours [32]. DNS in other geometries have been proposed, such as homogeneous RB, where the flow is fully periodic and a background temperature gradient is imposed. This geometry is easy to simulate [62], but presents exponentially growing solutions and does not have a boundary layer, thus not showing any transition [137]. Axially homogeneous RB, where the two plates of the cylinder are removed, the side-walls kept, and a background temperature gradient is imposed to drive the flow has also been simulated (e.g. in Ref. [43]). This system does not have boundary layers on the plates and does not show the sought after transition. Therefore, it seems necessary to keep both horizontal plates, having at least one wall-bounded direction. The simplest geometry we can simulate with these requirements is a parallelepiped box, periodic in both wall-parallel directions, which we will call “rectangular” RB for simplicity. Rectangular RB is receiving more attention recently [42, 138–140], due to possibility to reach higher Ra as compared to

more complex geometries. It is additionally the geometry that is closest to natural applications, where there are commonly no sidewalls.

For TC, we have one naturally periodic dimension, the azimuthal extent. The axial extent can be chosen to be either bounded by end-plates, like in experiments, or to be periodic. Axial end-plates have been shown to cause undesired transitions to turbulence if TC is in the linearly stable regime [141], or to not considerably affect the flow if TC is in the unstable regime [142]. Large Re DNS of TC focus on axially periodic TC, bounding the flow only in the radial direction [60, 143]. Therefore, the choice of having a single wall-bounded direction for DNS of both TC and RB seems justified.

2.3 Numerical scheme

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

The nondimensional Navier-Stokes equations with the Boussinesq approximation for RB read in vector notation:

$$\nabla \cdot \mathbf{u} = 0, \quad (2.1)$$

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \sqrt{\frac{\text{Pr}}{\text{Ra}}} \nabla^2 \mathbf{u} + \theta \mathbf{e}_x, \quad (2.2)$$

$$\frac{\partial \theta}{\partial t} + \mathbf{u} \cdot \nabla \theta = \sqrt{\frac{1}{\text{PrRa}}} \nabla^2 \theta, \quad (2.3)$$

where $\mathbf{u}$ is the nondimensional velocity and $\mathbf{e}_x$ is the unitary vector in the anti-parallel direction to gravity, which is also the plate-normal direction.

As mentioned previously, the two horizontal directions are periodic and the vertical direction is wall-bounded. The spatial discretization used is a conservative second-order centered finite difference with velocities on a staggered grid. The pressure is calculated at the center of the cell while the temperature field is located on the u_x grid. This is to avoid the interpolation error when calculating the term $\theta \mathbf{e}_x$ in equation (2.2), and thus to exactly conserve the transformation of potential energy into kinetic energy. The scheme is energy conserving in the limit $\Delta t \rightarrow 0$. A two-dimensional (for clarity) schematic of the discretization is shown in figure 2.2. For the case of thermal convection, an additional advantage of using FDS is present: the

Figure 2.2: Location of pressure, temperature and velocities of a 2D simulation cell. The third dimension (z) is omitted for clarity. As on an ordinary staggered scheme, The velocity vectors are placed on the borders of the cell and pressure is placed in the cell center. The temperature is placed on the same nodes as the vertical velocity, to ensure exact energy conservation.

absence of pressure in the advection/diffusion equation for scalars can cause very sharp gradients in the temperature (scalar) field (§3) and low-order schemes fare better in this situation.

Time marching is performed with a fractional-step third-order Runge-Kutta (RK3) scheme, in combination with a Crank-Nicholson scheme [124] for the implicit terms. A second-order Adams-Bashforth (AB2) method is also implemented in the code. However, in all production runs the RK3 method takes precedence over AB2 even though the total RK3 time step includes three substeps as compared to one for AB2. The theoretical stability limit of AB2 and RK3 are CFL numbers lower than 1 and $\sqrt{3}$, respectively. In practice, the maximum CFL numbers of AB2 and RK3 are approximately 0.3 and 1.3, respectively. Because of three times higher amount of substeps in RK3, the computational cost is proportionally higher compared to AB2. Nevertheless, RK3 is more efficient as the progression in physical time per computational cost is better. In addition, even though the Crank-Nicholson integration with $\mathcal{O}([\Delta t]^2)$ error is the weakest link, the $\mathcal{O}([\Delta t]^3)$ error of RK3 decreases the total error significantly compared to the $\mathcal{O}([\Delta t]^2)$ error of AB2. In addition, RK3 is self-starting at each time step without decreasing the accuracy and without needing additional information in the restart file. AB2 would require two continuation files per quantity.

The pressure gradient is introduced through the “delta” form of the pressure [144]: an intermediate, nonsolenoidal velocity field $\mathbf{u}^*$ is calculated using the nonlinear, the viscous and the buoyancy terms in the Navier-Stokes equation, as well as the pressure at the current time sub-step:

$$\frac{\mathbf{u}^* - \mathbf{u}^j}{\Delta t} = \left[\gamma_l H^j + \rho_l H^{j-1} - \alpha_l \mathcal{G} p^j + \alpha_l (\mathcal{A}_x^j + \mathcal{A}_y^j + \mathcal{A}_z^j) \frac{(\mathbf{u}^* + \mathbf{u}^j)}{2} \right], \quad (2.4)$$

where the superscript j denotes the sub-step, $\mathcal{A}_i$ is the discrete differential relationship for the viscous terms in the i th-direction, $\mathcal{G}$ the discrete gradient operator and H^j all explicit terms. The coefficients γ_l , ρ_l and α_l depend on the time marching method used. The pressure required to enforce the continuity equation at every cell is then calculated by solving a Poisson equation for the pressure correction ϕ :

$$\nabla^2 \phi = \frac{1}{\alpha_l \Delta t} (\nabla \cdot \mathbf{u}^*), \quad (2.5)$$

or in discrete form:

$$\mathcal{L} \phi = \frac{1}{\alpha_l \Delta t} (\mathcal{D} \mathbf{u}^*), \quad (2.6)$$

where $\mathcal{D}$ the discrete divergence operator, and $\mathcal{L}$ is the discrete Laplacian operator, $\mathcal{L} = \mathcal{D} \mathcal{G}$. The velocity and pressure fields are then updated using:

$$\mathbf{u}^{j+1} = \mathbf{u}^* - \alpha_l \Delta t (\mathcal{G} \phi), \quad (2.7)$$

and

$$p^{j+1} = p^j + \phi - \frac{\alpha_l \Delta t}{2\text{Re}} (\mathcal{L} \phi), \quad (2.8)$$

making $\mathbf{u}^{j+1}$ divergence free.

The original numerical scheme treats all viscous terms implicitly. This would result in the solution of a large sparse matrix, but this is avoided by an approximate factorization of the sparse matrix into three tridiagonal matrices; one for each direction [37]. The tridiagonal matrices are then solved using Thomas' algorithm, with a Sherman-Morrison perturbation if the dimension is periodic, in $\mathcal{O}(N)$ time. The calculation is thus simplified at the expense of introducing an error $\mathcal{O}(\Delta t^3)$. This method was originally developed and used for small Reynolds number problems, and without having in mind that data communication between different processes could be a bottleneck. The first parallelization scheme with MPI was a 1D-domain "slab" decomposition, visualized in the figure 2.3(a). The main bottlenecks were found in the all-to-all communications present in the pressure-correction step and the tridiagonal solver in the direction in which the domain is decomposed (cf. table 2.1 for more details). Slab decompositions are easy to implement, but are limited in two ways: First, the number of MPI processes cannot be larger than N , the amount of grid points in one dimension. A hybrid MPI-OpenMP decomposition can take this

Figure 2.3: Left panel: Slab-type domain decomposition using four MPI processes. Right panel: Pencil-type domain decomposition using twelve MPI processes.

limit further, but scaling usually does not go further than $\mathcal{O}(10^4)$ cores. Second, the size of the “halo” (or ghost) cells becomes very significant with increasing number of cores. Halo cells are cells which overlap the neighbor’s domain, and whose values are needed to compute derivatives. In the limit of one grid point per processor, halo cells are of the size of the domain in a second-order scheme, and even larger for higher order schemes.

2D-domain decompositions, also known as “pencil” decompositions, mitigate these problems. A schematic of this decomposition is shown in figure 2.3(b). To implement this decomposition, the 2DECOMP [145] library has been used, and extended upon to suit the specifics of our scheme. The limit on the amount of processes is now raised to N^2 , and the size of the halo cells on every core decreases with increasing amount of cores, so the amount of communication per core decreases. However, for a pencil decomposition solving all the tridiagonal matrices requires all-to-all communications for two directions, instead of one direction, as in the case of slab decomposition. As mentioned previously, solving the tridiagonal matrices involves large data communication, especially in the context of pencil decompositions. In this chapter we attempt to eliminate them as far as possible and at the same time implement an efficient pencil domain decomposition by arranging the data to gain advantage of the inherent anisotropy with respect to the grid point distributions.

2.4 Constraints on the timestep

In the new scheme, solving the tridiagonal matrices in the horizontal directions is avoided by integrating not only the advection terms but also the viscous terms explicitly. A major concern is that this can cause the temporal stability issues that the

implicit integration used to negate. In this section we argue that for high Ra , using the Courant-Frederich-Lewy (CFL) [135] time-step size constraint is sufficient. The CFL condition ensures the stability of the integration of the advection terms, and for high Ra it additionally ensures stability of the viscous terms. The grid point distribution in the wall-normal direction is different compared to the periodic directions. Namely, it is nonuniform in the wall-normal direction, with clustering of points near the boundaries in order to adequately resolve the boundary layers. As the periodic directions are homogeneous, no such clustering is required and the grid point distribution can be uniform. As a consequence, the minimum grid spacing in the wall-normal direction is much smaller than in the horizontal directions. Because of the scaling of both the time-step constraints, the viscous terms in the wall-normal direction do require implicit integration for all Ra .

In this semi-implicit method, both viscous terms and the nonlinear terms are integrated explicitly. This requires two stability constraints on the time-step: one due to the nonlinear terms, and one due to the horizontal viscous terms. For the nonlinear terms, the definition of the CFL condition is given by:

$$\Delta t_{\mathbf{u} \cdot \nabla \mathbf{u}} \leq \mathcal{C}_1 \min_{\forall \mathbf{x} \in X} \frac{1}{\frac{|u_x|(\mathbf{x})}{\Delta x(\mathbf{x})} + \frac{|u_y|(\mathbf{x})}{\Delta y(\mathbf{x})} + \frac{|u_z|(\mathbf{x})}{\Delta z(\mathbf{x})}}, \quad (2.9)$$

where $\mathcal{C}_1$ is the integration scheme dependent Courant number, $\mathbf{x}$ is the position vector, X is the complete domain and $|\cdot|$ gives the absolute value. Here Δx gives the (nondimensional) grid spacing in the x direction at position $\mathbf{x}$. The wall-normal direction is x and the wall parallel directions are y and z (cf. figure 2.2).

The additional constraint originates from the viscous terms, and is given by:

$$\Delta t_{v \nabla^2 \mathbf{u}} \leq \text{Re } \mathcal{C}_2 \min_{\forall \mathbf{x} \in X} (\Delta y(\mathbf{x}) + \Delta z(\mathbf{x}))^2, \quad (2.10)$$

where $\text{Re} = \sqrt{Ra/Pr}$ is the Reynolds number based on the free-fall velocity, and $\mathcal{C}_2$ a number which depends on the integration scheme and the number of dimensions treated explicitly. This condition only needs to be satisfied in the horizontal directions, and not in the vertical direction, as the time integration of the vertical second derivatives is kept implicit. This is because $\Delta x(\mathbf{x})^2$ can be very small, and the resulting time-step would make the simulation infeasible.

We can now compare the two CFL constraints, and show that the nonlinear constraint is more restrictive than the viscous constraint in the homogeneous directions. As $|u_z|$ and Δz are strictly positive, we have:

$$\frac{\text{Re } \mathcal{C}_2}{\frac{|u_x|(\mathbf{x})}{\Delta x(\mathbf{x})} + \frac{|u_y|(\mathbf{x})}{\Delta y(\mathbf{x})} + \frac{|u_z|(\mathbf{x})}{\Delta z(\mathbf{x})}} < \frac{\text{Re } \mathcal{C}_2}{\frac{|u_y|(\mathbf{x})}{\Delta y(\mathbf{x})} + \frac{|u_z|(\mathbf{x})}{\Delta z(\mathbf{x})}}. \quad (2.11)$$

Including the wall-normal grid spacing in the CFL condition gives a smaller time-step than only using horizontal spacing, and thus the expression on the right is an upper bound on the time-step. If we then use that the grid is uniformly spaced, and equally spaced in both horizontal directions, we can simplify the expression as $\Delta y(\mathbf{x}) = \Delta z(\mathbf{x}) = \Delta y$. We also know that the dimensionless velocity is $|u| \sim \mathcal{O}(1)$ by normalization. Using all of this, we obtain:

$$\Delta t_{\mathbf{u} \cdot \nabla \mathbf{u}} \sim \mathcal{O}(\Delta y), \quad (2.12)$$

for the nonlinear CFL condition and

$$\Delta t_{v \nabla^2 \mathbf{u}} \sim \mathcal{O}(\text{Re } \Delta y^2), \quad (2.13)$$

from the CFL criterion for the viscous terms. If we assume $\text{Pr} \sim \mathcal{O}(1)$, we can get a bound on the viscous time-step as a function of Ra , $\Delta t_{v \nabla^2 \mathbf{u}} \sim \mathcal{O}(\text{Ra}^{\frac{1}{2}} \Delta y^2)$.

To compare both bounds, we need an estimation for Δy . For a resolved DNS, Δy should be similar to the smallest physical length scale in the system. Several length scales can be chosen in the thermal convection problem. The first choice stems from homogeneous turbulence, where the most commonly used length scale that determines the numerical resolution is the Kolmogorov length scale, $\eta_K = \nu^{3/4} \varepsilon^{-1/4}$, where ε is the viscous dissipation rate. For RB, we can obtain an estimate for the Kolmogorov scale by using that the volume and time averaged viscous dissipation rate can be expressed directly as a function of Nu , Ra and Pr [26, 27]:

$$\langle \varepsilon \rangle_{V,t} = \frac{\nu^3}{L^4} \text{Ra} \text{Pr}^{-2} (\text{Nu} - 1). \quad (2.14)$$

For high Ra simulations, $\text{Nu} \gg 1$. Using again that $\text{Pr} \sim \mathcal{O}(1)$, we can obtain an estimate for η_K , and thus the grid spacing as $\Delta y = \eta_K / L \approx 1/(\text{Ra} \text{Nu})$. If we assume $\text{Nu} \sim \text{Ra}^\gamma$ we can now compare both CFL constraints on the time step, obtaining $\gamma \leq 1$ as a requirement for the nonlinear CFL to be more restrictive on the time step than the viscous CFL constraint.

In RB convection, another restrictive length scale naturally arises, i.e. that of thermal plumes. These are conceptualized as detaching pieces of thermal boundary layers. The thickness of a thermal boundary layer can be approximated by $\lambda \approx 1/(2\text{Nu})$. Using this as an estimate for Δy in equations (2.9) and (2.10) give another bound: $\gamma \leq 1/2$. Trivial upper bounds in RB convection give a physical upper bound of $\text{Nu} \sim \text{Ra}^{1/2}$ [3], indicating that for the mild assumptions made, the criteria $\gamma \leq 1/2$ is always satisfied. This signifies that the scaling of $\Delta t_{\mathbf{u} \cdot \nabla \mathbf{u}}$ is more restrictive than $\Delta t_{v \nabla^2 \mathbf{u}}$, which results in that using only the nonlinear CFL constraint in the time-marching algorithm, inherently satisfies the stability constraints imposed by the explicit integration of the horizontal components of the viscous terms. Including the vertical nonuniform grid in this derivation makes this statement even more valid, as

the used CFL time step is based on this grid (cf. equation 2.9). Inherent to the big-O notation is the absorption of the coefficients and offsets. This makes this derivation only valid for high Ra flows. For low Ra, the solver will be unstable as the viscous constraint is not satisfied in this regime.

In addition, we note that the previous analysis can be applied for the scalar (temperature) equation as long as $\text{Pr} \sim \mathcal{O}(1)$. If $\text{Pr} \gg 1$, which is the case in some applications, such as many oils or the Earth's mantle, the CFL constraint on the horizontal conductive terms becomes $\Delta t_{\kappa \nabla^2 T} \sim \mathcal{O}(\text{Pr}^{\frac{1}{2}} \text{Ra}^{\frac{1}{2}} (\Delta y)^2)$, which means a stricter restriction on the time-step than equation (2.13). This means that the Ra of the flow required to make $\Delta t_{\mathbf{u} \cdot \nabla \mathbf{u}} \leq \Delta t_{\kappa \nabla^2 T}$ will be higher.

2.5 Code parallelization

In the previous section, we reasoned that for large Ra the implicit integration of the viscous terms in the horizontal direction becomes unnecessary. The calculation becomes local in space as the two horizontal directions no longer require implicit solvers to calculate the intermediate velocity field $\mathbf{u}^*$. In this case it is worth decomposing the domain such that the pencils are aligned in the wall-normal (x) direction, i.e. that every processor possesses data from x_1 to x_N (cf. figure 2.4). Halo updates must still be performed during the computation of $\mathbf{u}^*$, but this memory distribution completely eliminates all the all-to-all communications associated to the viscous implicit solvers, as for every pair (y, z) , a single processor has the full x information, and is able to solve the implicit equation in x for the pair (y, z) without further communication.

All-to-all communications are unavoidable during the pressure correction step, as a Poisson equation must be solved. As the two wall-parallel directions are homogeneous and periodic, it is natural to solve the Poisson equation using a Fourier decomposition in two dimensions. Applying a Fourier transform to the variables ϕ and the right side in equation (2.5) reduces the pressure correction equation to:

$$\left(\frac{\partial^2}{\partial x^2} - \omega_{y,j}^2 - \omega_{z,k}^2 \right) \mathcal{F}(\phi) = \mathcal{F} \left[\frac{1}{\alpha_l \Delta t} (\mathcal{D} \mathbf{u}^*) \right] \quad (2.15)$$

where $\mathcal{F}(\cdot)$ denotes the 2D Fourier transform operator, and $\omega_{y,j}$ and $\omega_{z,k}$ denote the j -th and k -th modified wavenumbers in y and z direction respectively, defined as:

$$\omega_{y,j} = \begin{cases} \left(1 - \cos \left[\frac{2\pi(j-1)}{N_y} \right] \right) \Delta_y^{-2} & : \text{for } j \leq \frac{1}{2}N_y + 1 \\ \left(1 - \cos \left[\frac{2\pi(N_y - j + 1)}{N_y} \right] \right) \Delta_y^{-2} & : \text{otherwise} \end{cases} \quad (2.16)$$

Figure 2.4: Domain decomposition of a $16 \times 12 \times 10$ grid using 12 distributed memory processes on a 4×3 process grid. Only data that is exclusive to one process is shown; i.e. the single gridpoint-sized halos are not shown in this figure. The pencils are a) x , b) y or c) z oriented.

and $\omega_{z,k}$ is defined in an analogous way. A modified wavenumber is used, instead of the real wavenumber, to prevent the Laplacian operator having higher accuracy in some dimensions. In the limit $\Delta y \rightarrow 0$, the modified wavenumbers converge to the real wavenumbers.

By using a second order approximation for ∂_x^2 , the left hand side of the equation is reduced to a tridiagonal matrix, and thus the Poisson equation is reduced to a 2D FFT followed by a tridiagonal (Thomas) solver. This allows for the exact solution of the Poisson equation in a single iteration with $\mathcal{O}(N_x N_y N_z \log[N_y] \log[N_z])$ time complexity. Due to the domain decomposition, several data transposes must be performed during the computation of the equation. The algorithm for solving the Poisson equation is as follows:

1. Calculate $(\mathcal{D}\mathbf{u}^*)/(\alpha_l \Delta t)$ from the x -decomposed velocities.
2. Transpose the result of (1) from a x -decomposition to a y -decomposition.
3. Perform a real-to-complex Fourier transform on (2) in the y direction.
4. Transpose (3) from a y -decomposition to z -decomposition.
5. Perform a complex-to-complex Fourier transform on (4) in the z direction.
6. Transpose (5) from a z -decomposition to a x -decomposition.
7. Solve the linear system of equations (2.15) with a tridiagonal solver in the x -direction.
8. Transpose the result of (7) from a x -decomposition to a z -decomposition.
9. Perform a complex-to-complex inverse Fourier transform on (8) in z direction.
10. Transpose (9) from a z -decomposition to a y -decomposition.
11. Perform a complex-to-real inverse Fourier transform on (10) in y direction.
12. Transpose (11) from a y -decomposition to a x -decomposition.

The last step outputs ϕ in real space, decomposed in x -oriented pencils, ready for applying in equations (2.7)-(2.8). Once the Poisson equation is solved, the corrected velocities and pressures are computed using equations (2.7)-(2.8), the temperature and other scalars are advected and the time sub-step is completed. The algorithm outlined above only transposes one 3D array, instead of three velocity fields, making it very efficient. Figure 2.4 shows a schematic of the data arrangement and the transposes needed to implement the algorithm. We wish to highlight that this algorithm also uses all possible combinations of data transposes. It can be seen from figure 2.4

	Slab		Pencil	
	Halo	A2A	Halo	A2A
$\mathbf{u}^*$ computation	2	6	2	0
Pressure correction	8	2	10	6
Scalar equation	3	2	2	0
Total	13	10	14	6

Table 2.1: Number of communications necessary for the computation of all the terms per timestep of the different codes. Here, A2A is short for all-to-all communications. Halo updates involve updating all halo cells, which requires more, but smaller, communications in the case of the pencil code. The difference between the details of the halo and all-to-all for the slab and pencil codes have not been taken into account. It can be seen that the pencil code contains the majority of the communications in the pressure (Poisson) solver.

that the x to z transposes and the z to x transposes need a more complex structure, as a process may need to transfer data to other processes which are not immediate neighbors. The non-overlapping of data before and after transposes is most striking for e.g. process 10 in figure 2.4 with no overlap at all between x and z oriented pencils. These transposes are absent in the 2DECOMP library on which we build. These transposes have been implemented using the more flexible all-to-all calls of the type ALLTOALLW, instead of the all-to-all MPI calls of the type ALLTOALLV used for the other four transposes. A complete list of the used libraries can be found in table 2.2 at the end of the chapter.

2.6 Computational performance

For optimal scaling conditions, each processor should have an equal amount of work, and the communication to computation ratio should be minimal. In our case, as we do not have iterative solvers, each grid point has the same amount of work, as long as the amount of points in every processor is the same there is perfect load balancing. We also reduce the communication as far as possible. Not only the number of all-to-all communications are reduced, but also the halo communications as the halo is only one grid point wide. Table 2.1 presents the reduction in the number of communications when going from the slab decomposition with fully implicit viscous terms to the pencil decomposition with semi-implicit viscous terms. It is worth noting that the communications are not exactly the same: halo updates involve communications to four neighbors in the pencil decomposition, while only two neighbors are involved in the slab decomposition. However, the size of the halos is much smaller, so less data is transferred. Conversely, for the all-to-all communications, not all processes exchange

data with each other in the pencil code, while all processes do so in the slab code. The total memory consumption of the code is approximately $M \approx 15 \times 8 \times N_x \times N_y \times N_z$. Here M is the total used memory in bytes of all processes without MPI overhead. The number of allocated 3D arrays is 14, with additional 1D and 2D arrays of which the memory consumption will not exceed that of one 3D array in the intended cases with large grids.

The left panel of figure 2.5 shows the strong scaling of the code for 2048^3 and 4096^3 grids on the Curie Thin Nodes system. Linear scaling can be seen up to 32K cores for the 4096^3 grid, with some scaling loss for 64K cores. The right panel of figure 2.5 shows the weak scaling of the code for 2^{23} points from 2 to 16K cores. The data in these plots is obtained by using only MPI parallelism, but hybrid OpenMP/MPI schemes are also available in the code. The choice between pure MPI or hybrid OpenMP/MPI depends heavily on the system on which the code is running. In addition, the presence of OpenMP will allow for a faster porting of the codes to a GPU architecture, in case it becomes viable for our application.

Finally, it must be noted that not only the scaling of the code is excellent, but also the absolute performance. The computational cost per physical time step is very low. In the end, this is what counts.

Figure 2.5: (a) Strong scaling of the code for 2048^3 and 4096^3 degrees of freedom n_{dof} . Here n_c is the number of cores used. The dashed lines indicate linear behavior. The walltime per timestep t_w (in seconds) is accounted for a full timestep, i.e. three sub-timesteps when using the RK3 integrator. (b) Weak scaling of the code for 8.3 Million (2^{23}) points per core. The dashed is a least squares linear fit to the corresponding data points. Time is measured in seconds.

2.7 Summary and prospects

In this chapter, we have presented a parallelization scheme of a second-order centered finite difference method with minimal communication. Only six transposes are

Figure 2.6: a) The heat flux Nu as a function of the driving Ra for a cylindrical, slab decomposed domain and a Cartesian, pencil decomposed domain. In both cases $Pr = \mathcal{O}(1)$. The cylinder was simulated with an aspect ratio of $\Gamma = 1/3$, while the lateral size in the periodic case was sufficiently large to approximate infinite aspect ratio. The GL theory [35] is additionally shown with a solid line. The error bars are based on the temporal convergence of Nu . b) An instantaneous temperature field at height $x = 0.001$ for $Ra = 10^{11}$, where white and black indicate hot and cold fluid, respectively.

needed for every fractional time-step, and for large enough grids, the code's strong scaling is linear up to 32K cores, with slight performance loss from 64K cores. We emphasize that 64K cores is over half the total number of cores of the Curie Thin nodes system. The code will probably scale well for even larger grids (8096^3) on systems with larger amount of cores, as do similar codes based on the 2DECOMP library [145]. In addition, the absolute performance is excellent. The wall-time per physical time is very low and substantial progress can be made with few computational resources.

The performance of this code allows simulation of flows at high driving. For the application to Rayleigh-Bénard convection, we refer to figure 2.6(a), where the heat flux Nu as a function of the driving Ra can be seen. In this plot, Nu can be compared between the cylindrical, slab decomposed domain, the Cartesian, pencil decomposed domain and the theoretical prediction of the GL-theory [35]. The theoretical prediction is based on a fit to experimental data and thus implies an indirect comparison to experiments as well. The cylindrical domain in numerical simulations is used specifically to facilitate a comparison to experiments at the cost of increased time complexity of the pressure correction algorithm and the limitation of a one-dimensional domain decomposition (slab), as compared to the proposed Cartesian code. As a quantification of the difference in computational demands of these code: The highest $Ra = 10^{12}$ data point for the cylindrical and the Cartesian simulations have cost 5M and 1M CPU-hours, respectively. This difference, in favor of the Cartesian method, is amplified by the higher temporal convergence of the Cartesian simulation, judging

Purpose	Library
I/O	HDF5
FFT	FFTW (Guru interface)
Linear algebra	BLAS, LAPACK/MKL/ESSL/LibSci/ACML
Distributed memory parallelism	MPI + 2DECOMP
Shared memory parallelism	OpenMP

Table 2.2: The used libraries for the specified purposes are indicated in this table.

from the smaller error bar size and the use of more degrees of freedom in the Cartesian geometry, as the system volume is slightly larger for identical Γ . The heat flux shows negligible differences, which shows that it is largely independent of the side-wall boundary conditions. Even though the impermeable no-slip wall in the cylindrical case differs largely from the lateral periodicity in the Cartesian case, the heat flux appears unaffected. This indicates that at least for the global quantities, there is no apparent reason to spend more computational resources on a cylindrical simulation, and one can safely resort to the proposed method while maintaining the possibility of comparing to experiments. Even without that possibility, the lateral periodicity is closer to natural applications of RB convection as it approximates infinite aspect ratio, which by itself warrants the use of the Cartesian domain. The prospected analysis of RB convection is not limited to global quantities such as the heat flux. The highly parallel I/O and high resolution facilitates the study of local quantities. An unfiltered snapshot of the temperature field close to the lower boundary for $Ra = 10^{11}$ is shown in figure 2.6b, where the small scale temperature fluctuations that are required to be properly resolved, can be seen. These small scales can straightforwardly be studied using spectral analysis, or other techniques (cf. Ref. [32]).

The use of this code in Refs. [146, 147] has already allowed us to push the limits in Taylor-Couette simulations to $Re \sim \mathcal{O}(10^5)$, never simulated previously. Its use in future RB simulations is expected to allow us to achieve the large drivings required for entering the “ultimate” regime. The scheme, in combination to a multiple resolution strategy for the scalar field (§3), has been used for simulating double diffusive convection [148], achieving the driving parameters relevant for oceanic convection. Due to the flexibility of finite difference schemes, we expect to be able to build further additions on to this code. The possibility of adding a Lagrangian phase, which can be either tracers, one-way or even two-way coupled particles is detailed in Ref. [149]. Other possibilities include adding rough walls using immersed boundary methods [150], or adding mixed Neumann-Dirichlet boundary conditions.

A multiple-resolution strategy for Direct Numerical Simulation of scalar turbulence *

A numerical procedure to simulate low diffusivity scalar turbulence is presented. The method consists of using a grid for the advected scalar with a higher spatial resolution than that of the momentum. The latter usually requires a less refined mesh and integrating both fields on a single grid tailored to the most demanding variable, produces an unnecessary computational overhead. A multiple resolution approach is used also in the time integration in order to maintain the stability of the scalars on the finer grid. The method is the more advantageous the less diffusive the scalar is with respect to momentum, i.e. particularly well suited for large Prandtl or Schmidt numbers. But even in the case of equal diffusivities the present procedure gives CPU time and memory occupation savings. The reason is that the absence of the pressure term in the scalar equation leads to much steeper gradients in the scalar field as compared to the velocity field.

*Based on: Y. Yang, R. Ostilla-Mónico, E. P. van der Poel, D. Lohse and R. Verzicco, *A multiple-resolution strategy for Direct Numerical Simulation of scalar turbulence*, in preparation. Initial proof of concept and coding by Ostilla-Mónico. Tricubic interpolation schemes and DDC implementation by Yang. Further debugging and RB implementation done by van der Poel. Writing and discussion done by everybody.

3.1 Introduction

Countless phenomena in Nature and technology involve one or more scalar fields that are advected and diffused by a turbulent flow. The dilution of pollution in the atmosphere [151], the transport of nutrients in oceans [152], the cooling or heating of devices [153] and the buoyancy-driven currents generated by natural- [27, 154] and double-diffusive [155, 156] convection are just few examples among many.

Numerical simulations have proven to be very helpful in unraveling the complex physics behind these phenomena [87] even if the calculations have shown to be more demanding than expected, taking up to millions of CPU hours in recent studies [131].

The common understanding of the problem is that in three-dimensional turbulent flows, there is a cascade from the largest towards the small spatial scales up to a lower limit that is determined by the diffusivity. As each field has its own diffusivity, these scales can have different magnitudes. In direct numerical simulation (DNS) the mesh size must be smaller than the smallest among them: This requirement quickly renders DNS infeasible. Denoting as η_K the smallest (Kolmogorov) scale of the momentum field, we can calculate the analogous quantity for a scalar field S as $\eta_B = \eta_K / \text{Sc}^{1/2}$, also called the Batchelor scale, with $\text{Sc} = \nu / \kappa_S$ the Schmidt number defined as the ratio of the kinematic viscosity ν and the scalar diffusivity κ_S , respectively. In some cases, like sugar in water, the Schmidt number exceeds 10^3 resulting in a Batchelor scale of $\eta_B \simeq \eta_K / 30$. With equal grid resolutions for the scalar and the momentum fields, this entails that the momentum field is resolved by a factor of approximately 30 in each direction. The problem is exacerbated by the fact that a scalar is described by only a single quantity, while momentum is a vector field satisfying the incompressibility condition or other related constraints. This implies that the solution of the momentum alone generally takes an order of 90% of the total CPU time of a simulation and therefore resolving it on an unnecessary fine mesh is not desirable.

The above scenario essentially derived from dimensional analysis, however, does not give the complete picture since it does not account for the structure of the equations. In fact, the naïve comparison between the Kolmogorov and Batchelor scales suggests that for $\text{Sc} \approx 1$, $\eta_K \simeq \eta_B$ although in practice the resolution requirements for the momentum and the scalar fields are not the same. Visual evidence of the latter statement can be obtained from the instantaneous snapshots of figure 3.1 showing horizontal cross-sections of temperature and vertical velocity in a thermally driven turbulent flow. In this flow, the fluid hotter than the average temperature (0.5 in nondimensional units) generates upward buoyancy and therefore positive vertical velocity (and vice versa). Although the two fields are very well correlated on the large-scales, the sharp fronts of the scalar field do not have an analogous counterpart in the momentum distribution and this results in a different resolution requirement for scalar and momentum. We will see that the main reason for this difference is the presence of the pressure term in the momentum equation that makes the dynamics nonlocal and

tends to smooth the intense steep fronts. A problem related to the nonlocal equations for momentum is their high computational cost and the detrimental implications on the parallel performance. Therefore, the possibility of using different meshes for momentum and scalars opens the door to very large gains in performance, not only by reducing the amount of operations, but also the communication of data among processors and the total memory usage. This consideration motivates the present chapter that describes a strategy for efficiently simulating scalar driven turbulent flows with different spatial resolutions for momentum and scalar fields.

Figure 3.1: A horizontal plane halfway between the plates for a Rayleigh-Bénard simulation in a Cartesian geometry at $Ra = 10^{10}$ and Prandtl number $Pr = 1$. *a)* vertical velocity, red indicating rising fluid while blue indicates falling fluid, *b)* temperature, red indicating hot fluid and blue indicating cold fluid. Even though the Prandtl number is one, much sharper gradients can be seen in the right panel.

In this study, the multiple resolution strategy will be mainly applied to Rayleigh-Bénard (RB) convection, the flow of a fluid vertically confined by a top cold and a bottom hot plate. RB is a particularly suitable example for the present application since the flow is driven by the temperature (scalar) field whose diffusivity can be changed by the Prandtl number Pr . In addition, analytical exact relations are available for this problem that can be used to check the correctness of the numerical results. It is worth mentioning that in RB convection the forcing comes from the heated and cooled surfaces where viscous and thermal boundary layers develop. Since they become thinner as the forcing strengthens, the resolution requirements in these boundary layers become more stringent than in the bulk. An extensive analysis of the problem can be found in Ref. [44] where all the details, estimates and guidelines for numerical simulations are given. Here, it suffices to mention that a nonuniform mesh is required in the wall normal direction such to cluster the nodes within the boundary layers. Nevertheless, even if the grid spacing at the wall is much finer than that in the

bulk, the volume of fluid within these layers is at most a few percent of the total and the nodes allocated there are only a small fraction of the whole mesh.

We will additionally show another numerical example. Namely, double diffusive convection (DDC), in which the flow is driven by two scalars with very different diffusivities and with opposite, stabilizing and destabilizing, effects on the flow. In this case the multiple resolution strategy is even more advantageous and it allows for the simulation of flow regimes that otherwise would be out of reach.

The organization of the chapter is the following. In the next section we describe the governing equations and the numerical method. §3.3 quantifies the differences of momentum and scalar gradients and presents some analytical exact relations for RB. The section closes with the results of reference simulations obtained on a standard single grid. In §3.4 the multiple resolution strategy and numerical details are explained. Finally, §3.5 discusses the results and the computational performance of the method for RB flow and double diffusive convection. Closing remarks are reported in §3.6.

3.2 Governing equations and numerical method

The incompressible Navier–Stokes equations with the Boussinesq approximation for thermal convection are the basis for this chapter. They can be found in equations 2.1-2.3. Deviations with the rest of the thesis of definitions used in this chapter are the following. Here, β_T the isobaric thermal expansion coefficient and κ_T the thermal diffusivity of the fluid, T_h and T_c the temperature at the hot and cold plates, respectively. These require a more specific notation, as double diffusion convection involves another scalar field. The Prandtl number Pr , which is the temperature analogue of the Schmidt number, is defined as $Pr = \nu / \kappa_T$.

The integration of the system is performed by a fractional timestepping [157] with the modifications proposed in Ref. [37]. In short, a provisional velocity $\hat{u}_i$ is computed from the previous field u_i^n using the old pressure p^n

$$\frac{\hat{u}_i - u_i^n}{\Delta t} = -\partial_i p^n - N_i^{n+1/2} + D_i^{n+1/2}, \quad (3.1)$$

$N_i^{n+1/2}$ contains the nonlinear terms and the temperature forcing while $D_i^{n+1/2}$ has the viscous terms: The former are computed explicitly in time, the latter implicitly. The flow incompressibility is then enforced by a pressure correction that takes the form of a Poisson equation $\nabla^2 \phi = \partial_i \hat{u}_i$ whose solution is the most computationally demanding step, especially on nonuniform grids. In addition, the Poisson equation is nonlocal and this has consequences on code parallelization, requiring the largest amount of communication. Once the scalar ϕ is obtained, the velocity $\hat{u}_i$ is projected onto the solenoidal field u_i^{n+1} and the new pressure p^{n+1} can be computed. The

advancement of the temperature is performed directly through

$$\frac{\theta^{n+1} - \theta^n}{\Delta t} = -M^{n+1/2} + V^{n+1/2}, \quad (3.2)$$

where, again, $M^{n+1/2}$ contains the explicit nonlinear terms and $V^{n+1/2}$ the implicit diffusive terms.

All the variables are discretized by central second-order finite-differences on a staggered grid and the time advancement of the solution is obtained by a low-storage third-order Runge-Kutta scheme. Further details can be found in Ref. [37].

3.3 Pressure effects and heat transfer in RB

As mentioned in the introduction, the Prandtl number gives the ratio of momentum to thermal diffusivity, and even if Pr is of order unity, temperature and momentum do not have the same gradient magnitudes (cf. figure 3.1). We quantify this statement in figure 3.2(a) by showing instantaneous temperature θ and vertical velocity u_z profiles across a vertical line from a RB simulation: Much steeper gradients, can be seen in the temperature field. These steep gradients are smoothed in the vertical velocity, owing to the pressure effects and this lowers the resolution requirements of momentum with respect to temperature. This observation is further corroborated by figure 3.2(b) showing the probability density functions of $\partial_z \theta$ and $\partial_z u_z$ computed in the bulk of the flow without the boundary layers. Extreme gradients can be seen to be more likely for θ thus evidencing a more intermittent behavior. This behavior has been extensively studied, and it is a well established fact that the intermittency corrections to the structure function exponents are much larger for scalars than for velocity [28, 158]. Indeed, these sharp fronts become much sharper with increasing Reynolds number, and thus increasing small-scale intermittency [159–164].

We have argued that the absence of the pressure term in the scalar equation is the reason for the localized steep gradients and this idea can be confirmed by the Burgers equation:

$$\partial_t u + u \partial_x u = \nu_B \partial_{xx} u, \quad (3.3)$$

which is often used to test numerical schemes since it is a simple one-dimensional partial differential equation that still retains the essential features of the more complex Navier-Stokes equations: The unsteady term, a quadratic nonlinear term and a strictly dissipative viscous term [165].

A one-to-one comparison with equation (2.2), however, evidences the absence of a pressure term and this causes the solution $u(x, t)$ to develop very sharp discontinuities in a finite time and for finite values of the diffusivity ν_B .

As an example, in figure 3.3, a solution obtained for an initial condition $u(x, 0) = \sin x$ in the domain $-\pi \leq x < \pi$ and $\nu_B = 5 \times 10^{-6}$ is shown. The gradient at $x = 0$

Figure 3.2: *a)* Instantaneous θ and u_z profiles as a function of the vertical coordinate z/L for $Ra = 10^{10}$, $Pr = 1$ RB simulation. *b)* PDF of $\partial_z \theta$ and $\partial_z u_z$ for the same simulation in the bulk.

becomes so steep that a fine nonuniform mesh clustered at the centre of the domain is necessary to properly capture the solution (figure 3.3(a)). For underresolved meshes (figure 3.3(b)) the solution unphysically overshoots the initial extrema $u_{min} = -1$ and $u_{max} = 1$ and spurious oscillations are generated in the region of the steep gradient (figure 3.3(c)) resembling the behavior of underresolved scalar fields. A very similar phenomenon is observed in a simulation with an underresolved temperature field as shown in figure 3.4.

In RB flow, one of the interesting quantities is the heat flux Q transferred from one plate to the other. In nondimensional form this is the Nusselt number, $Nu = Q/\kappa_T(T_h - T_c)L^{-1}$. This is not only interesting from a physical point of view, but also as a monitoring variable since it has been observed [94] that when the separately calculated Nusselt number converge and are grid independent, at least all quantities up to second order statistics are properly resolved.

There are several ways to calculate Nu , either by measuring the convective heat transport in the system

$$Nu(z) = \sqrt{RaPr} \langle u_z \theta \rangle_{A,t} + 1, \quad (3.4)$$

or by using the exact relationships derived from global balances [26] of kinetic energy,

$$\varepsilon_v = \nu U_f^2 L^{-2} \langle [\partial_i u_j]^2 \rangle_{V,t} = \nu^3 L^{-4} (Nu - 1) Ra Pr^{-2}, \quad (3.5)$$

and thermal energy,

$$\varepsilon_\theta = \kappa_T (T_h - T_c)^2 L^{-2} \langle [\partial_i \theta]^2 \rangle_{V,t} = \kappa_T (T_h - T_c)^2 L^{-2} Nu. \quad (3.6)$$

Here the subscripts t , A and V denote, respectively, averages in time, horizontal homogeneous planes and the whole fluid volume, and U_f the free-fall velocity $U_f =$

Figure 3.3: Spatial profiles at various times of the solution of the Burgers equation for $\nu_B = 5 \times 10^{-6}$: dashed $t = 0$, dotted $t = 0.2$, chaindot $t = 0.4$ and solid $t = 0.8$. *a)* resolved simulation with $\Delta x = 10^{-4}$, *b)* underresolved simulation with $\Delta x = 4 \times 10^{-4}$, *c)* enlargement of *b)* in the region of the steep gradient.

$\sqrt{\beta g(T_h - T_c)L}$. Although equation (3.4) depends on z , once the equilibrium is reached its value becomes constant. This condition is requested to assess the statistical convergence of the results.

From here on, we denote Nu with a subscript, either $Nu_{u_z\theta}$, Nu_{ε_v} or Nu_{ε_θ} which specifies the particular equation, i.e. (3.4)–(3.6) respectively, with which Nu is calculated. In addition, we also denote the Nusselt number calculated by the temperature gradient at the wall as Nu_{θ_w} . All definitions are equivalent analytically, but they involve gradients or square gradients of the variables that, when calculated numerically, can deviate from each other if the simulations do not have enough spatial resolution to capture the smallest flow scales: Their comparison can thus be used as a test for the adequacy of the mesh [94].

Figures 3.5(a) and 3.5(b), show the ratios $Nu_{\varepsilon_\theta}/Nu_{u_z\theta}$ and $Nu_{\varepsilon_v}/Nu_{u_z\theta}$ for RB simulations performed on the same grid for momentum and temperature at $Ra = 10^9$

Figure 3.4: *a)* Snapshot of an underresolved flow field for $Ra = 10^9$ and $Pr = 1$. The characteristic “wiggles” of the underresolved temperature field can be clearly appreciated (see arrows). *b)* Snapshot of a properly resolved velocity field.

and $Pr = 1$ or $Pr = 10$. Resolutions between $96^2 \times 192$ and $384^2 \times 768$ were used, the larger number corresponding to the vertical (wall-bounded) direction. An aspect ratio of $\Gamma = 1$ was used in both directions, meaning that the computational domain is cubic. Points were clustered near the wall using a Chebychev-like distribution according to the prescriptions of Ref. [44]. The Kolmogorov scale is computed from the kinetic energy dissipation rate using $\eta_K/L = (v^3/\varepsilon_v)^{1/4}$ and the Batchelor scale $\eta_B/L = \eta_K/LPr^{-1/2}$. As mentioned above, the various expressions for Nu should be equivalent, their ratios however, approach the unity limit only when the normalized mesh sizes Δ/η_K and Δ/η_B decrease and they do not converge at the same rate. In particular it can be noted that $Nu_{\varepsilon_v}/Nu_{u_z\theta}$ tends to unity for larger grid spacings than $Nu_{\varepsilon_\theta}/Nu_{u_z\theta}$ even for $Pr = 1$ and this corroborates our hypothesis that a finer resolution is needed for the scalar than for momentum. Using an identical mesh to spatially discretize both momentum and the scalars therefore produces an overhead in computational resources that is redundant.

At the highest resolution, all the definitions converge to the same value (within an uncertainty of 2–3%), therefore we will refer to it as Nu_{ref} without specifying the particular expression and figure 3.5(c) and 3.5(d) show the convergence of $Nu_{u_z\theta}$ to this asymptotic value.

Figure 3.5: (a) ratio between different ways of calculating Nu against grid size for a rectangular RB simulation with $Ra = 10^9$ and $Pr = 1$. Red squares are $Nu_{\epsilon_v}/Nu_{u_z\theta}$, blue circles are $Nu_{\epsilon_\theta}/Nu_{u_z\theta}$. (b) same as (a) for $Pr = 10$. Nu_{ϵ_θ} is plotted against $\max(\Delta/\eta_B)$ while Nu_{ϵ_v} is plotted against $\max(\Delta/\eta_K)$. For $Pr = 1$, $\eta_B \equiv \eta_K$. (c) convergence to an asymptotic value of $Nu_{u_z\theta}$ for $Ra = 10^9$ and $Pr = 1$. (d): same as (c) for $Pr = 10$.

3.4 The multiple resolutions strategy

3.4.1 Multiple resolution strategy in space

In this subsection we present a method to decouple the spatial discretization of the scalars and the momentum, which allows for large computational savings. This is achieved by refining every cell of a base mesh $\mathcal{M}^i$ times in each i -th direction. A simplified two-dimensional sketch of this procedure is shown in figure 3.6. On the left, the location of the scalars and velocities in the standard single mesh is shown for a staggered arrangement. There, the velocity components are at the centers of the cell faces, while the pressure and the scalar are discretized at the center of the cell volume. The right panel shows a case with velocity and pressure on the base grid,

Figure 3.6: Location of pressure, temperature and velocities of a 2D simulation cell. The third dimension (z) is omitted for clarity. As on an ordinary staggered scheme, the velocity vectors are placed on the borders of the cell and pressure is placed in the cell center. The temperature is placed on the same nodes as the vertical velocity, to ensure exact energy conservation.

and a doubly refined ($\mathcal{M}^x = \mathcal{M}^y = 2$) mesh for the scalar, which is temperature in the RB case.

The method works as follows. We first generate the refined mesh over which the scalar field is discretized and then a coarser mesh is obtained by taking only one out of $\mathcal{M}^i$ nodes in the i -th direction. Note that when the mesh is uniform in space this is equivalent to start from the coarse cells and split them into $\mathcal{M}^i$ identical parts. For a nonuniform mesh, however, this naive splitting would result in a staircase distribution of the metrics for the fine grid with constant coefficients within each coarse element and with jumps across its boundaries. These discontinuities would locally decrease the accuracy of the discretization to first order and introduce spurious oscillations in the resolved fields. The difference between the two methods is shown in figure 3.7(a) for a mesh obtained by a Chebychev-like distribution with 96 base nodes and a refinement factor of eight. In this chapter, most numerical examples are obtained using the same $\mathcal{M}^i$ in every direction therefore, unless otherwise specified, from here on we will use only $\mathcal{M}$ to indicate the isotropic refinement factor without specifying the direction. However, this is not required for the method to work and the same procedure can be applied to refinement levels different in each direction depending on the particular flow physics. An example will be shown in §3.5.2.

In order to advect the scalar, the velocity has to be interpolated from the base mesh onto the refined grid at the centers of the faces of the refined cells. This is achieved using a tri-cubic Hermite spline interpolation, taking a stencil of four points in every direction for a total of sixty-four points in three dimensions which, according to our numerical tests, is the minimum required. At the top and bottom boundaries, one-sided interpolation is used, which in principle is less accurate, but is performed on a much finer grid, and thus the amplitude of the error is much smaller than in the bulk. The accuracy of Hermitian interpolation has proven to be sufficient in turbu-

lent flows, and it is comparable to that of B-splines [166]. Hermitian interpolation, however, is preferred in this method as B-splines are much more computationally expensive. Preliminary simulations have shown that a linear interpolation using a two point stencil is not sufficient, because it results in a spatially interpolated velocity field which has equal fluxes inside every base cell, and different at the base cell boundaries (figure 3.7(b)). This lack of homogeneity results in spurious oscillations in the scalar field, in particular around local maxima and minima of velocity. These oscillations are visualized in figure 3.8.

Figure 3.7: (a) Normalized metric $\Delta x/N_x$, where N_x is the amount of grid points for a Chebychev-type grid clustering for a refined-mesh generated ($\mathcal{M} = 8$) from a base mesh by splitting the base cells (squares), and the base mesh generated from the refined mesh (diamonds). The first method causes a staircase-like metric, which leads to spurious oscillations. (b) Comparison on interpolated velocity v from a base mesh to the refined mesh ($\mathcal{M} = 8$) using linear interpolation (squares) and cubic Hermite splines (diamonds). Both interpolations coincide at the base mesh points. The underlying basis for the interpolation is also plotted.

The spatially interpolated velocity can then be used to advance equation (2.3), and compute the values of the scalars at the new time. If a scalar couples back to the momentum field, like in the case of RB flow, a spatial filter must be applied to calculate a “coarsened” scalar. In this case, an averaging using equal weights within each refined cell is used. This averaged scalar is then used in equation (2.2) to advance momentum and pressure. Notice that in this case the scalar field is interpolated from a fine mesh onto a coarser one, therefore the previous problem of having equal fluxes between neighboring cells is not encountered.

We stress that the interpolation of a velocity field between two different grids is a very dangerous operation since its effect is equivalent to that of a low-pass filter, which usually leads to loss of energy and generation and destruction of information. This is catastrophic in the DNS of turbulent flows where the dynamics are based on

Figure 3.8: (a) Pseudocolor plot of temperature at the mid-height when using a refinement of $\mathcal{M} = 3$ and linear interpolation for the velocities. Spurious oscillations every three points can be seen all over the domain. (b) Zoom-in of the region inside the black square of (a).

the energy cascade through the scales. It has even more serious consequences in a RB flow where the balance between thermal (potential) and kinetic energy determines the heat transfer. Nevertheless, if the base mesh already captures the smallest momentum structures, the field is smooth at the scale of the grid cell and an interpolation kernel that is continuous enough does not alter the energy content of the field.

Indeed, the interpolated velocity on the refined grid is *not* solenoidal when the tricubic Hermitian interpolation is used[†]. There are several ways of addressing this problem. One could apply a “minimum energy” correction, by solving a Poisson equation for a velocity correction, and using the local divergence as source term. However, this would involve solving a Poisson equation on the fine grid. While the multiple resolutions strategy would remain favorable, this option would negate one of the main advantages of the method. A second option is to remove the interpolation of the vertical velocity in the vertical direction. Instead, to obtain this velocity on the refined grid, the continuity equation (2.1) is integrated separately over each grid cell using the interpolated horizontal velocities for the horizontal derivatives and the vertical velocity on the base mesh as boundary condition. This would result in a solenoidal velocity field on the refined mesh with much less computational effort as the first option. The last option is to use the tricubic interpolation “as-is”. This nonsolenoidal field has not resulted in apparent problems for the simulations in this chapter. The divergence is very small as long as we are in the DNS range. However,

[†]A linearly interpolated velocity does remain solenoidal on the fine grid. However, we have clearly seen that other spurious effects are generated, rendering it unusable.

we anticipate that this could become a problem at higher drivings.

The previous discussion suggests that the proposed multiple resolution procedure can only work if the coarse mesh is fine enough to fully resolve the momentum field. In §3.5 numerical results will confirm this statement showing that when the base mesh adequately resolves the momentum field good results and CPU time saving can be obtained by refining only the grid for the scalar. On the other hand, if the coarse grid does not fully resolve the momentum field even very large values of $\mathcal{M}$ do not lead to correct results.

3.4.2 Multiple resolution strategy in time

The multiple resolution in space entails that the node spacing for the scalars (Δ_S) is smaller than that for the momentum (Δ_U) and this has immediate consequences on the stability of the time integration because of the explicit terms. Due to the Courant–Friedrichs–Lewy condition [135], $\Delta t \cdot \max[U/\Delta_S] \leq \mathcal{C}_{CFL}$, in fact, the time step must decrease by a factor equal to the refinement $\mathcal{M}$ because $\min[\Delta_S] = \min[\Delta_U]/\mathcal{M}$. As this small Δt is not needed by the base mesh for momentum and pressure, the usage of the current approach becomes disadvantageous very rapidly, especially in high Sc flows requiring high values of $\mathcal{M}$. However, a multiple resolution strategy can be applied also in time, by advancing the more expensive momentum and pressure with a larger time-step and the scalar with a smaller one, using a temporally interpolated velocity. In this way, the stability of the explicit terms in the scalar equation is retained without the penalization of an unnecessary small integration step for all the other equations.

The integration of the scalar equation is therefore performed in $\mathcal{L}$ sub-steps, and at each intermediate l time level the velocity is linearly interpolated through

$$\bar{q}^l = \frac{\mathcal{L}-l}{\mathcal{L}} \bar{q}^n + \frac{l}{\mathcal{L}} \bar{q}^{n+1}, \quad (3.7)$$

where $\bar{q}^n$ is the spatially interpolated velocity at time step n . A simple linear interpolation is used, which is enough to ensure correctness as is demonstrated in §3.5. This velocity is then used to advect the scalar(s) for every sub timestep using equation (2.3) until the scalars have been advanced to the time t^{n+1} . Then, the velocity can be advanced a further time-step and the procedure repeated. If the maximum possible CFL is used for the velocity equations, which is usually the case, then $\mathcal{L} \geq \mathcal{M}$ must be satisfied to ensure stability.

3.5 Results and computational performance

In this section we will present the results of the multiple resolution method, and the associated saving in computational time and memory usage. A more extensive

analysis will be performed in the first part for RB flow while, in the second part, additional results with anisotropic refinements will be shown for DDC flow.

3.5.1 Rayleigh–Bénard flow

A series of rectangular RB simulations with aspect ratio $\Gamma = 1$ were run to validate and to demonstrate the benefits of the described method. Meshes of $96^2 \times 192$, $128^2 \times 256$ and $192^2 \times 384$ (only for $\text{Pr} = 1$) were used for momentum, the Ra was kept constant at 10^9 while Pr was taken $\text{Pr} = 1$ or $\text{Pr} = 10$. In order to minimize the computational costs $\mathcal{L} = \mathcal{M}$ was always used except for a specific set of runs in which the effects of $\mathcal{L}$ were isolated.

Figure 3.9(a,b) shows the ratio between the different definitions of Nu and the maximum refinement level $\mathcal{M}$ while the bottom panels report the convergence of $\text{Nu}_{u_z\theta}$ to the asymptotic reference value, calculated from a wiggles-free simulation such as the one seen in Figure 3.8(b). The raw numerical values can be found in table 3.2 at the end of the chapter.

As mentioned before, the multiple resolution strategy only works if the base mesh is sufficiently fine to fully resolve the momentum field. Looking at figure 3.5(a) we can see that at $\text{Pr} = 1$ the $96^2 \times 192$ mesh is not sufficiently fine, and the different Nu definitions do not show a monotonic convergence of the Nusselt ratios to the asymptote. It is interesting to note that for $\mathcal{M} = 4$ the Nu ratios get close to one, although the absolute values of Nu are wrong and do not indicate a convergence towards the reference grid independent value. On the other hand, the $192^2 \times 384$ grid yields a converged value of $\text{Nu}_{\varepsilon_v}$ even though that resolution is not enough for the computation of $\text{Nu}_{\varepsilon_\theta}$ that involves squared temperature gradients. For this case a refinement factor $\mathcal{M} = \mathcal{L} = 2$ for the temperature gives an appropriate resolution as shown by the Nusselt numbers that converge to the reference value. Although a factor two in space and time might seem to produce only limited benefits, we should consider that it implies a grid for the momentum and pressure with 2^3 less elements than for the temperature. In addition, the momentum equations are solved only once every other time sub-step therefore, even if there is an overhead introduced by the interpolation of the fields, the CPU time savings are substantial. In our case the standard simulation on the single grid $384^2 \times 768$ required for the integration of dimensionless time unit a wall-time of 36.4 minutes on 96 processors, for a total of 58.2 CPU hours using 13 GB of RAM memory. Using $\mathcal{L} = \mathcal{M} = 2$, one dimensionless time unit required a wall-time of 36.7 minutes on 48 processors for a total of 29.4 CPU hours using 4.9 GB of RAM memory.

The method becomes even more advantageous as the Prandtl number increases. In fact, from equations (2.2)–(2.3) we see that the nondimensional diffusivities of momentum and temperature, read $\text{Re} = \sqrt{\text{Ra}/\text{Pr}}$ and $\text{Pe} = \sqrt{\text{RaPr}}$, respectively. Therefore for $\text{Pr} > 1$ the momentum field smoothens while the temperature field devel-

Figure 3.9: (a) Ratio between different ways of calculating Nu against grid size for the two base meshes and increasing spatial refinement for $Pr = 1$. (b) same as (a) for $Pr = 10$. (c) convergence to an asymptotic value of $Nu_{u_z\theta}$ for increasing refinement and $Pr = 1$. (d): same as (c) for $Pr = 10$. Circles are for base meshes of $96^2 \times 192$, while diamonds are for $192^2 \times 384$ base meshes. On the top panels, blue indicates the ratio $Nu_{\epsilon_\theta}/Nu_{u_z\theta}$ and red the ratio $Nu_{\epsilon_v}/Nu_{u_z\theta}$.

ops sharper gradients. This results in larger Kolmogorov η_K and smaller Batchelor η_B scales that need different meshes to be properly resolved. Figure 3.5(b) shows that at $Pr = 10$ the increased momentum diffusivity makes even the relatively coarse grid $128^2 \times 256$ adequate for the description of the momentum field. On the other hand, the same mesh is clearly too coarse for the scalar field as the ratio $Nu_{u_z\theta}/Nu_{\epsilon_\theta}$ strongly deviates from one. This grid, however, can be used to advance the momentum and to generate a refined mesh to advect the temperature. For this case the convergence of the Nusselt numbers to the reference value is obtained for $\mathcal{M} = \mathcal{L} = 3$ that yields a computational gain around a factor 7 and a reduction of RAM memory by a factor 3.5 when compared to the reference cases using a single mesh.

Before concluding this section we point out that for all simulations we have used a refinement factor for the time step $\mathcal{L} = \mathcal{M}$. Values of $\mathcal{L}$ smaller than $\mathcal{M}$ can be used provided the CFL number for momentum is reduced so that the scalar integration remains stable; this increases the number of time steps needed to advance

the simulation over the same physical time resulting in an increased computational cost. On the other hand, further increasing $\mathcal{L}$ beyond $\mathcal{M}$ does not modify the results within statistical error and empirical evidence supporting this statement can be found in table 3.3 at the end of the chapter.

3.5.2 Double diffusive convection

Double-diffusive convection (DDC) is a system where two scalars with very different diffusivities are coupled to the flow field, one of which is stabilizing and the other destabilizing. A relevant example of this system is the ocean, where the scalars are temperature ($Pr \approx 7$) and salinity ($Sc \approx 700$). The former being warmer at the top surface and cooler at the bottom stabilizes the flow while the latter has the opposite effect because a higher salinity at the top boundary results in a denser, sinking fluid. A snapshot of the flow in a DDC system for a geometry similar to RB can be seen in figure 3.10. Very sharp gradients of salinity can be observed, while the temperature field is in a quasi-diffusive state.

In this case, the computational gains associated with a multiple resolution can be even larger than before, owing to the very large Sc number of salt in water. In the simulations of Ref. [148], the temperature is discretized without further refinement, for salinity a factor $\mathcal{M}^x = \mathcal{M}^y = 3$ is used for the horizontal directions while in the vertical direction it is $\mathcal{M}^z = 2$. The anisotropic refinement is necessary to cope with the unstable salinity field that is organized into thin vertical fingers with horizontal gradients steeper than in the vertical direction (figure 3.10(a)). Also the time step is refined by a factor $\mathcal{L} = 3$ in order to maintain the integration of the salinity equation stable without penalizing the evolution of momentum and temperature.

Similar to the RB case, the results in terms of heat transfer, salinity fluxes and turbulence statistics agree within the uncertainty of 2–3% with those obtained using a single refined grid for all the variables. Nevertheless, using the present numerical approach momentum and temperature equations are solved on a mesh with $3^2 \cdot 2$ less nodes than that for salinity and 3 times less frequently in time; with respect to the single grid approach this leads to a reduction of CPU time by a factor of 5 for a grid of $144 \times 144 \times 144$ with refinement factors $\mathcal{M}^x = \mathcal{M}^y = 3$ and $\mathcal{M}^z = 2$, when compared to resolving the full flow field with a grid of $432 \times 432 \times 288$. A decrease of RAM memory usage by more than 50% is also achieved by using the strategy.

Before concluding this section it is worthwhile to discuss briefly why in DDC it is possible to simulate a flow with a Schmidt number of 700 without using a refinement factor $\sqrt{Sc} \simeq 27$. The DDC equations in nondimensional form read

Figure 3.10: Instantaneous snapshot of (a) salinity ($Sc_s = 700$), (b) temperature ($Pr = 7$) and (c) vertical velocity in a DDC simulation at drivings of $Ra_s = 5 \cdot 10^7$ and $Ra_T = 10^6$. This results in $Le = 100$ and $R_\rho = 2$.

$$\partial_t u_i + u_j \partial_j u_i = -\partial_i p + \sqrt{\frac{Pr_S}{Ra_S}} \partial_{jj} u_i + (R_\rho \theta - S) \delta_{iz}, \quad (3.8)$$

$$\partial_t \theta + u_j \partial_j \theta = Le \sqrt{\frac{1}{Pr_S Ra_S}} \partial_{jj} \theta, \quad (3.9)$$

$$\partial_t S + u_j \partial_j S = \sqrt{\frac{1}{Pr_S Ra_S}} \partial_{jj} S. \quad (3.10)$$

where the flow parameters are defined as $Ra_T = g\beta_T \Delta T L / (\nu \kappa_T)$, $Pr_T = \nu / \kappa_T$, $Ra_S =$

$g\beta_S\Delta SL/(\nu\kappa_S)$ and $\text{Pr}_S = \nu/\kappa_S$, $\text{Le} = \text{Pr}_S/\text{Pr}_T$ and $R_p = \text{Ra}_T\text{Le}/\text{Ra}_S$.

It can be noted that the diffusivity of momentum $\text{Re} = \sqrt{\text{Pr}_S/\text{Ra}_S}$ increases with Pr_S . Therefore for large enough values the flow does not fully transition to turbulence. On the other hand, the equations for salinity and temperature are linear and they can not sustain the cascade without a turbulent velocity field. This is indeed the case for the flow parameters of the present numerical example (see also Ref. [148]) where the fully turbulent three dimensional cascade cannot be achieved and a factor $\mathcal{M} = \sqrt{\text{Sc}} \simeq 27$ is not required for salinity. Even so, the multiple resolutions strategy results in a substantial gain factor in computational time and RAM memory occupation when compared against the single grid strategy.

3.6 Summary and conclusions

In this chapter we have presented a numerical strategy for the direct numerical simulation of turbulent flows with active and/or passive scalar fields without overresolving the momentum equation and its pressure correction. This is certainly the case of flows with scalar diffusivity smaller than the kinematic viscosity (Pr or $\text{Sc} > 1$). Substantial computational time and memory occupation savings are even obtained for equally diffusive fields with Schmidt numbers of order unity. The different requirements for spatial discretization of scalars with respect to momentum originate not only from the diffusivity but also from the pressure. Its nonlocal effect was found to smoothen the momentum gradients and thereby reduce the resolution requirements with respect to resolving the scalar field. This scenario modifies the picture obtained from dimensional analysis that compares only the Kolmogorov and the Batchelor scales.

To reduce computational costs, a multiple resolutions strategy was developed in which momentum is discretized on a base mesh while scalars are discretized on a refined mesh. To solve the scalar diffusion–advection equation, momentum is spatially interpolated onto the refined grid by tricubic Hermitian splines. The scalar is advanced in time, and if necessary, coarsened to couple it back to the momentum equations. Due to stability constraints on the nonlinear terms, the scalar is advanced in time using a refined timestep. Velocity is linearly interpolated in time for all the intermediate timesteps. The optimal amount of substeps $\mathcal{L}$ coincides with the grid refinement factor $\mathcal{M}$, when it is isotropic, or with $\max[\mathcal{M}^i]$ when it is anisotropic.

The method was applied to Rayleigh–Bénard convection, and decoupling the grid resolutions was found to result in computational speedups of around one-and-a-half to two times for Prandtl unity, and seven for $\text{Pr} = 10$. This strategy was also applied to high Sc flows, also resulting in computational advantages of approximately five. Due to the large costs, both in operations, memory usage and in communication associated to solving the Poisson equation, we expect the gains to increase for larger grids and larger drivings. This is because the Poisson solver is the most expensive

part of advancing the Navier–Stokes equations in time, and this does not scale linearly with the amount of points, while the scalar diffusion-advection equations do. We expect gains of about three to four times for RB simulations at $\text{Pr} = 1$ and $\text{Ra} = 10^{12}$ with production grids of about 1 billion points and $\mathcal{M} = 2$, planned for the future. Also- the memory consumption is heavily reduced, by a factor 2.6x with a refinement of two, and this makes some simulations possible on supercomputers with a lower memory per core and decreases the dependence on high CPU–memory bandwidth.

It is crucial that the base mesh is fine enough to correctly resolve the momentum field. Adding more refinement to the scalar mesh when the velocity grid is insufficient does not give an improvement of the quality of the results, and it might even lead to the suppression of small scales that violate energy conservation. This method could in principle be additionally applied to flows with $\text{Pr} < 1$. Obviously, in this case the velocity field should be solved on a mesh finer than that of the scalar. Although explicit numerical tests have not been attempted, we expect that the computational overhead introduced by the interpolation and coarsening of the fields overcomes the advantages produced by solving the scalar equation on a coarser mesh.

$N_x \times N_y \times N_z$	Pr	$\text{Nu}_{u_z\theta}$	Nu_{θ_w}	$\text{Nu}_{\varepsilon_v}$	$\text{Nu}_{\varepsilon_\theta}$
$96 \times 96 \times 192$	1	66.8	67.2	71.0	59.7
$128 \times 128 \times 256$	1	64.9	64.6	67.1	60.5
$192 \times 192 \times 384$	1	63.2	63.2	64.1	61.3
$256 \times 256 \times 512$	1	63.8	63.6	64.6	62.5
$384 \times 384 \times 768$	1	64.0	63.6	64.3	63.2
$96 \times 96 \times 192$	10	68.4	67.9	68.6	60.8
$128 \times 128 \times 256$	10	65.5	65.2	65.7	61.0
$192 \times 192 \times 384$	10	63.2	63.0	63.1	61.0
$256 \times 256 \times 512$	10	63.6	63.9	63.6	62.4
$384 \times 384 \times 768$	10	63.4	63.9	63.4	63.3

Table 3.1: Details of grid resolution used for standard single grid runs. Simulations were run until $\text{Nu}_{u_z\theta}$ achieved 1% temporal convergence. All the simulations are performed at $\text{Ra} = 10^9$ and $\Gamma = 1$. The first column shows resolution, the second Pr, while the other four show the results of the different definitions of Nu.

$N_x \times N_y \times N_z$	$\mathcal{M}$	Pr	$Nu_{u_z\theta}$	Nu_{θ_w}	Nu_{ε_v}	Nu_{ε_θ}
$96 \times 96 \times 192$	2	1	65.5	65.4	68.4	63.0
$96 \times 96 \times 192$	3	1	65.6	65.3	69.3	69.5
$96 \times 96 \times 192$	4	1	65.4	65.4	66.0	64.9
$128 \times 128 \times 256$	2	1	64.4	64.4	66.7	66.7
$128 \times 128 \times 256$	3	1	64.4	64.4	66.9	66.9
$192 \times 192 \times 384$	2	1	63.5	63.4	62.6	64.5
$96 \times 96 \times 192$	2	10	66.6	64.8	60.0	66.0
$96 \times 96 \times 192$	3	10	64.5	64.5	63.5	63.5
$96 \times 96 \times 192$	4	10	65.4	65.0	64.2	64.2
$128 \times 128 \times 256$	2	10	64.3	64.2	64.7	63.0
$128 \times 128 \times 256$	3	10	64.6	64.1	62.2	64.8

Table 3.2: Details of grid resolution used for multiple resolutions runs. Simulations were run until $Nu_{u_z\theta}$ achieved 1% temporal convergence. All the simulations are performed at $Ra = 10^9$ and $\Gamma = 1$. The first column shows resolution, the second shows the refinement of the scalar grid in all directions, the third Pr, while the other four show the results for the different definitions of Nu. For all simulations $\mathcal{L} = \mathcal{M}$.

$\mathcal{L}$	$\mathcal{C}_{CFL}$	$Nu_{u_z\theta}$	Nu_{θ_w}	Nu_{ε_v}	Nu_{ε_θ}
1	0.6	64.5	64.6	67.3	64.0
2	1.2	64.4	64.4	66.8	63.5
3	1.2	64.6	64.3	67.2	63.5

Table 3.3: Details of the testing for the temporal multiple resolutions. Simulations were run until $Nu_{u_z\theta}$ achieved 1% temporal convergence. All the simulations are performed at $Ra = 10^9$ and $\Gamma = 1$ on a grid $128 \times 128 \times 256$ with $\mathcal{M} = 2$. The first column shows the time refinement level $\mathcal{L}$, the second the maximum CFL computed on the momentum grid, while the last four show the results of the different definitions of Nu.

Connecting flow structures and heat flux in turbulent Rayleigh-Bénard convection*

The aspect ratio (Γ) dependence of the heat transfer (Nusselt number Nu in dimensionless form) in turbulent (two-dimensional) Rayleigh-Bénard convection is numerically studied in the regime $0.4 \leq \Gamma \leq 1.25$ for Rayleigh numbers $10^7 \leq Ra \leq 10^9$ and Prandtl numbers $Pr = 0.7$ (gas) and 4.3 (water). $Nu(\Gamma)$ shows a very rich structure with sudden jumps and sharp transitions. We connect these structures to the way the flow organizes itself in the sample and explain why the aspect ratio dependence of Nu is more pronounced for small Pr . Even for fixed Γ different states (with different resulting Nu) can exist despite turbulence, between which the flow can or cannot switch. In the latter case the heat transfer thus depends on the initial conditions.

*Based on: E.P. van der Poel, R.J.A.M. Stevens, D. Lohse, *Connecting flow structures and heat flux in turbulent Rayleigh-Bénard convection*, Phys. Rev. E R.C. **84** (4) 045303 (2011) [167]

4.1 Introduction

The physicists' view on fully developed turbulence has been dominated by Kolmogorov's seminal work [45], postulating universality of the small scales. Real-world flows however have walls and boundaries. How do these geometric properties affect the global transport characteristics of the flow such as heat or momentum transfer? The common view is that in the fully turbulent state, due to the large fluctuations of the system, the phase space is fully explored by the dynamics of the flow and that universality implies an at most weak dependence on the boundary conditions, clearly without any jumps in global transport properties.

Only recently the community became aware of the possibility of the coexistence of different turbulent states, with first or second order phase transitions in between them. Examples include different turbulent states in von Kármán flow ("French washing machine" [48]), in magnetohydrodynamic turbulence in a closed system (von Kármán turbulent liquid sodium experiment) [46], in turbulent rotating Rayleigh-Bénard (RB) flow [47], or in turbulent rotating spherical Couette flow [49], and possibly even in high Rayleigh number turbulent RB flow in a cylindrical cell of aspect ratio $\Gamma = 1/2$ [50, 55] and $\Gamma = 0.23$ [80]. That transitions between different flow states occur in closed flows at low degree of turbulence has been well known and explored in the context of spatial-temporal chaos and pattern formation, see e.g. [51], but that they also occur between turbulent states clearly came as a surprise.

In this chapter we will numerically show that different turbulent states with first and second order phase transitions in between them and even coexistence of different turbulent states also exist in an even simpler geometry, namely in a two-dimensional (2D) RB sample. The advantages of the 2D geometry are (i) that a flow visualization is much easier, (ii) that the complicated axial and toroidal dynamics of 3D RB flow [87] does not complicate or even obscure the flow field analysis, and (iii) that it is numerically cheaper so that a good resolution in the aspect ratio Γ (i.e. many different runs with different Γ) becomes feasible. These features will enable us to reveal the connection between the flow organization and the heat-transfer properties. However, we stress that these connections also exist in 3D RB flow, and working them out from experimental measurements had been pioneered by Xia and coworkers [168, 169].

The main control parameter of this study will be the aspect ratio Γ , whose effect on the turbulent RB flow has not yet been extensively studied, with only a few theoretical and numerical studies [170–172]. The main reason for this short-coming is that it is experimentally very difficult to vary Γ in 3D cylindrical samples, as each Γ requires a new sample. That is why in experiment the Γ resolution has hitherto been insufficient to detect transitions between different turbulent states. In their review Ahlers *et al.* [87] conclude, based on a small number of experiments with few different Γ [78, 79, 173], that the "weak Γ -dependence [of the heat transfer] suggests an insensitivity to the nature of the large-scale convection". We will show that in 2D

Figure 4.1: $Nu(\Gamma)$ for $Ra = 10^8$ and (a) $Pr = 4.3$ and (c) $Pr = 0.7$ (averaging time $> 10^3 t_E$). The accompanying figures (b) and (d) show the respective relative time the system is in the single roll state (SRS), double-roll state (DRS), triple-roll state (TRS), and quadruple-roll state (QRS). Additionally, the extend of time that no roll state could be identified is indicated.

RB this is definitely *not* the case.

One may argue that the flow phenomena in 3D are different and richer, which is correct. However, various 2D RB flow simulations [38, 41, 174–179] have revealed the value of this approach for a better understanding of turbulent RB convection and the analogies to 3D RB flow. In ref. [178] we could even reveal a one-to-one analogy between the flow organization in our 2D numerical simulations and in experiments in a quasi-2D sample of the same aspect ratio $\Gamma = 1$.

The code on which the results in this chapter are based is a fourth order finite difference discretization of the incompressible Oberbeck-Boussinesq equations. It has been described and tested in detail in ref. [177]. The velocity boundary conditions on the walls are no-slip. The (relative) temperature is fixed at $\Delta/2$ at the bottom plate and $-\Delta/2$ at the top plate, with adiabatic side-wall conditions. The grid resolution obeys the strict criteria formulated in ref. [94]. The imposed initial condition is a single roll state with a linear temperature profile. Times are given in multiples of large eddy turnover times $t_E := 4\pi/|\omega_c(t)|$, where ω_c is the center vorticity.

4.2 Results

In fig. 4.1 we show $\text{Nu}(\Gamma)$ for $\text{Ra} = 10^8$ and $\text{Pr} = 0.7$ and 4.3, resulting from a very large averaging time of more than $10^3 t_E$, for which we have checked statistical convergence. For the lower Pr the curve shows variations in Nu of up to 35%, with abrupt jumps and sharp transitions. From visual inspection of flow movies we deduce that these jumps are associated with transitions in the overall flow organization from one to two vertically stacked rolls (at $\Gamma \approx 0.9$) and from two to three rolls (at $\Gamma \approx 0.55$). We automatize this flow analysis by measuring the zeros in the vorticity along the center vertical axis, i.e., the zeros in $\omega(x = D/2, z)$. A state is not counted if its life time is shorter than t_E . The results for the relative time in a certain state is shown in fig. 4.1. For $\text{Pr} = 0.7$ this analysis confirms that the transitions are rather sharp, with the coexistence of different roll states only in a small Γ -range. Next to the jumps, relatively sharp transitions in $\text{Nu}(\Gamma)$ can be observed. As an example we discuss the 35% increase in Nu from $\Gamma = 0.45$ to $\Gamma = 0.55$, namely from $\text{Nu} = 16$ to $\text{Nu} = 24$. This coincides with a developing instability of the triple roll state (TRS): The sample becomes too wide for three rolls so that the three-roll structure from time to time breaks down. This breakdown shuffles warm fluid upwards and cold fluid downwards, leading to a larger temperature gradient across the thermal boundary layers (BLs) and thus to increased heat flux. Typical snapshots of the temperature field in this regime are shown in fig. 4.2.

The enhanced vortex mobility at $\Gamma = 0.55$ as compared to $\Gamma = 0.45$ can also be deduced from the positions of the vortex centers, which we identify by a direct ellipse-fit [180] coupled with a vortex criterium based on the nonzero imaginary part

Figure 4.2: Snapshots of the temperature field for $Ra = 10^8$ and $Pr = 0.7$ for (a) $\Gamma = 0.45$ with the flow in a very stable TRS and (b,c) $\Gamma = 0.55$ with the flow in an unstable TRS. The top and bottom rolls in (b) grow until collision (c), which causes enhanced mixing and heat transport. The positions of the roll centers are automatically tracked and their PDFs as function of (x, z) are shown in (d) for $\Gamma = 0.45$ and (e) for $\Gamma = 0.55$.

Figure 4.3: Two temperature snapshots for $Ra = 10^9$, $Pr = 4.3$, and $\Gamma = 0.93$. The system is either in the SRS (a) or DRS (b). Heat transport efficiency differs between these states, see fig. 4.4.

of the velocity gradient tensor's eigenvalues. The 2D probability functions (PDFs) of these positions are visualized in fig. 4.2d (for $\Gamma = 0.45$) and fig. 4.2e (for $\Gamma = 0.55$). While in the former case we see three pronounced sharp peaks, reflecting the stability of that flow configuration, in the latter case the peaks are smeared out, showing the vortex mobility which contributes to the enhanced heat flux.

We now come to the case of large $Pr = 4.3$. Here the transitions in $Nu(\Gamma)$ are much smoother as compared to the $Pr = 0.7$ case (compare figs. 4.1b and d) with wide Γ regimes of coexistence between different states, between which the dynamical evolution of the flow meanders, as e.g. seen from temperature field snapshots of fig. 4.3 and the time series of the Nusselt number. For these larger Pr the dynamics is much richer as the flow keeps on switching between the different states. The reason for this lies in the plume dynamics: Whereas for $Pr = 0.7$ the larger thermal diffusivity tends to smoothen out temperature differences between different flow parcels, for larger $Pr = 4.3$ the plumes keep their thermal energy for a longer time. Thus the plumes, which feed the competing rolls as described in ref. [178], have a longer life time, which leads to more lively roll dynamics. Therefore a 100% dominance of a certain roll state, common for small Pr , does not occur.

Based on the state analysis, the heat flux can be conditionally averaged on the SRS, DRS, or TRS. The results for these conditional heat fluxes are shown in fig. 4.4. For the vertically arranging vortices it again holds that the stable states with n rolls enable larger heat transfer than the stable states with $n+1$ rolls. For $n=1$ and $n=2$ the difference is about 5% for $Ra = 10^9$, $Pr = 4.3$. Remarkably, that value is similar to what one would expect for the 3D situation, based on an extrapolation

Figure 4.4: Conditionally averaged $Nu(\Gamma)$ for the various states SRS, DRS, and TRS, which can be identified at $Ra = 10^9$ and $Pr = 4.3$. For fixed Γ the flow jumps in between these different states.

towards $Ra = 10^9$ of the Nu measurements for the SRS and DRS in ref. [181] (for $4 \cdot 10^9 \leq Ra \leq 10^{11}$), which roughly gives 3%.

We also found a case for which the final state and thus Nu depend on the initial conditions of the flow field, see fig. 4.5 for $Ra = 10^7$ and $Pr = 0.7$, which according to ref. [38] is already turbulent. The unstable TRS initial condition for $\Gamma = 0.63$ falls back to the DRS, whereas for initial DRS condition at $\Gamma = 0.64$ the flow remains in this DRS (with lower Nu) for longer than $3000 t_E$. It remains to be seen whether this explicit dependence on initial conditions can also be found at larger Ra .

We finally address the question why Nu is much more sensitive to the flow organization at small Pr as compared to large Pr , see again fig. 4.1. The first reason for this finding is the organization of the thermal BL and kinetic BL: For large Pr the thermal BL is nested in the kinetic one. Thus modifications of the bulk flow are buffered by the kinetic BL and hardly lead to a different thermal BL thickness λ_θ and therefore to hardly any change in $Nu \approx L/(2\lambda_\theta)$. In contrast, for low Pr the thermal BL is thicker than the kinetic one and is therefore fully exposed to bulk flow modifications, leading to a much stronger dependence of $Nu \approx L/(2\lambda_\theta)$ on the flow organization. The second reason for the larger sensitivity of Nu at smaller Pr is the larger thermal diffusivity, leading to a thermal smoothening of the plumes. As discussed above this results in sharper transitions between different states. Our interpretation is supported by fig. 4.6, in which we plot $Nu(\Gamma)$ vs a normalized Reynolds number $Re_z(\Gamma)$, where $Re_z = u_{z,rms}L/\nu$, which represents the bulk flow. For $Pr = 4.3$ there is hardly any dependence of Nu on $Re_z/\langle Re_z \rangle$, whereas for $Pr = 0.7$ this dependence is major. Here $\langle Re_z \rangle$ is the average Reynolds number of the shown Γ range $0.4 \leq \Gamma \leq 1.25$.

Figure 4.5: $Nu(\Gamma)$ for $Ra = 10^7$ and $Pr = 0.7$. For $\Gamma \approx 0.64$ the Nusselt number depends on the initial conditions, see text for details.

Figure 4.6: $Nu(\Gamma)$ vs. $Re_z(\Gamma)/\langle Re_z \rangle$ for $Pr = 0.7$ (red squares) and $Pr = 4.3$ (blue bullets) at $Ra = 10^8$.

4.3 Conclusion

In conclusion, we could clearly identify different turbulent states, corresponding to different roll structures. It is remarkable that these features, which have been associated to lower Reynolds and Rayleigh number flow in the regime of spatial-temporal chaos with much less dynamical degrees of freedom, survive for such high Ra . It seems that the turbulent states 'live' on low-dimensional structures. The different turbulent states are associated with different overall heat transfer. Transitions between the states – either dynamically or as function of the control parameter Γ – thus imply jumps and sharp transitions in $Nu(\Gamma)$. Based on the flow organization, we understand why these variations are larger for lower Pr and why the overall flow dynamics is richer at larger Pr , for which the plumes can keep their thermal identity for a longer time. The next step will be to push the present results to much higher Ra in order to see whether these features survive. Based on our analysis for $Ra = 10^8$ and 10^9 we presume that this could be the case as the stability of the states and the variation in $Nu(\Gamma)$ is higher for $Ra = 10^9$ compared to $Ra = 10^8$ at $Pr = 4.3$. Additionally, large-scale roll states have been distinguished up to $Ra = 10^{10}$ [178] and can probably be found for even higher Ra .

Flow states in two-dimensional Rayleigh-Bénard convection as a function of aspect ratio and Rayleigh number*

In this numerical study on two-dimensional Rayleigh-Bénard convection we consider $10^7 \leq Ra \leq 10^{12}$ in aspect ratio $0.23 \leq \Gamma \leq 13$ samples. We focus on several cases. First we consider small aspect ratio cells, where at high Ra number we find a sharp transition from a low Ra number branch towards a high Ra number branch, due to changes in the flow structure. Subsequently, we show that the influence of the aspect ratio on the heat transport decreases with increasing aspect ratio, although even at very large aspect ratio of $\Gamma \approx 10$ variations up to 2.5% in the heat transport as a function of Γ are observed. Finally, we observe long-lived transients up to at least $Ra = 10^9$, as in certain aspect ratio cells we observe different flow states that are stable for thousands of turnover times.

*Based on: E.P. van der Poel, K. Sugiyama, R.J.A.M. Stevens, D. Lohse, *Flow states in two-dimensional Rayleigh-Bénard convection as a function of aspect ratio and Rayleigh number*, Phys. Fluids. **24** (8) 085104 (2012) [182]

Figure 5.1: a) Nu versus Ra for $Pr = 1$ in aspect ratio $\Gamma = 0.23$ (orange circles), $\Gamma = 1/3$ (lime diamonds), $\Gamma = 1/2$ (green squares), $\Gamma = 2/3$ (blue upward pointing triangles), $\Gamma = 1$ (purple pentagrams) and $\Gamma = 2$ (red downward pointing triangles) samples. b) Re_2 versus Ra for $Pr = 1$ and in $\Gamma < 1$ samples. The averaging time ranges from $4000 t_E$ to $200 t_E$.

5.1 Introduction

To better understand geo- and astrophysical phenomena it is important to know the heat transfer in the high Ra number regime. Nowadays, most experimental and numerical measurements of the heat transfer, indicated by the Nusselt number Nu , in 3D agree up to $Ra \approx 2 \times 10^{11}$ (see Ref. [87] for detailed references) and these data are well described by the Grossmann-Lohse (GL) theory [35, 66, 68, 70]. Unfortunately, there are considerable unexplained differences in the heat transfer measurements for higher Ra [30, 31, 50, 80, 89, 94, 99, 100, 113, 114, 183–187].

Explaining the differences between the high Ra number measurements is subject of an ongoing discussion [31, 80, 87, 94, 183]. The difficulty is that experiments in the high Ra number regime are very challenging as it requires very large setups that operate under high pressures [50, 89, 100, 186, 187], or use liquid helium near its critical point [30, 80, 99, 113, 114, 184, 185]. Therefore only a few setups in the world can perform high Ra number experiments and testing the influence of some effects, e.g. the influence of the aspect ratio, is very time consuming [80]. In 3D simulations it is difficult to study the problem, as these simulations are very CPU time intensive [31].

One possibility to limit the required computational time is to study the influence of several effects in 2D RB convection in order to select the most interesting cases that need to be studied in 3D. One may wonder whether the dynamics of 3D RB con-

Figure 5.2: Ra_c versus Γ , both on logarithmic scale. A least-squares fit, which is indicated by the black solid line, gives $Ra_c \sim \Gamma^{-2.44}$. The blue and red dashed lines give $Ra_c \sim \Gamma^{-2}$ and $Ra_c \sim \Gamma^{-3}$, respectively.

vection are sufficiently captured in 2D simulations. This question has been addressed by Schmalzl *et al.* [188] and they showed that in relatively large aspect ratio cells, where several convection rolls can form next to each other, and for $Pr \gtrsim 1$ 2D RB convection global quantities such as the Nu number and the Re number show similar behavior in 3D. Therefore 2D simulations have been used to investigate a number of aspects observed in 3D convection [31, 38, 41, 176, 177, 179, 189–191].

It has been argued that the differences between high Ra number experiments are due to the formation of different turbulent states. Experimental indications for coexistence of different turbulent states in RB convection are found by several authors [50, 169, 183, 185, 187, 192–194] and are discussed theoretically by Grossmann and Lohse [55]. It has been shown by Xi & Xia [169] and Weiss & Ahlers [194] that in a $\Gamma = 0.5$ sample the flow can be either in a single roll state (SRS) or in a double roll state (DRS), each with a specific heat transport. Later §4 confirmed this effect in 2D simulations and showed that the flow state, and thus Nu, can strongly depend on the aspect ratio. Experiments by Roche *et al.* [80] show that the transition towards a regime in which a strong heat transfer enhancement as function of Ra is found strongly depends on the aspect ratio and the experiments by Niemela & Sreenivasan [183] reveal the presence of a low and a high Ra number branch.

Using a direct numerical simulation scheme for $10^7 \leq Ra \leq 10^{12}$ we show that also in small aspect ratio 2D RB convection there is a low and a high Ra number branch for the heat transport and that the transition at the critical Rayleigh number Ra_c between the branches increases with decreasing aspect ratio. Subsequently, we study the heat transport as function of the aspect ratio at fixed Ra. Bailon-Cuba *et al.* [172] have studied the effect on Nu of increasing the aspect ratio in 3D numerics and found that Nu depends on the number of horizontally stacked rolls. Now, we try to estimate how large the aspect ratio should be before finite size effects become

unimportant.

The objective of this paper is to study the phenomena associated with varying Ra and Γ to a large extent. The corresponding observations of the double branching in $Nu(Ra)$ and vanishing variations in $Nu(\Gamma)$ at large Ra and Γ can be found in chapters III and IV, respectively. Furthermore, in chapter V we will discuss some long-lived transient effects we observe at $Ra = 10^9$ and $Pr = 0.7$. These three cases have overlapping origin and secondary effects, such as multi-stability and roll break-up.

In the case of long-lived transients, the exhibited multiple roll states with different corresponding Nu and Re , survive for such long times, that the roll state can either be interpreted as a transient or as stable. This classification is very difficult, as the insuperable finite run time of simulations makes it impossible to ascertain that the observed state is not a transient. To overcome the ambiguity between transient and multi-stability, the cases for which this classification is unclear will be termed as transients and these will be annotated with the simulation run time. This time is an indication of the stability of the observed states. We conclude the paper with a discussion of the presented results.

5.2 Numerical method

The code on which the results in this chapter are based is a fourth order finite difference discretization of the incompressible Oberbeck-Boussinesq equations. The velocity boundary conditions on the walls are no-slip. The (relative) temperature is fixed at $\Delta/2$ at the bottom plate and $-\Delta/2$ at the top plate, with adiabatic side-wall conditions. The code has been described and tested in detail by Sugiyama *et al.* [38, 176, 177] and this code was used to explain the non-Oberbeck Boussinesq effects observed in 3D experiments of Ahlers *et al.* [176], and Zhou *et al.* [179, 190] and Sugiyama *et al.* [178] found a good agreement between results obtained using this 2D code and experiments performed in quasi-2D RB samples. The grid resolution we used obeys the strict criteria formulated in refs. [44, 94]. The Nusselt number Nu is calculated with four different procedures. The Nu used in this study is the average of the definitions given by equations 8-11. As the Nusselt number should not be dependent on the procedure by which it is calculated, comparing the results of the different procedures is an indication of the numerical error. For all data points in this study the error calculated by comparing the results is smaller than dot size. The time convergence of Nu is checked by comparing the time-averages over half the duration of the simulation and the full duration. Again, the resulting error is for most cases smaller than dot size. However, this error is not necessarily monotonically decreasing with increasing simulation time due to slow trends and rare events. For an indication of the uncertainty associated with the calculation of the numerical quantities, the typical averaging time will be annotated with the data. The used unit of time is the large

Figure 5.3: Flow visualization for the flow in a $\Gamma = 0.23$ sample with $\text{Pr} = 1$ at (a) $\text{Ra} = 10^8$, (b) $\text{Ra} = 10^9$, (c) $\text{Ra} = 10^{10}$, (d) $\text{Ra} = 10^{11}$, and (e) $\text{Ra} = 10^{12}$. The velocity field is represented by the vectors and, red and blue indicate high and low temperature, respectively. Note that the colormap is not constant. For $\text{Ra} = 10^{11}$ the activity of the rolls is increased and at $\text{Ra} = 10^{12}$ the roll structure appears to be completely broken down.

eddy turnover time, given by $t_E \equiv 4\pi/|\langle \omega_c \rangle|$, where ω_c is the vorticity at the center of a roll.

5.3 High Rayleigh number convection

Figure 5.1a shows the heat transport as function of Ra for different aspect ratio cells. Just as in the experiments of Niemela & Sreenivasan [183] a low and a high Ra number branch is observed and the Nu difference is larger for the low aspect ratio cells. One can see that the Ra number at which the transition from the low to the high branch sets in increases with decreasing aspect ratio. To find the transitional Ra number Ra_c we extrapolated the low branch, which scales approximately as $Nu \sim Ra^{0.30}$, and fitted the points found in the transition region with a power law. The intersection of the resulting lines gives Ra_c , which is calculated for $0.23 \leq \Gamma \leq 2/3$. Figure 5.2 shows that Ra_c scales approximately as $Nu_c \sim \Gamma^{-2.44}$, although the Γ -range is of course very limited. This is very similar to the result obtained by Roche *et al.* [80], who performed high Ra number experiments in different aspect ratio samples and observed a sharp increase in the heat transfer, which sets in beyond a critical Ra that scales as $Ra_c \sim \Gamma^{-2.50}$. However, we note that both data sets would also be in reasonable agreement with a Γ^{-3} scaling, which would be equivalent to saying that a Ra number based on the diameter d and not the height L of the cell is constant [80].

The transitional Ra numbers we find are well below the value at which the transition towards the ultimate state is expected [87] and therefore it is important to know what effect is responsible for the sharp increase in the heat transport. To answer this question we visualized the flow field for the simulations in the aspect ratio $\Gamma = 0.23$ sample, where the transition is most pronounced. Figure 5.3 reveals that for low Ra there are vertically stacked stable rolls. The flow structure is substantially different in the higher Ra number cases. For $Ra = 1 \times 10^{11}$ the increased temperature gradients in the corner rolls indicate that they are more active than at lower Ra , i.e. the corner rolls exchange more thermal energy with the large-scale flow. As this increases the effective plate area that contributes to the heat transport, this leads to heat transport enhancement. For even higher Ra the rolls (partially) break up due to increased buoyancy forces. The plumes break up the rolls and at the same time have a decreased travel distance towards the opposite plate. This leads to a higher heat transport. In order to verify this picture we calculated Re_2 , where $Re_i \equiv u_i^{RMS} L / \nu$ is the Reynolds number based on the root mean square velocity with the index $i = 1, 2, a$ indicating horizontal, vertical and absolute velocity, respectively. Figure 5.1 shows that the transition in the Nu number coincides with a strong increase in the vertical velocities. Therefore we can conclude that the transition we see here is due to a transition between different turbulent states - the breakdown of the corner roll - and is not a transition towards the ultimate regime.

When we compare the 2D results with the measurements of Roche *et al.* [80] we notice that the Ra number at which the sharp increase in the heat transfer is observed happens at a lower Ra in 2D than in 3D. Another difference is that we observe a low and a high Ra number branch for the heat transfer in 2D, whereas no high Ra number branch is observed in the experiments of Roche *et al.* [80]. However, we note that Niemela & Sreenivasan [183] did observe two branches and it could well be that this second branch could also be found in the Roche *et al.* [80] experiments at higher Ra. Although one should be careful with comparing the results from 2D and 3D RB convection in small aspect ratio samples, as we will discuss in detail below, we emphasize that it is important to keep in mind is that not every increase in the scaling of the heat transport as function of Ra that is observed indicates a transition towards the ultimate regime, as we showed here for the 2D case.

Again we stress that one should be careful with a direct comparison between 2D and 3D results in small aspect ratio cells. For small aspect ratio cells the dynamics in 2D and 3D RB convection can be different as vertically stacked rolls are formed. In 2D vertically stacked rolls can lead to a larger reduction of the heat transport than in 3D RB convection as warm (cold) fluid in the bottom (top) part of the cell is more likely to be trapped than in 3D. In fact experiments and simulations of 3D RB convection, e.g. Bailon-Cuba *et al.* [172], show a weaker aspect ratio dependence than observed in the 2D simulations (section 5.4).

5.4 Large aspect ratio

To find the critical horizontal length of the system at which the heat transport becomes nearly independent of the aspect ratio we extend the dataset for $Ra = 10^8$ and $Pr = 4.3$ of §4 towards large Γ to include horizontally stacked rolls and the corresponding transitions between them. The most remarkable observation is that the transitions between the horizontal roll states have a different shape than the transitions between vertical roll states, see figure 5.4a and §4. The amplitudes of the Nu variation over the transitions are surprisingly large, especially the transition between the SRS and the horizontal DRS. What cannot be extracted from this figure is that the lifetime of the transient states increases close to a jump.

Figure 5.4b reveals that the ratio $f(\Gamma) \equiv n/\Gamma$ approaches a constant value of approximately 0.8 at large Γ , where n is the number of large-scale rolls in the system. Here we define that for vertically stacked rolls $n \leq 1$ and for horizontally stacked rolls $n \geq 1$. Comparing with $Nu(\Gamma)$ in figure 5.4a, it can be seen that there is a strong correlation between Nu and n/Γ . This indicates that the asymmetric deformation of the rolls is connected to Nu, which can be demonstrated using the concept of plumes driving the bulk flow and transporting the heat. When a roll is horizontally elongated, the ratio between the number of rolls n and Γ decreases, this results in a lower Nu as

Figure 5.4: a) Nu as a function of Γ for $Pr = 4.3$ and $Ra = 10^8$. The depicted $1 < \Gamma < 12$ range captures the SRS up to the horizontally stacked 10RS ($n = 10$), each represented by a cluster of points from low to high Γ . b) n/Γ approaches a constant value of approximately 0.77. c) The function $f(\Gamma) \equiv Re_2 / (Re_1 n / \Gamma)$. The error on the time-convergence is smaller than the dot size as the averaging time is more than $1000 t_E$.

Figure 5.5: a) The amplitude of the jumps between different in roll states in $Nu(\Gamma)$, ΔNu_n^{n+1} and the $C/(\Gamma + D)$ scaling as a function of n . Here the scaling constants $C = 6.9$ and $D = 1$. b) The Reynolds number Re_a as a function of Γ appears to asymptotically approach a constant $Re_{a,\infty}$ value at high Γ . The fit with equation (5.2) is plotted as the dashed line.

the number of thermal hotspots per horizontal plate length decreases as $1/\Gamma$ for fixed n . This explains the similarity of the $Nu(\Gamma)$ profiles for fixed n between the $Nu(\Gamma)$ plot in figure 5.4a and the $f(\Gamma)$ plot in 5.4b. In addition, it appears that the amplitudes of the Nu jumps between these plots are similar. The amplitudes decreases for each consecutive transition from n to $n + 1$. This can be explained by using identical reasoning for the profile for fixed n , applying to a transition. We then get that the jump amplitude ΔNu_n^{n+1} between a n and $n + 1$ roll state scales as

$$\Delta Nu_n^{n+1} \sim \frac{n+1}{\Gamma} - \frac{n}{\Gamma} = \frac{1}{\Gamma}. \quad (5.1)$$

In figure 5.5a ΔNu_n^{n+1} , extracted from $Nu(\Gamma)$ in figure 5.4a, is plotted together with a scaled function $C/(\Gamma + D)$. The offset in the denominator stems from the fact that the reasoning behind the derivation of the scaling is only valid for $n \geq 1$. The agreement between these plots is very good and therefore the fit can be used to extrapolate ΔNu_n^{n+1} to higher Γ . Using the asymptotic values for Nu and n/Γ , which are 24.92 ± 0.06 and 0.77 ± 0.01 respectively, the Γ_c where the jump magnitude is less than 1% of Nu is found to be $\Gamma_c = 26 \pm 1$, which corresponds to $n \approx 20$.

Not only $Nu(\Gamma)$, but also $Re_a(\Gamma)$ can be used for extrapolating. Figure 5.5b shows that Re_a increases with Γ and approaches an asymptotic $Re_{a,\infty}$. Similar to $Nu(\Gamma)$ and for $n \geq 1$, the trend is well approximated by

$$Re_a^{fit}(\Gamma) = Re_{a,\infty} \left(1 - 0.01 \frac{\Gamma_c}{\Gamma}\right), \quad (5.2)$$

where Γ_c is the aspect ratio where the function $Re_{12}^{fit}(\Gamma)$ is 99% of $Re_{a,\infty}$. Using

Figure 5.6: Nu versus Re_1 (a) and Re_2 (b) for $Ra = 10^8$ and $Pr = 4.3$. Different n are indicated by the colored symbols, see legend figure 5.5b. A negative correlation between Nu and Re_1 and a positive correlation between Nu and Re_2 can be seen.

the Γ 's just after a jump results in $\Gamma_c = 22 \pm 1$, which is close to the prediction based on $Nu(\Gamma)$, considering the quantity used for extrapolation is very different.

The loss of Γ dependence is accompanied by an increase in multi-stability of the roll states. For large Γ the transients for Γ 's near a jump in n become very long-lived. As an example, for $\Gamma = 13.6$ both the $n = 10$ and $n = 11$ roll states survive for longer than $3000 t_E$. For comparison, a typical transient state for this $Ra = 10^8$ and $Pr = 4.3$ is less than $100 t_E$. The corresponding Nu differs substantially between these roll states at $Nu = 24.68$ and $Nu = 25.11$ for $n = 10$ and $n = 11$, respectively. Thus, even though the Nu dependence on Γ decreases monotonically for larger Γ per roll state, which can be seen in the $Nu(\Gamma)$ plot shown in figure 5.4, at large Γ different roll states have overlapping stable regions in Γ , meaning that hysteresis effects become important. Thus, in spite of the proper extrapolations, multi-stability might prevent a solid indication for a Γ_c , at which the Γ dependence of global properties is lost.

The effect of horizontal roll asymmetry is further highlighted by the plots in figure 5.6. The deformation indirectly results in decreasing Nu by decreasing Re_2 . Figure 5.6b shows that Nu and Re_2 are positively correlated. For $\Gamma \geq 1.1$, Re_2 decreases monotonically with increasing Γ due to roll asymmetry up to the Γ where n jumps to $n + 1$. In contrast, Nu is negatively correlated with Re_1 , see figure 5.6a, which can be explained by a flux conservation argument similar to the one presented by Grossmann and Lohse [170]. Considering the large-scale circulation (LSC) to be of simple elliptical shape, the horizontal flux has to be equal to the vertical flux. Normalizing with the height of the system, the flux balance is

$$f(\Gamma) \equiv \frac{Re_2}{Re_1 n / \Gamma} = 1. \quad (5.3)$$

Indeed, figure 5.4c reveals that this function is in the order of 1 over the studied

Γ range, which explains the negative correlation between Nu and Re_1 by relating Re_1 to Re_2 .

5.5 Long-lived transients

This chapter differs from the previous two in the sense that it does not vary a single control parameter to an large extent. Instead, a phenomenon is presented in the form of very long-lived transients. In §4 we showed that for $Ra = 10^7$ and $Pr = 0.7$ the final state and thus Nu can depend on the initial conditions of the flow field. Whether this feature of moderate Ra number RB convection can be found for high Ra number flows is an important and open question. Multiple states have been reported for high Ra 3D experiments by Roche *et al.* [195] and Weiss & Ahlers [194], where the system dynamically switches between two meta-stable states, each with a different Nu . In addition, Ahlers *et al.* [50] showed multiple $Nu(Ra)$ scalings, dependent on minor external temperature variations. However, many details of multiple states in RB flow and their effect on Nu are still unknown.

We now analyze multi-stable states at $Ra = 10^9$ and $Pr = 0.7$ in 2D, where the largest roll in the flow is in general significantly smaller than the limiting dimension of the enclosing boundaries. This qualification implies that simple roll states are broken down. These turbulent states with broken-down rolls are named uncondensed, where the notion of condensation is followed from [196]. Here, a state is named condensed when the largest roll in the system is of system-size, i.e. is spectrally condensed with the energy piled-up in a scale close to system-size. In RB flow the dynamics of the coherent structures differ substantially between condensed and uncondensed states. In the uncondensed case the largest rolls are no longer stationary on a time scale shorter than a turnover time. Instead, they are mobile and cause thermal plumes to move through high-shear central regions, which is very different from the condensed states where plumes crawl along the sidewall. Whether the uncondensation is an effect of the possible inverse energy cascade or a result of a growing buoyancy forces compared to inertial forces or both, is not known and beyond the scope of this paper. Nevertheless, the condensation terminology is used in this chapter to highlight the similarity between condensation in two-dimensional RB flow and classical 2D [197] and thin layer [196] turbulence.

The uncondensed roll states for high Ra number flows are composed of small and mobile rolls. Therefore an advanced identification algorithm is required to obtain statistics on the roll state for these cases. In the remainder of this section we first discuss the vortex detection algorithm of §4 in detail before we apply it to a set of simulations at $Ra = 10^9$ and $Pr = 0.7$, where very long-lived transients are found.

Figure 5.7: Example vortex detection of a flow field snapshot for $Ra = 10^9$, $Pr = 4.3$ and $\Gamma = 0.85$. (a) Flow visualization with the temperature and velocity indicated by color and vectors respectively. (b) Mapped by vortex criterium and sign of vorticity. Blue and red indicate clockwise and counter clockwise rotation, respectively. Green indicates hyperbolic field. (c) End results of the algorithm where the ellipses are colored by direction of rotation. The DRS exhibited by the flow field is captured accurately by the vortex detection algorithm.

5.5.1 The vortex detection algorithm

In order to analyze the large-scale flow structure we look at the second invariant of the velocity gradient tensor $A_{ij} \equiv \partial_j u_i$. The criterion of a positive second invariant [198, 199], formally known as the Q-criterion, is used to identify vortex regions. For incompressible two-dimensional flow the criterion results in

$$A_{11}^2 + A_{12}A_{21} < 0. \quad (5.4)$$

A segmentation algorithm is employed to connect the grid points encompassed by the vortex regions after the grid resolution is reduced. The purpose of the grid reduction is to decrease the computational cost of the segmentation. Although some information is lost in the process, it is only detrimental for small structures, has little effect on the LSC structure and the reduction value can be adjusted. The edge points are used in a direct ellipse-fit to model the vortices in the flow as ellipses. In general, this shape is more fitting for larger structures and as detecting these is the main purpose of this algorithm, it seems justified to use ellipses. The direct output consists of the six coefficients of the quadratic conic section. These coefficients are used to calculate the center coordinates, the tilt angle and the radii of the ellipse. It requires five floating points and an additional boolean for the direction of rotation, to store the information of a single vortex. The operation of the algorithm is visualized

in figure 5.7. Using this method we can now store all information about the main flow structures for long simulations at $Ra = 10^8$ in only 0.15 GB, whereas storing the complete flow field over the same time-interval would require 1000 GB. This opens the possibility to study rare events of which the information is usually lost.

5.5.2 Different states in the turbulent regime

Figure 5.8 shows Nu as a function of Γ . In this figure the colored symbols indicate the observed roll state using the vortex detection algorithm described above. The uncondensed SRS and uncondensed DRS states are distinct from each other by their Nu and the number of equal sized largest vortices. A correlation between the roll state and Nu can be distinguished as the points are clustered by Nu and the roll state. The simulation we ran for $\Gamma = 0.950$ snapped into a SRS state after $750 t_E$, unlike neighboring points, which remained in the uncondensed SRS state for longer than $2200 t_E$. Forcing the system in a condensed SRS by using the steady roll state solution of $\Gamma = 0.950$ reveals that there is a possibility of multi-stability around this point as this state remains stable for longer than $1800 t_E$, see figure 5.8b. However, for Γ 's further away from $\Gamma = 0.950$, the SRS does not survive and the system immediately becomes uncondensed. This happens for e.g. $\Gamma = 1.100$, where this break down occurs within one turnover time t_E . Thus there appears to be hysteretic behavior not only over the jumps between the different roll states (§4), but also over the transition to condensed states.

The SRS has a higher Nu than the uncondensed SRS. This is unexpected, as flow field movies seem to reveal enhanced mixing and heat transport due to the presence of the secondary roll in the uncondensed SRS. However, a closer investigation suggests that the thermal plumes are not directly transported to the opposite boundary layer in the uncondensed SRS, which is the case for the SRS. For the TRS (triple roll state) and DRS, this effect is opposite. Here, the break up of the simple roll states increases Nu , similar to the effect seen in chapter III.

In contrast, the $Nu(\Gamma)$ dependence within the uncondensed SRS, uncondensed DRS and DRS regions appears to be absent. However, large Nu variations can be seen at the TRS region, where due to an increased restriction of the flow, the largest scale of the flow approaches the length of the limiting dimension of the system and thereby a return of strong aspect ratio dependence. A collection of probability density functions (PDFs) of the x and z coordinates of the vortex centroids for specific and relevant roll states can be found in figure 5.8. These plots are based on the output of the vortex detection algorithm. In figure 5.8d a clear fingerprint of the 'orbiting rolls' uncondensed SRS can be observed as a large central peak with a concentric ring. The latter represents the smaller roll(s) rotating around the large central roll. Distinct from this figure is the uncondensed DRS PDF in figure 5.8c, which reveals that even different uncondensed states can be distinguished. In contrast, the SRS PDF has three

Figure 5.8: (a) $Nu(\Gamma)$ for different states for $Pr = 0.7$ and $Ra = 10^9$. The error on the time-convergence is smaller than the dot size as the averaging time is more than $1000 t_E$. (b) Zoom at multi-stability region $0.90 \leq \Gamma \leq 1.00$. 2D PDF plots of the x and z coordinates of the vortex centroids for (c) $\Gamma = 0.73$ (uncondensed DRS), (d) $\Gamma = 0.945$ (uncondensed SRS) and (e) $\Gamma = 0.95$ (SRS). In (e) the original algorithm output is convoluted with a Gaussian for illustrative purpose. This results in the peaks being displayed wider than they are.

sharp peaks, which are shown in figure 5.8e. The PDFs reveal that the mobility of the rolls increases for high Ra uncondensed roll states, as the peaks are more smeared out for these cases.

5.6 Discussion and Conclusion

To summarize, here we considered three cases of two-dimensional Rayleigh-Bénard convection in direct numerical simulations. First, we showed that in small aspect ratio 2D RB convection there are two branches for the heat transport as function of Ra. A lower branch for relatively low Ra and a higher branch for high Ra. By necessity, there is a strong increase of the heat transport in the transition region. This transition takes place for higher Ra and is stronger when the aspect ratio is smaller. We show that the heat transport enhancement coincides with the transition from a flow state with vertically stacked stable rolls to a regime in which the thermal driving becomes strong enough to (partially) destroy the rolls. We discuss the similarities and difference with respect to the experiments of Roche *et al.* [80] and Niemela & Sreenivasan [183] and although one cannot directly compare the 2D and 3D results in this case it is clear from this example that one should be careful in identifying an increase of the heat transport scaling as function of Ra as the transition towards the ultimate regime.

Second, we showed that the influence of the aspect ratio on the heat transport decreases with increasing aspect ratio, although even at a very large $\Gamma = 10$ variations up to 2.5% are observed due to changes in the flow structure. Extrapolating $Re_a(\Gamma)$ towards high Γ gives $\Gamma_c = 22 \pm 1$, where aspect ratio dependence of global properties is less than 1% of their asymptotic values. Using the jumps in $Nu(\Gamma)$, a value of $\Gamma_c = 26 \pm 1$ is found.

Finally, we observe very long-lived transients / different turbulent states at $Ra = 10^8$ and $Pr = 4.3$ for certain very large aspect ratios and at $Ra = 10^9$ and $Pr = 0.7$. In the latter regime rare random events cause the system to switch between states. The probability of these events occurring, the stability of the resulting state and the effect on Nu appear to be very sensitive to the control parameters. In particular, the aspect ratio Γ has a large influence on these phenomena; varying Γ reveals a rich phase space for a given Ra and Pr. For these parameters the flow is so turbulent that the different states with their rare events can only be identified with the use of an advanced vortex detection algorithm, which has revealed the possibility of hysteretic behavior over the transition to condensed states.

The effect of velocity boundary conditions on the heat transfer and flow topology in two-dimensional Rayleigh-Bénard convection*

The effect of various velocity boundary condition is studied in two-dimensional Rayleigh-Bénard convection. Combinations of no-slip, stress-free and periodic boundary conditions are used on both the sidewalls and the horizontal plates. For the studied Rayleigh numbers Ra between 10^8 and 10^{11} the heat transport is lower for $\Gamma = 0.33$ than for $\Gamma = 1$ in case of no-slip sidewalls. This is, surprisingly, the opposite for stress-free sidewalls, where the heat transport increases for a lower aspect ratio. In wider cells the aspect ratio dependence is observed to disappear for $Ra \geq 10^{10}$. Two distinct flow types with very different dynamics can be seen, mostly dependent on the plate velocity boundary condition, namely roll-like flow and horizontal zonal flow, which have a substantial effect on the dynamics and heat transport in the system. The predominantly horizontal zonal flow suppresses heat flux and is observed for stress-free and asymmetric plates. Low aspect ratio periodic sidewall simulations with a no-slip boundary condition on the plates also exhibit zonal flow. In all the other cases, the flow is roll-like. In two-dimensional Rayleigh-Bénard convection, the velocity boundary conditions thus have large implications on both roll-like and zonal flow that have to be taken into consideration before the boundary conditions are imposed.

*Based on: E.P. van der Poel, R. Ostilla-Mónico, R. Verzicco, D. Lohse, *Effect of velocity boundary conditions on the heat transfer and flow topology in two-dimensional Rayleigh-Bénard convection*, Phys. Rev. E **90** (1) 013017 (2014) [132]

Figure 6.1: Temperature field snapshots for different simulations. Red and blue indicate hot and cold fluid, respectively. The color varies between $\theta = 0.2$ and $\theta = 0.8$. $Ra = 10^{11}$ and $\Gamma = 1/2$ for lateral periodicity, showing zonal flow (left panel); $Ra = 10^{10}$ and $\Gamma = 0.33$ for no-slip sidewalls, showing roll structures (center panel); and $Ra = 10^{10}$ and $\Gamma = 0.33$ for stress-free sidewalls (right panel). The plates are no-slip in all cases.

6.1 Introduction

RB convection is used as a simple model for all types of natural convection, regardless of geometry. For 2D RB, at a moderate $Ra = 10^8$, the heat flux is expected to be independent of the aspect ratio, and thus of the sidewall boundary conditions, beyond $\Gamma \gtrsim 26$ (§5). This value of Γ is expected to be lower for 3D RB [172]. Low aspect ratio applications with a no-slip BC on the lateral walls, such as cooling fins and domestic heating, have moderate Rayleigh numbers ($Ra < 10^{10}$) that are accessible with contemporary direct numerical simulations (DNS). However, nature is dominated by flows with large aspect ratios and inaccessible high Ra [33].

In both experiments and numerics, the aspect ratio Γ is commonly reduced to decrease the volume of the setup, as Ra depends only on the height of the system. In simulations, reducing the aspect ratio for fixed Ra decreases the computational complexity by $\mathcal{O}(\Gamma^2)$ in three-dimensions, while in experiments it means a smaller setup volume. In both cases it makes higher Rayleigh numbers more accessible. Despite the additional effort required for large aspect ratio, research in this direction has been done in simulations [172] and experiments [79, 200, 201]. However, these endeavors were all limited in Ra due the large aspect ratios used. In simulations

Figure 6.2: Compensated $Nu/Ra^{2/7}$ as a function of Ra for stress-free and no-slip side-walls and no-slip plates. The data are for aspect ratios $\Gamma = 1$ and $\Gamma = 0.33$. As expected, the stress-free Nu is consistently higher than for no-slip for the same value of Γ . For stress-free boundary conditions, the heat transport is higher for $\Gamma = 0.33$ than for $\Gamma = 1$ for all of the evaluated Ra , while for no-slip this is only observed at high Ra .

one can approximate infinitely large Γ by using periodic boundary conditions at the sidewalls. This leads to the question of how large the simulated domain has to be to sufficiently approximate infinite Γ , as a truly infinite domain can in principle support any wavenumber while a periodic domain allows only for multiples of the fundamental one imposed by its size. This is addressed in this study in 2D RB, which is expected to require a larger domain than 3D and therefore is more demanding in terms of computational resources.

Different temperature boundary conditions at the plates were studied by [41], where no significant difference between constant flux and isothermal plates was found in the higher Ra regime. Therefore, in this chapter we focus only on the *velocity* boundary conditions. High Rayleigh number applications of RB usually do not have a no-slip lateral wall BC. Such lateral walls are unfortunately unavoidable in experiments due to flow confinement, but it is not required in numerics, although numerics tend to use no-slip sidewalls when replicating or complimenting experiments. Removing the no-slip BC on the lateral wall is actually beneficial in simulations, as it reduces computational requirements due to the absence of the viscous BL and therefore no need to cluster grid points in the wall-normal direction. In any case, boundary conditions must be chosen in numerical studies and one has to chose the boundary best suited for the intended study, but also the computational demand and possible introduced artifacts have to be taken into account.

Despite its perceived importance, the effect of the velocity boundary conditions on the lateral walls has not been systematically studied for RB even though it is expected to have a significant effect on the roll state, absolute heat flux, and kinetic energy of the flow. In numerics, any expression which can be mathematically for-

mulated can be used as a boundary condition, but here we focus on the three most physical options: no-slip (NS), stress-free (SF) and periodic (PD). For no-slip and stress-free sidewalls, an additional temperature BC has to be imposed which in our case is adiabatic.

Many recent studies on RB convection focus on the so-called “ultimate regime” [29, 55, 62, 80, 202], a regime of RB flow where the boundary layers are expected to become fully turbulent. It is expected that the scaling of integral quantities in this regime can be extrapolated to the very high Ra numbers present in geo- and astrophysical natural convection. In this chapter, we address the question of how the lateral wall boundary conditions affect the flow and how we can extrapolate the results obtained to flows at arbitrary large driving, such as those in the ultimate regime. We find that, in essence, when one strives to model the high Ra applications of natural convection, the no-slip lateral wall BC and the low aspect ratios of experiments and simulations may obscure phenomena which are seen in large aspect ratio convection found in nature. This research focuses on two-dimensional RB and it must be noted that three-dimensional RB might behave differently. In specific cases, qualitative arguments result in the expectation that three-dimensional RB does not show phenomena at all that are very strong in two-dimensional RB (§8).

One of these phenomena is zonal flow, which is a flow state with most of the kinetic energy stored in the horizontal motion [203, 204]. The topology consists of two shearing layers of fluid, one at the top and one at the bottom, that move in opposite horizontal directions. Zonal flow strongly suppresses heat flux, and, correspondingly, the heat flux as a function of time behaves very differently. It can be either bursting or sustained. In the first case quiescent periods of negligible convective heat flux are interrupted by large bursts, while in the second case the heat flux is more sustained. Even in the sustained case, the heat flux is much lower than would be expected in the more conventional roll-like flow state with identical control parameters. Zonal flow is observed with stress-free, asymmetric and no-slip plates, though for no-slip plates, the size of the period in laterally periodic simulations has to be small.

The organization of the manuscript is as follows: First, the boundary conditions are formulated and their consequences on the numerical algorithm are evaluated. Then, simulations dominated by roll-like dynamics are presented in both thin ($\Gamma < 1$) and wide ($\Gamma > 1$) cells. Here, we compare the heat flux in no-slip, stress-free and periodic sidewalls as function of Ra. We quantify the behavior of the heat flux as function of Γ for periodic boundary conditions in order to find the aspect ratio for which periodicity does not introduce any artifacts. Finally, we study the effect of stress-free plates, both in an asymmetric setup with only one stress-free plate, and also with both plates having stress-free velocity boundary conditions. Here the heat flux as a function of time is dominated by large bursts with quiescent intervals. For all simulations a Prandtl number equal to unity is used, unless stated otherwise, to

Figure 6.3: a) Nu as a function of Γ for stress-free sidewalls and no-slip plates. The data are for $Ra = 10^8$. At $\Gamma \approx 1$ there is a transition region between a roll state with one roll and a roll state with two horizontally aligned rolls, which is reflected by hysteretic jumps in Nu. b) Compensated $(Nu - 1)/Ra^{2/7}$ as a function of Ra for stress-free and periodic sidewalls and no-slip plates. Data are depicted for $\Gamma = 1.5$ and $\Gamma = 2$. The effect of the aspect ratio on Nu disappears for high Ra while the effect of the sidewall boundary condition remains.

prevent the nesting of the kinetic into the thermal boundary layer and vice versa, and to reduce the parameter space to a manageable size.

6.2 Numerical method

The direct numerical simulations (DNS) were performed with a two-dimensional version of a second order finite difference scheme [105, 128]. The underlying numerical scheme has been used for simulations of three-dimensional RB [84, 172], Taylor-Couette [134] and other flows [205]. The two-dimensional version of the code was validated by comparison to a fourth order finite difference code [177] that on its turn was compared with quasi two-dimensional experiments. Specifically, the $Nu(Ra)$ data for $\Gamma = 0.33$ with no-slip boundary conditions can be compared one-to-one with the fourth order code and turn out to be equal within error (§5). In addition, results for no-slip boundary conditions in a $\Gamma = 1$ cell at $Pr = 1$ agree well with the fourth order compact scheme of [40]. Details of the simulations can be found at the end of this chapter.

The boundary conditions chosen are either no-slip, i.e., $u_i = 0$ at the walls; stress-free walls, i.e., $u_i n_i = 0$, where n_i is the vector normal to the wall; and $\partial_\tau u_i = 0$, where τ is the direction tangent to the wall and there is lateral periodicity, i.e., $u_i(x = 0, z) = u_i(x = D, z)$. The temperature boundary condition on the plates are isothermal in all cases. For the no-slip and stress-free sidewalls, as an additional temperature

boundary condition we chose adiabaticity, i.e., $\partial_n \theta = 0$.

The use of different boundary conditions has a significant bearing on the algorithm to be chosen to solve the Boussinesq equations. The main difference is that for stress-free and periodic boundary conditions, grids with uniformly spaced points can be used without loss of efficiency. In contrast, for the no-slip condition, resolving the sharp gradients in the resulting boundary layers with a uniform grid distribution will overresolve the bulk. It is therefore more efficient to use a nonuniform grid to cluster points near the boundary layers. However, solving an equation on a nonuniform grid is generally more costly in terms of computational requirements when compared to solving the same equation on an equally sized uniform grid. This is by virtue of the uniform grid that allows for the use of a Fourier transform to solve the pressure equation to impose the incompressibility of the flow.

6.3 Roll dominated convection

6.3.1 Thin cells

For stress-free sidewalls, Nu for $\Gamma = 0.33$ is higher than for $\Gamma = 1$, which is in contrast with the no-slip case, where Nu for $\Gamma = 1$ is higher than for $\Gamma = 0.33$. It must be emphasized that this strong aspect ratio dependence is a 2D effect not observed in 3D [172]. Even for $\Gamma < 1$ it is observed in 3D experiments that there is no difference in Nu between $\Gamma = 1$ and $\Gamma = 1/2$ cells for identical Ra and Pr [83, 101]. This is despite the fact that in both 2D and 3D the amount of vertically stacked rolls changes with decreasing aspect ratio [86].

The observation that the dependence of Nu on Γ differs between the no-slip and free-slip sidewall boundary conditions can be rationalized as follows. In the stress-free case, the aspect ratio $\Gamma = D/H$ can be interpreted as the ratio between the proportion of the enclosing wall that draws energy out of the system (no-slip plates) and the proportion that has no effect on the flow (stress-free sidewall). With decreasing Γ , this ratio decreases and thus there is less drag experienced by the flow at lower Γ , resulting in a higher Nu for stress-free sidewalls. In case of no-slip sidewalls, following the same reasoning, one expects that the Nu does not depend on Γ provided that the flow structure remains the same. The difference in Nu for no-slip sidewall between thin and square ($\Gamma = 1$) cells must then be a result of a changing flow state. While in $\Gamma = 1$ cells a single roll is present, in $\Gamma = 0.33$ cells there are four vertically stacked rolls, see figure 6.1b. In 2D, the heat flux through the system depends on the amount of vertically stacked rolls (§4), which explain the difference in Nu.

There are exceptions to this trend, as there are specific cases in which an aspect ratio reduction resulted in an increased heat flux for no-slip walls [206]. In addition, for the no-slip sidewall data seen in figure 6.2, Nu for $\Gamma = 0.33$ is lower than Nu for $\Gamma = 1$ for most of the Ra range explored. However, at $Ra = 4.64 \times 10^{10}$ it is the

Figure 6.4: a) Nu vs Γ for periodic sidewalls and no-slip plates for $Ra \in \{10^8, 10^9, 10^{10}, 10^{11}\}$, see the legend in b). Jumps in Nu can be seen around $\Gamma \approx 1.25$, $\Gamma \approx 1.25$, $\Gamma \approx 1.10$ and $\Gamma \approx 1.05$ for $Ra = 10^8$, $Ra = 10^9$, $Ra = 10^{10}$ and $Ra = 10^{11}$, respectively. The Nusselt number statistics at lower Γ than the jump are more difficult to converge than the other data points due to the bursting nature of $Nu(t)$ and have a larger error. They are included to indicate the change of flow state. In b) Nu is compensated with $Nu(\Gamma = 3)$.

opposite, which has been attributed to the break up of the large-scale rolls in the flow (§5).

We can further quantify the trend of $Nu(\Gamma)$ for thin cells and stress-free sidewalls, and compare against the no-slip case. For no-slip sidewalls, $Nu(\Gamma)$ shows relatively large jumps between vertically stacked roll states with Nu generally invariant with Γ (for $\Gamma < 1$) provided that the roll state does not change (§4). In figure 6.3a the corresponding results for stress-free sidewalls can be seen. In contrast to the no-slip case, no jumps can be seen and Nu decreases monotonically with Γ up to $\Gamma = 0.95$. At $\Gamma \approx 1$ the flow transitions from a roll state with one to a roll state with two horizontally aligned rolls. There appears to be multi-stability in this transition region. The absence of jumps for $\Gamma < 1$ can be directly attributed to the fact that for $\Gamma \leq 0.95$ the system is exclusively in a single roll state while for $\Gamma = 1$ the system is in a roll state with two horizontally arranged rolls, resulting in a jump in Nu.

6.3.2 Wide cells

Small Γ cells are dominated by the presence of the sidewall. However, even if one could expect this dependence to progressively vanish for the case of large Γ , Nu for 2D RB systems with no-slip sidewalls has a strong Γ dependence up to very large values of Γ (§5) (i.e. $\Gamma \lesssim 26$ for $Ra = 10^8$). Here we repeat the analysis of §5, but now for cells with lateral periodicity, to check whether the Γ dependence is still present at such high values of Γ and study the scaling of $Nu(Ra)$.

Figure 6.5: Temperature field snapshots for $Ra = 2.15 \times 10^8$ and $\Gamma = 1.5$ with no-slip plates and stress-free sidewall boundary conditions of two different statistically steady states. The colormap ranges from $0 \leq \theta \leq 1$. The area averaged mean temperature $\langle \theta \rangle_{A,t}$ is 0.44 (left panel) and 0.56 (right panel).

In figure 6.3b Nu against Ra for laterally periodic and stress-free sidewalls are compared for $\Gamma = 1.5$ and $\Gamma = 2$. Nu for stress-free sidewalls is higher than for periodic sidewalls. This difference can be attributed to two effects, namely the roll state imposed by the impermeable walls and the drag from the sidewall. The amount of horizontally stacked rolls for periodic sidewalls, in contrast to impenetrable sidewalls (NS and SF sidewalls), is restricted to even numbers. At $\Gamma = 2$, for the studied parameter range, the periodic simulations showed two horizontally stacked rolls while the stress-free simulations showed three rolls. For both simulations, the initial conditions consisted of two rolls, to ensure that the heat flux is not affected by a different roll state.

Nu heavily depends on the amount of horizontally stacked rolls (§4) and this effect most likely contributed to the difference in Nu between the evaluated cases. However, there could also be other causes of the difference in Nu . In order to find out, $\Gamma = 1.5$ was simulated for the same Ra as for $\Gamma = 2$. At this aspect ratio both laterally periodic and stress-free sidewall simulations have a roll state consisting of two rolls. It can be seen that the difference in Nu between PD and SF is smaller, as expected, and that the difference in stress at the boundaries alone results in a lower Nu for laterally periodic cells as compared to stress-free sidewalls.

The figure shows that Nu becomes Γ -independent for both BC's at sufficiently large Ra . This finding adds the conclusion that not only laterally periodic cells lose the Γ dependence, but also that this is valid for stress-free sidewalls as well at $\Gamma \approx 2$ for $Ra \geq 10^{10}$. We now focus on the aspect ratio dependence of periodic sidewall simulations at different Ra .

Periodic boundary conditions are used to approximate infinite aspect ratio, i.e. an

Figure 6.6: Temperature field snapshots with velocity vectors superimposed for stress-free plates and periodic sidewalls for $Pr = 1$ and at $Ra = 10^6$ (left panel) and $Ra = 10^8$ (right panel) in a $\Gamma = 2$ cell. The temperature ranges from $0 \leq \theta \leq 1$. The size of the arrows is proportional to the absolute velocity. The flow is roll-like in a) and zonal in b).

absence of finite-size effects on a finite size domain. Thus, the aspect ratio in periodic sidewall simulations does not reflect a physical domain but instead the period size of the computational domain. This aspect ratio cannot be arbitrarily small for two reasons: i) there must always be an even number of horizontal rolls in a periodic system, and ii) wavelengths larger than the domain are not simulated and thus not accounted for. However, as the aspect ratio is proportional to the computational cost, it is of interest to study the minimum aspect ratio $\Gamma_{\min}$ that still produces physical solutions. When considering three dimensional (3D) flows with a large-scale circulation (LSC), periodicity can be imposed in two distinct dimensions. The periodic dimensions can either be parallel or perpendicular to the vorticity vector of the LSC. It is expected that parallel periodicity has less effect on the flow than perpendicular periodicity. Parallel periodicity is often used in Taylor-Couette simulations [134], where, unlike in 3D RB [207], the orientation of the LSC is known *a priori*. In 2D RB this periodicity is unavoidably imposed in the perpendicular direction and thus a strong effect is expected.

In figure 6.4 Nu as function of the period Γ is shown for four different Ra . One would expect that $\Gamma_{\min} \approx 2$ as the minimum number of rolls is two and the aspect ratio of one roll is approximately unity (§5). It is therefore surprising that a weak dependence of Nu , i.e. $\leq 5\%$, on Γ is seen from $\Gamma_{\min}$ significantly lower than two, where $\Gamma_{\min}$ is indicated by the jump in $Nu(Ra)$. For $Ra = 10^9$ the aspect ratio dependence is larger than for higher Ra . This is in particular visible in figure 6.3b. At $Ra = 10^9$, Nu differs approximately 8% between $\Gamma = 1.5$ and $\Gamma = 2$, while this difference vanishes at $Ra = 10^{10}$. $\Gamma_{\min}$ appears to decrease for increasing Ra . We expect this to be a result of a weaker LSC (§8) and decreased structure size at higher Ra .

We wish to highlight a peculiarity observed for stress-free sidewall and no-slip plates, namely that the mean temperature can be $\langle \theta \rangle_{A,t} \neq 0.5$. This can be seen in more detail in figure 6.5. Even though there is top bottom symmetry in the boundary conditions and in the equations there is a deviation from the expected value $\langle \theta \rangle_{A,t} = 0.5$. As the system is not turbulent enough, it might take infinite time for the system to explore all possible states and the symmetry can be spontaneously broken due to the different flow states. The system is in a horizontally stacked double roll state where the hot plumes are moving up at the center of the no-slip plate and the cold plumes move down along the stress-free sidewalls. In this case $\langle \theta \rangle_{A,t} > 0.5$, as the hot plumes are well mixed by turbulence while the cold plumes seem to lose their heat through molecular diffusion, see figure 6.5a. A similar but opposite effect can be obtained in other realizations of the same system with different initial conditions. In steady state axisymmetric convection with stress-free plates and sidewalls [208] the core temperature is smaller than 0.5 in case of a rising central plume.

We have checked the dependence of the deviation of the mean temperature from 0.5 on the central plume location by performing the transformation $u_i(x, z) \mapsto u_i(x, L - z)$ and $\theta(x, z) \mapsto 1 - \theta(x, L - z)$ on the hot solution of $\Gamma = 1.5$, $Ra = 2.15 \times 10^8$. This transformation flips the velocity and temperature fields upside-down and inverts the temperature. While before the transformation in statistically steady state $\langle \theta \rangle_{A,t} = 0.54 > 0.5$, converging the simulation with the transformed field results in $\langle \theta \rangle_{A,t} = 0.46 < 0.5$, of which a snapshot can be found in figure 6.5b. This indicates that the deviation from 0.5 is a flow state effect heavily dependent on the initial condition. Even though the time and volume averaged heat flux through the system is identical in both cases, the area-averaged and local temperature strongly differ between these two flow states.

6.4 Zonal flow

6.4.1 Stress-free plates

Until now we have focused on the case with no-slip plates and varied the sidewall boundary conditions. Of course, another degree of freedom of the boundary conditions are the horizontal plates. Using a stress-free boundary condition instead of no-slip results in huge differences in both flow topology and heat flux. Stress-free plates are used in theory to simplify boundary conditions, as well as infinite (periodic) systems. This BC is a critical requirement for theorems that use the vanishing vorticity condition at the plates, which goes all the way back to original analysis by Rayleigh, but it is also used for more recent work, such as the finite-Pr upper bound theorem of [209] that gives $Nu \leq 0.2891 Ra^{5/12}$.

We performed simulations with (horizontal) stress-free plates and used lateral periodicity with $\Gamma = 2$ to approximate an infinite system. For $Ra \gtrsim 10^7$ the flow

Figure 6.7: a) Nu as a function of dimensionless time in free-fall time units at $\Gamma = 1/2$, for $Ra = 1 \times 10^8$ and $Ra = 1 \times 10^{11}$, NS plates and PD sidewalls. At $Ra = 10^8$ we observe bursting behavior while at $Ra = 10^{11}$ we do not: The zonal flow is bursting for lower Ra and sustained for higher Ra. Note the large difference between the time scale of the bursts at $Ra = 10^8$ and the fluctuations at $Ra = 10^{11}$. b) Probability density function of the time interval between the bursts Δt for $Ra = 10^7$ and $Ra = 10^8$.

topology consists of two shearing layers with predominantly horizontal motion. The flow at the lower half of the domain moves in opposite direction as the top. This is because the total momentum must be conserved due to the absence of momentum transport to the boundaries. The flow is in a state for which Nu shows bursts with long “quiet” intervals where $Nu(t) \approx 1$. This flow state is referred to as *zonal flow* [52, 53, 203, 204], similar to the zero-wavenumber flows observed in toroidal plasmas and planetary atmospheres, e.g. on Jupiter. The strong horizontal motion is driven by the so-called “shearing mechanism”. Plumes emitted from the one plate move vertically at first until they are deviated horizontally by the opposite plate, driving the horizontal motion.

Depending on Pr, there is a threshold Ra beyond which the flow transitions from roll-like to zonal flow. Hysteresis is observed at this transition [204]. In figure 6.6 snapshots can be seen of the flow below and above this threshold at $Pr = 1$. At $Ra = 10^6$ the flow is still roll-like; a large-scale circulation with accompanying plumes. Increasing Ra to $Ra = 10^8$ the flow transitions to a zonal flow. In the corresponding snapshot in figure 6.6b the flow is in the $Nu(t) \approx 1$ interval between bursts, in which a linear temperature gradient can be seen with strong horizontal flow. This interval phase is interrupted by large bursts in Nu(t). During these burst phases there is high mixing before the interval phase is re-initiated. Zonal flow is only observed in two dimensions. In our three-dimensional simulations using SF plates, periodic sidewall and a Cartesian geometry with $\Gamma = 1$, no zonal-flow has been observed for $Ra \in \{10^7, 10^8, 10^9\}$. Bursts in Nu have been observed for wind-reversals [178] although in that case the bursts are not preceded by “quiet” i.e. $Nu \approx 1$ flow states.

The zonal flow state is detrimental for obtaining $Nu(Ra)$ scaling as Nu is close

Figure 6.8: Mean horizontal velocity $\langle u_x \rangle_{x,t}$, normalized by its maximum, as a function of vertical position z/L for different Ra (see legend) in a) $\Gamma = 1$ cells with lateral periodicity and no-slip plates, b) $\Gamma = 0.5$ cells with lateral periodicity and no-slip plates and c) $\Gamma = 2$ cells with lateral periodicity and asymmetric plates.

to one and, due to the intermittent nature of the bursts, time-averaged quantities are very hard to converge, requiring simulations of several tens of thousands of large eddy turnover times. In order to obtain a converged Nu to see how the system approaches the theoretical upper bounds, we prevent zonal flow by increasing Pr as this increases the shear between the bottom and top layer. Increasing to $Pr = 40$ prevents zonal flow for $Ra < 10^{10}$. In the low Ra regime the flow is composed of two rolls with very thin plumes streaks in between, very similar to infinite Pr flows with SF plates [210]. The absolute Nu for a given Ra is nearly double of that in the case of no-slip plates. However, the $Nu(Ra)$ scaling exponent is similar, namely 0.28, much smaller than the upper bound exponent of $5/12 \approx 0.42$ [209], rigorously derived for these boundary conditions.

6.4.2 Suppressed periodicity

Zonal flow is not inherent to the stress-free plate boundary condition. It is also observed for no-slip plates when Γ is too low for the lateral periodicity and the flow becomes dominated by artifacts. For $\Gamma < \Gamma_{min}$ the flow is zonal for all the studied Ra . First, we focus on $\Gamma = 1$, which is close to Γ_{min} where the flow transitions from zonal to roll-like, see figure 6.4. A strong characteristic of zonal-flow as compared to roll-like flow is that the mean horizontal velocity $\langle u_x \rangle_{x,t}$ as a function of z/L is nonzero [204]. This can be seen in figure 6.8a for $\Gamma = 1$. The two shearing layers are reflected in $\langle u_x \rangle_{x,t}$ by the two peaks with opposite velocity. The velocity profile seems nearly independent of Ra . Unlike with stress-free plates [204], the velocity in this case vanishes at the plates, inherent to the no-slip boundary condition. It thus appears that zonal flow is not intrinsic to stress-free plates. When the lateral period is too small to allow roll-like flow, the sideways deflected plumes have no freedom to return to their original plates. The plumes therefore have to move sideways, driving a zonal flow.

Decreasing the aspect ratio to $\Gamma = 0.5$ increasingly suppresses the flow. In figure 6.7a, $Nu(t)$ for two different Ra is depicted. $Nu(t)$ for $Ra = 10^8$ shows the Nu bursts with a peak value of approximately $Nu(t_{peak}) \approx 50$. For $Ra = 10^{11}$ the features of $Nu(t)$ are completely different. Here, large symmetric fluctuations around the mean can be seen, characteristic for common RB systems. A similar transition is seen for zonal flow between stress-free plates [204]. However, there the zonal flow type transitions from *bursting* to *sustained* when Pr is increased. Here, the transition between the bursting and the sustained Nu is at $Ra = 10^{10}$ for constant $Pr = 1$ and $\Gamma = 0.5$, with bursts found at lower Ra . At this same $Ra = 10^{10}$ the vertical profile of $\langle u_x \rangle_{x,t}$ starts to differ from the profiles at lower Ra (figure 6.8b). For lower Ra , the horizontal motion is only in one direction, with a maximum at mid-height. At higher Ra , the velocity near the plates opposes the motion at mid-height and three regions of different horizontal motion are present. This shows that also for zonal flow there are different states, strongly dependent on the boundary conditions and correspondingly Γ .

The scale of the buoyant thermal plumes decreases for both increasing Ra and increasing Pr , allowing for more freedom compared to the fixed periodic length scale. In the $\Gamma = 0.5$ case, increasing Ra prevents the bursting flow state. In the sustained zonal flow state, there are no bursts in Nu . Most likely it is the heat buildup during the stagnant phase that results in the bursts. This is supported by the fact that for larger $\Gamma = 1$, the zonal flow is additionally sustained. The flow-field snapshot of $Ra = 10^{11}$ is displayed in figure 6.1a. The flow topology in this snapshot differs markedly from typical RB (see e.g. figure 6.1b), even though $Nu(t)$ has a similar structure, its mean value is substantially lower, indicating that the suppression of heat flux still is significant at higher Ra .

The interval between the bursts strongly depends on Ra . In figure 6.7b, the probability density functions for $Ra = 10^7$ and $Ra = 10^8$ can be seen. The interval duration Δt is extracted using a peak finding algorithm that finds local maxima. The minimum peak height and minimum peak distance are tuned by hand for each Ra . For increasing Ra , the mean interval increases while the variation appears approximately constant. For $Ra > 10^8$ the mean Δt becomes so large that obtaining statistical convergence requires huge amounts of CPU time. It therefore remains unknown how the mean time interval between bursts increases up to the point that the bursting behavior disappears. In addition no converged Nu can be obtained as a result of the increasing time interval.

These low Γ PD sidewall simulations are the only cases we encountered with zonal flow when both plates are no-slip in two-dimensions. However, it has been observed in three-dimensional RB experiments in an annular cylinder [203], where all the enclosing boundary conditions are no-slip with periodicity introduced in the azimuthal direction.

Figure 6.9: a) Temperature field snapshot for asymmetric plates BCs and periodic side-walls at $Ra = 4.64 \times 10^8$. The top boundary is stress-free and the bottom boundary is no-slip. b) Nu as a function of Ra for asymmetric plate BC's and periodic sidewalls. Simulations where the initial conditions is taken from the lower Ra neighboring data point are indicated with rightward-pointing triangles and where the initial condition is taken from higher Ra are indicated with leftward-pointing triangles.

6.4.3 Asymmetric plate boundary conditions

The final variation we consider on the plates is using asymmetric velocity boundary conditions. These conditions are rarely studied, but have many applications; the ocean or a cooking pan can be thought of as having stress-free top at their free surfaces and a no-slip bottom. Asymmetric boundary conditions break the top-down symmetry in RB even in the Boussinesq approximation. In conjunction to asymmetric boundary conditions at the plates, we take a laterally periodic system to avoid sidewall effects as much as possible.

Snapshots of the flow-field are displayed in figure 6.9a. Here, it can be seen that we obtain partly zonal flow near the top plate where the BC is stress-free. Indeed, the system displays similar behavior to the case where both plates are stress-free, namely bursts in Nu with $Nu \approx 1$ intervals. The main difference between stress-free BCs and the asymmetric setup is obviously near the no-slip bottom plate. In symmetric zonal flow, the mechanism that drives zonal flow is conceptually understood as plumes from both plates driving the zonal flow at the opposite plate. However, the zonal flow present in this asymmetric setup has no plumes originating from the bottom plate, see 6.9a. This shows that even without these plumes, the zonal flow in the upper, stress-free, layer can be driven by the interaction between the stationary layer at the bottom and the descending cold plumes alone.

In our simulations, we see this mixed zonal-flow state for $Pr = 1$ and $Ra > 10^9$. For lower Ra , the system displays large-scale circulations without zonal flow, resulting in a more typical behavior of $Nu(t)$ fluctuating around the mean without periods where $Nu \approx 1$. The thermal plumes in this Ra regime have a different shape; the plumes originating from the no-slip plate are surrounded with high vorticity while

the others are not. The plumes that originated at the stress-free plate appear like long streaks that are less well mixed and have sharper gradients compared to their NS counterparts.

Figure 6.9b shows Nu as a function of Ra . As these Nusselt number data are very hard to converge, the typical averaging time is at least one order of magnitude larger than for roll-like flows. The difference between Nu with and without zonal flow can be clearly seen. Moving upwards in Ra , i.e. using the solution field from a lower Ra simulation as an initial condition, the flow transitions at $Ra = 10^9$. Moving backwards, the transition back towards a flow without zonal flow is at $Ra = 10^7$. This difference indicates that there is hysteretic behavior at this transition, similarly to the double stress-free plates case [204]. The vertical profile of $\langle u_x \rangle_{x,t}$ can be seen in figure 6.8c for the cases with asymmetric plates that have zonal flow. Below the forward transition at $Ra = 10^9$, the horizontal motion is exclusively in one direction. For higher Ra , similarly to the case described in the previous chapter, a layer is observed near the no-slip plate that has an opposite horizontal motion. At higher Ra , the plumes coming from the stress-free cold plate reach the no-slip plate and drive the zonal flow in the bottom of the cell, while at lower Ra the plumes do not reach that far into the flow and are dissipated before they can drive the zonal flow.

As the up-down symmetry is broken it is expected that the area and time averaged temperature $\langle \theta \rangle_{A,t}$ can deviate from the value of 0.5 commonly found in symmetric RB [38], similarly to what is observed in non-Oberbeck-Boussinesq RB convection [211]. This quantity is plotted as a function of Ra in figure 6.10a, where it can be seen that also within the Oberbeck-Boussinesq approximation the deviation from 0.5 can be substantial, as seen here with asymmetric plate boundary conditions. In addition, there is no clear dependence on Ra except for a large jump that corresponds to the transition between roll-like and zonal flow. It appears that for roll-like flow at lower Ra , the plate with the stress-free BC (in this case the cold plate) has a dominant effect on the bulk temperature, as $\langle \theta \rangle_{A,t} < 0.5$. The absence of the viscous boundary layer on this plate must therefore have a stronger effect on $\langle \theta \rangle_{A,t}$ than the increased vorticity at the no-slip plate. At the stress-free plate, the full thermal boundary layer is exposed to the LSC while at the no-slip plate it is (partly) nested in the viscous boundary layer. In contrast, in case of zonal-flow at higher Ra , there is a negligible deviation of the mean temperature from the symmetrical value of 0.5.

In figure 6.10b the vertical temperature profiles $\langle \theta \rangle_{x,t}$ as function of z/L can be seen for various Ra . The no-slip and stress-free boundary layers are located near $z/L = 0$ and $z/L = 1$, respectively. For $Ra = 10^7$ and $Ra = 10^8$ the bulk profile is clearly colder than 0.5. The two different boundary layer profiles significantly differ from each other for both these Ra . The no-slip plate boundary layer is less steep and larger than the stress-free one. A small overshoot in θ can be seen for $Ra = 10^7$, which is typical for low Ra RB and not too small Pr . The boundary layer profile for

Figure 6.10: a) The area -and time averaged temperature $\langle \theta \rangle_{A,t}$ as a function of Ra for asymmetric plate boundary conditions. Only the runs where the initial condition is taken from a lower Ra are included. b) The horizontal- and time-averaged temperature $\langle \theta \rangle_{x,t}$ as a function of the vertical coordinate z/L for $Ra = 10^7$, $Ra = 10^8$ and $Ra = 10^9$. The $Ra = 10^9$ data in this plot are taken from a simulation with zonal flow while the others are in a roll-like state. The dashed black line indicates $\langle \theta \rangle_{x,t} = 0.5$. For both panels, the asymmetry is introduced by making bottom plate (i.e. $z/L = 0$) no-slip, while the top plate (i.e. $z/L = 1$) is stress-free.

$Ra = 10^9$ deviates strongly from typical RB BL profiles [179]. It must be noted that this is a time average and so this profile is affected by both flow phases; the zonal flow phase and the burst. As there is negligible vertical motion in the zonal flow region, a near linear temperature profile can be seen, confirming that the convective heat flux is negligible and that the heat flux is dominated by molecular diffusion.

6.5 Summary and Outlook

The velocity boundary conditions in two-dimensional Rayleigh-Bénard convection have a large effect on the flow topology and consequently, the Nusselt number. This is in contrast with the temperature boundary conditions, which have been shown to have negligible effects when switching between isothermal and constant flux boundary conditions on the plates [41].

The flow can be classified as roll-like and zonal. The roll-like flow state is composed of a large-scale circulation interacting with thermal plumes. The resulting $Nu(t)$ fluctuates around its mean. This flow state is most commonly observed when the horizontal plates are subject to a no-slip boundary condition, which is the case in experiments. The zonal flow state, however, differs substantially. When looking at the Nu time series, we see large bursts of Nu surrounded by “quiet” intervals where $Nu(t) \approx 1$. During these intervals, vertical motion is absent and the flow largely

moves horizontally. This is allowed by the use of lateral periodicity. Zonal flow is observed when either one or both plates have a stress-free boundary condition. Zonal flow is additionally observed for no-slip plates in a special case, i.e. when the sidewall is periodic and $\Gamma < \Gamma_{\min}$, and thus the flow has limited freedom. This results in a similar $Nu(t)$ structure. A difference between these cases is that zonal flow is observed *upwards* from a critical Ra, while for the low Γ case with lateral periodicity, the bursting behavior of $Nu(t)$ is only observed for a Ra *lower* than a critical Ra. In all cases, zonal flow is only observed for periodic sidewalls in two-dimensional RB.

We have quantified the effect of the sidewall on Nu for no-slip plates when the flow is roll-like using for no-slip sidewalls, stress-free sidewalls and lateral periodicity. As expected, Nu is higher for stress-free than for no-slip sidewalls over the evaluated Ra range. Surprisingly, in the stress-free case, Nu is higher for lower Γ , while the opposite happens for no-slip. This can be attributed to the absence of vertical roll states for stress-free sidewalls. In addition, stress-free boundary conditions result in heat flux, when compared to lateral periodicity for both $\Gamma = 1.5$ and $\Gamma = 2$ and for both of these boundary conditions the aspect ratio dependence of Nu disappears at high Ra.

From analyzing $Nu(\Gamma)$ for lateral periodicity and no-slip plates, we can conclude that below a certain $\Gamma_{\min}$ the flow becomes zonal. Roll-like flow is suppressed, resulting in a lower Nu than larger $\Gamma > \Gamma_{\min}$. The type of zonal flow that results depends strongly on Γ , as zonal flows with two and three shearing layers are observed for $\Gamma = 1$ and $\Gamma = 0.5$, respectively. $\Gamma_{\min}$ decreases for higher Ra, most likely due to the decreased viscous stresses on the thermal plumes. This allows the plumes to require less freedom to move alongside each other in opposite directions, allowing for roll-like flow.

Finally, in the case of asymmetric plate boundary conditions, where one horizontal plate has a no-slip boundary condition and the other plate a stress-free boundary condition, zonal flow can be observed from a critical Ra onwards, as was the case for two stress-free plates. Below this Ra, the flow remains roll-like, although the mean temperature is not 1/2 as the up-down symmetry is broken due to the different velocity boundary conditions. The plate with the stress-free boundary condition has a larger effect on the mean temperature and it therefore deviates from 1/2 towards the temperature of the SF plate. This same effect was also seen previously with stress-free sidewalls, even though the plate boundary conditions were equal. We wish to highlight that even though the effect is the same, they are due to very different mechanisms. The resulting vertical temperature profile is also completely different between the zonal flow and the roll-like flow regimes. In addition, we observed hysteretic behavior around the transition from roll-like to zonal flow, similarly to the case with two stress-free plates, reported in [204].

Choosing the boundary conditions for a simulation can be an involved, but very

relevant, consideration, as results have shown here. Based on computational performance, the laterally periodic simulations with stress-free plates would be the first choice; removing most boundary layers. In two-dimensions this can result in zonal flow with very little resemblance to roll-like RB convection, commonly observed in experiments. Zonal flow is avoided by introducing drag through the no-slip plate boundary condition. However, the roll-like convection that corresponds to this set of boundary conditions requires a minimum aspect ratio, otherwise zonal flow will emerge. Above this, the aspect ratio dependence, but not the boundary condition dependence, of the heat flux becomes negligible for $Ra \geq 10^{10}$, at least for stress-free and periodic sidewalls. Introducing asymmetry in the system, between either the plates or the sidewall and the plates, can result in zonal flow but also surprising effects as unexpected mean temperatures deviating from $1/2$. Most, if not all, of these boundary conditions effects are qualitatively expected to be nonexistent or at least much weaker in three-dimensions as compared to two-dimensions.

Table 6.1: The columns from left to right indicate Ra , Γ , the wall BC (BCw), the plate BC (BCp), the resolution in horizontal and vertical direction $N_x \times N_z$, the number of grid points in the thermal boundary layer $\#\{n \mid n \in \{1, 2, \dots, N_z\} \wedge Z(n) < L/(2Nu)\}$ (where $Z(n)$ is the vertical grid point distribution), the average Kolmogorov length scale in the flow compared to the largest grid length used somewhere in the grid $\max(\delta_x, \delta_z)/\eta$ with $\eta/L = Pr^{1/2}/[Ra(Nu - 1)]^{1/4}$, the mean Nu over the full simulation and the averaging time in free fall time units τ_f .

Ra	Γ	BCw	BCp	$N_x \times N_z$	N_{BL}	$\frac{\max(\delta_x, \delta_z)}{\eta}$	Nu	τ_f
10^7	2.00	PD	AS	512×256	11	0.47	21.6	750
2.15×10^7	2.00	PD	AS	512×256	10	0.59	25.8	900
4.64×10^7	2.00	PD	AS	512×256	9	0.76	32.0	900
10^8	2.00	PD	AS	512×256	8	0.95	37.0	900
2.15×10^8	2.00	PD	AS	1024×512	15	0.60	43.0	900
4.64×10^8	2.00	PD	AS	1024×512	13	0.76	52.3	1000
10^9	2.00	PD	AS	3072×1024	118	0.20	9.8	10000
2.15×10^9	2.00	PD	AS	3072×1024	128	0.25	8.6	14000
10^9	1.00	PD	NS	512×512	19	0.79	27.9	1700
10^9	1.20	PD	NS	512×512	18	0.96	29.1	1500
10^9	1.25	PD	NS	512×512	16	1.18	54.8	600
10^9	1.30	PD	NS	512×512	17	1.22	53.7	400
10^9	1.40	PD	NS	1024×512	11	0.66	53.7	1500
10^9	1.60	PD	NS	1024×512	11	0.74	51.0	1500
10^9	1.80	PD	NS	1024×512	12	0.82	48.5	1500
10^9	2.00	PD	NS	1024×512	12	0.91	48.3	1200
10^9	2.20	PD	NS	1024×512	12	1.00	47.9	1200
10^9	2.40	PD	NS	1600×512	12	0.70	47.6	900
10^9	2.60	PD	NS	1600×512	11	0.78	54.8	1000
10^9	2.80	PD	NS	1600×512	11	0.84	53.4	1300
10^9	3.00	PD	NS	1600×512	11	0.88	50.9	1200
10^{10}	1.00	PD	NS	1024×1024	28	0.85	59.1	400
10^{10}	1.05	PD	NS	1024×1024	51	0.86	49.2	500
10^{10}	1.10	PD	NS	1024×1024	32	1.08	102	1100
10^{10}	1.20	PD	NS	1024×1024	18	1.17	99	600
10^{10}	1.40	PD	NS	1440×1024	18	0.96	95.8	600
10^{10}	1.60	PD	NS	1440×1024	18	1.10	95.7	600
10^{10}	1.80	PD	NS	1440×1024	18	1.24	96.4	700
10^{10}	2.00	PD	NS	1440×1024	42	1.37	94.9	400
10^{10}	2.20	PD	NS	2048×1024	19	1.05	93.7	1000
10^{10}	2.40	PD	NS	2048×1024	19	1.15	95.3	1000
10^{10}	2.60	PD	NS	2048×1024	19	1.24	93.1	1100
10^{10}	2.80	PD	NS	2048×1024	19	1.34	93.3	1000
10^{10}	3.00	PD	NS	2048×1024	23	1.43	92.6	1000
10^{11}	1.00	PD	NS	2048×2048	61	0.82	77.9	300
10^{11}	1.05	PD	NS	2400×2048	50	0.92	198	200
10^{11}	1.10	PD	NS	2400×2048	51	0.95	189	200
10^{11}	1.40	PD	NS	2400×2048	29	1.23	197	300
10^{11}	1.80	PD	NS	2560×2048	30	1.48	196	200

Ra	Γ	BCw	BCp	$N_x \times N_z$	N_{BL}	$\frac{\max(\delta_x, \delta_z)}{\eta}$	Nu	τ_f
10^8	1.50	SF	NS	512×256	13	0.68	29.1	600
2.15×10^8	1.50	SF	NS	1024×512	23	0.41	36.1	400
4.46×10^8	1.50	SF	NS	1024×512	19	0.55	45.1	400
10^9	1.50	SF	NS	1024×512	16	0.70	56.0	400
2.15×10^9	1.50	SF	NS	2048×1024	30	0.45	66.1	400
4.64×10^9	1.50	SF	NS	2048×1024	25	0.58	83.7	400
10^{10}	1.50	SF	NS	3072×1536	36	0.49	101	300
10^8	2.00	SF	NS	512×256	9	0.90	29.7	500
2.15×10^8	2.00	SF	NS	576×320	11	1.03	36.4	600
4.46×10^8	2.00	SF	NS	1024×512	17	0.74	45.8	600
10^9	2.00	SF	NS	1024×512	15	0.95	56.8	500
2.15×10^9	2.00	SF	NS	1152×576	15	1.07	69.0	500
4.64×10^9	2.00	SF	NS	1280×640	15	1.22	81.9	600
10^{10}	2.00	SF	NS	2048×1440	41	0.98	101	500
10^8	1.00	SF	NS	512×512	18	0.47	33.4	400
2.15×10^8	1.00	SF	NS	512×512	17	0.57	35.4	500
4.46×10^8	1.00	SF	NS	512×512	19	0.74	44.5	500
10^9	1.00	SF	NS	512×512	11	0.94	54.6	500
2.15×10^9	1.00	SF	NS	1024×1024	29	0.61	70.1	600
4.46×10^9	1.00	SF	NS	1024×1024	23	0.79	92.9	500
10^{10}	1.00	SF	NS	2048×1441	35	0.49	103	200
2.15×10^{10}	1.00	SF	NS	2048×1441	28	0.64	135	200
4.64×10^{10}	1.00	SF	NS	2048×1441	22	1.00	180	300
10^{11}	1.00	SF	NS	3240×3072	59	0.66	217	100
10^8	0.33	SF	NS	512×512	16	0.16	37.8	500
2.15×10^8	0.33	SF	NS	512×512	13	0.20	46.5	500
4.46×10^8	0.33	SF	NS	512×512	11	0.26	57.0	500
10^9	0.33	SF	NS	1024×1024	35	0.17	73.5	200
2.15×10^9	0.33	SF	NS	640×768	18	0.35	97.8	400
4.46×10^9	0.33	SF	NS	640×768	15	0.45	125	400
10^{10}	0.33	SF	NS	1024×1280	27	0.36	154	500
2.15×10^{10}	0.33	SF	NS	1441×1600	31	0.33	199	400
4.64×10^{10}	0.33	SF	NS	2048×3072	66	0.29	240	100
10^{11}	0.33	SF	NS	3072×3456	69	0.25	280	200
10^8	0.30	SF	NS	512×512	17	0.15	38.5	400
10^8	0.35	SF	NS	512×512	17	0.17	37.3	500
10^8	0.40	SF	NS	512×512	18	0.19	36.1	500
10^8	0.45	SF	NS	512×512	18	0.21	35.0	500
10^8	0.50	SF	NS	512×512	19	0.23	34.0	500
10^8	0.55	SF	NS	512×512	19	0.26	33.1	500
10^8	0.60	SF	NS	512×512	20	0.28	32.0	400
10^8	0.65	SF	NS	512×512	20	0.30	31.5	500
10^8	0.70	SF	NS	512×512	21	0.32	31.0	500
10^8	0.75	SF	NS	512×512	21	0.34	30.5	500
10^8	0.80	SF	NS	512×512	21	0.36	29.6	400
10^8	0.85	SF	NS	512×512	21	0.38	29.5	500
10^8	0.90	SF	NS	512×512	22	0.40	28.5	400
10^8	0.95	SF	NS	512×512	22	0.43	28.8	500

Ra	Γ	BCw	BCp	$N_x \times N_z$	N_{BL}	$\frac{\max(\delta_x, \delta_z)}{\eta}$	Nu	τ_f
10^8	1.00	NS	NS	256×256	10	1.12	26.1	300
2.15×10^8	1.00	NS	NS	512×512	20	0.76	32.6	300
4.46×10^8	1.00	NS	NS	512×512	18	1.00	40.8	400
10^9	1.00	NS	NS	512×512	19	1.33	50.5	800
2.15×10^9	1.00	NS	NS	1024×1440	52	0.85	61.5	400
4.46×10^9	1.00	NS	NS	1024×1440	44	1.08	75.3	400
10^{10}	1.00	NS	NS	1024×1440	37	1.45	98.0	200
2.15×10^{10}	1.00	NS	NS	2048×2048	55	0.94	125	200
4.64×10^{10}	1.00	NS	NS	3072×3072	85	0.80	145	100
10^{11}	1.00	NS	NS	3072×3072	72	1.04	187	200
10^8	0.33	NS	NS	256×256	15	0.36	19.2	1000
2.15×10^8	0.33	NS	NS	512×512	13	0.34	23.2	1000
4.46×10^8	0.33	NS	NS	512×512	14	0.38	29.8	900
10^9	0.33	NS	NS	512×512	24	0.76	36.6	300
2.15×10^9	0.33	NS	NS	512×576	17	0.49	46.3	200
4.46×10^9	0.33	NS	NS	512×1024	33	0.63	59.3	300
10^{10}	0.33	NS	NS	768×1440	43	0.59	87.9	200
2.15×10^{10}	0.33	NS	NS	768×1440	34	0.77	120	300
4.64×10^{10}	0.33	NS	NS	2048×2048	26	1.01	172	300
10^{11}	0.33	NS	NS	2048×3072	63	0.51	200	100
10^6	0.50	PD	NS	256×256	65	0.07	2.61	90000
10^7	0.50	PD	NS	512×512	113	0.07	3.41	300000
10^8	0.50	PD	NS	512×512	96	0.13	4.32	200000
10^9	0.50	PD	NS	1024×1024	171	0.13	5.79	20000
10^{11}	0.50	PD	NS	2048×3072	105	0.43	95.4	200
10^{12}	0.50	PD	NS	3072×4096	73	0.67	282	100
10^8	1.50	PD	NS	512×256	15	0.66	26.1	600
2.15×10^8	1.50	PD	NS	1024×512	24	0.42	33.1	400
4.46×10^8	1.50	PD	NS	1024×512	20	0.54	41.1	400
10^9	1.50	PD	NS	1024×512	17	0.69	51.3	400
2.15×10^9	1.50	PD	NS	2048×1024	31	0.44	63.3	400
4.64×10^9	1.50	PD	NS	2048×1024	27	0.56	75.5	400
10^{10}	1.50	PD	NS	3072×1536	38	0.48	94.4	300
10^8	2.00	PD	NS	512×256	15	0.66	26.1	600
2.15×10^8	2.00	PD	NS	512×256	9	1.11	31.2	2600
4.46×10^8	2.00	PD	NS	512×256	8	1.42	38.9	2400
2.15×10^9	2.00	PD	NS	1024×512	10	1.17	61.1	1100
4.64×10^9	2.00	PD	NS	1024×512	10	1.50	76.3	1000
10^{11}	2.20	PD	NS	4096×2048	31	1.11	187	200
10^{11}	2.60	PD	NS	4096×2048	31	1.32	188	200
10^{11}	3.00	PD	NS	4096×2048	31	1.52	186	200

Logarithmic mean temperature profiles and their connection to plume emissions in turbulent Rayleigh-Bénard convection*

Two-dimensional simulations of Rayleigh-Bénard convection at $Ra = 5 \times 10^{10}$ show that vertical logarithmic mean temperature profiles can be observed in regions of the boundary layer where thermal plumes are emitted. The profile is logarithmic only in these regions and not in the rest of the boundary layer where it is sheared by the large-scale wind and impacted by plumes. In addition, the logarithmic behaviour is not visible in the horizontal average. The findings reveal that the temperature profiles are strongly connected to thermal plume emission and support a perception that parts of the boundary layer can be turbulent, while others are not. The transition to the ultimate regime, in which the boundary layers are considered to be fully turbulent, can therefore be understood as a gradual increases in fraction of the plume-emitting ('turbulent') regions of the boundary layer.

*Based on: E.P. van der Poel, R. Ostilla-Mónico, R. Verzicco, S. Grossmann, D. Lohse, *Logarithmic mean temperature profiles and their connection to plume emissions in turbulent Rayleigh-Bénard convection*, Phys. Rev. Lett. under review (2015).

Figure 7.1: Instantaneous (top panel) and time-averaged (bottom panel) temperature fields. Examples of the three different regions are indicated in the bottom panel. In the panels red and blue indicate hot and cold fluid, respectively.

7.1 Introduction

Most theories assume that from a critical Rayleigh number Ra_c onwards, the boundary layer (BL) transitions from laminar to turbulent [34, 35, 54, 55, 66] and base their scaling laws on either a time- and space averaged laminar [34, 35] or turbulent [3, 26, 27, 35, 54, 55, 66] BL profile. In the regime of laminar BLs, the mean temperature profile is assumed to be of Prandtl-Blasius-Pohlhausen (PBP) type [70, 88, 212, 213] while in the turbulent case a logarithmic (log) profile is expected [54, 214], analog to turbulent temperature boundary layers in wall turbulence [59]. For $Ra < Ra_c$, BL profile measurements reveal a profile that is similar to the expected PBP profile when measured at horizontal regions where the flow conditions most closely match the assumptions required to analytically obtain the PBP profile [86, 179, 189, 191]. However, the lateral dependence is strong [179] and deviations from the PBP profile are observed [43, 215, 216].

Lateral local mean temperature log profiles have been found in experiments and direct numerical simulations (DNS) down to a Rayleigh number of $Ra = 10^{12}$ [64, 217, 218]; a Ra where the BL is expected to more closely resemble a laminar profile instead of a logarithmic (turbulent) profile. The log profiles were found near the sidewall in the experiments and numerics, with the log amplitude and fit quality decreasing towards the center of the cell. In cylindrical setups with $\Gamma = \mathcal{O}(1)$ the plumes are commonly ejected from the boundary layer close to the sidewall, resulting in a larger heat flux in the corners [219]. The finite size of the cylindrical setup forces the thermal plumes to be emitted near the sidewall due to the large-scale circulation

of system size. The log profiles could either be an effect of the sidewall or the plume emission or both, as momentum is injected into the RB flow either by the no-slip wall or the thermal plumes. In order to separate these effects, we avoid sidewalls by using lateral periodicity and thereby focus only on the contribution to the logarithmic profile by the thermal plumes. Two-dimensional simulations are used to aid visualization and identification of plume emission locations. Even though two-dimensional (2D) RB differs from three-dimensional (3D) RB in terms of integral quantities for finite Pr (§8), the theoretical arguments for logarithmic profiles are not specific to 3D RB. Furthermore, the two-dimensional domain is more suitable to study the horizontal dependence of the boundary layer profile than the three-dimensional domain. The locations of plume emission on the one hand and large-scale circulations on the other hand are more straightforwardly identified. In addition, converging local 3D statistics of a sufficiently turbulent flow, which cannot be averaged over any spatial dimension, remains unfeasible to this date due to the required computational cost.

The data are obtained from an energy conserving second order finite difference method [105, 128] converted to 2D. The code was validated previously (§6) using other 2D RB codes and quasi 2D experiments. Resolution checks are performed by checking the consistency of the Nusselt number calculated in five different ways (equations 8-11), local inspection on spurious oscillations and comparing with simulations performed with different codes. The number of grid points in the used $Ra = 5 \times 10^{10}$, $Pr = 1$, aspect ratio $\Gamma = 4.8$ DNS is 11520×2304 with grid point clustering at the steep gradients near the horizontal plates. The aspect ratio is $\Gamma = 4.8$ as this stabilizes the large-scale rolls in the system. For lower $\Gamma = 2$ and comparable $Ra = 10^{10}$ it is found that the heat flux approximates the heat flux at infinite aspect ratio [41]. However, this aspect ratio is insufficient for the analysis presented here, as the horizontal organization of the flow is not static at $\Gamma = 2$. In order to average in time, the temperature conditioned in a plume ejecting region, the flow organization is required to be static. The total averaging time is 1000 free-fall time units. As the local averages take a very long time to converge, a horizontal moving average with a window of $0.01L$ is used.

7.2 Flow topology

It is common in RB theories to assume that there is no horizontal dependence. RB flow can then be conceptually decomposed into boundary layers and a bulk [35]. Some authors include an additional mixing zone as an intermediate region [98]. However, taking a perspective from channel or pipe flows, where the complete domain can be considered to be a BL, the RB BL corresponds to the inner BL region and the bulk to the outer BL region. This is because in fully developed channel and pipe flow the complete domain is considered to be influenced by the boundary. In addition, these

Figure 7.2: a) Mean temperature profiles for three distinct boundary layer regions and horizontally averaged. The black dashed line is a fit to the logarithmic part of the profile. There is a logarithmic like profile visible in the ejecting mean temperature profile. The region is approximately one decade in width; namely for $0.02 \leq z \leq 0.2$. A zoom can be seen in the inset.

Figure 7.3: The Richardson number Ri , the log amplitude $-A$, the fit residual R and the log quality P as a function of the horizontal coordinate x . The plotted quantities are normalized by their maxima. It can be seen that there is a strong correlation between plume ejecting regions and logarithmic mean temperature profiles.

systems are statistically homogeneous in directions parallel to the boundary. In RB flow, this is not the case as it is strongly horizontally (and vertically) inhomogeneous due to the self-organization into large-scale rolls. The result of this inhomogeneity is that different regions, which are separated horizontally, have very distinct dynamics. We divide the boundary layer horizontally into three regions, namely *ejecting*, *impacting* and *wind shearing* [60]. In the ejecting region thermal plumes are emitted while in the impacting region the wind and plumes from the opposite boundary impact the BL. In between is the wind shearing region that is sheared by the large-scale wind. The velocity is predominantly vertical in the ejecting and impacting region while in the wind shearing it is horizontal. These regions are specific to either the bottom or top boundary layer. In figure 7.1 (top panel) the instantaneous temperature field can be seen. large-scale rolls and small scale plumes can be distinguished. As the rolls are nearly stationary, the roll structure and the plume emission spots can clearly be observed in the mean temperature field in figure 7.1 (bottom panel). The three horizontal regions are sketched on top of this figure, where it can be seen that the ejecting region for one BL is similar to the impacting region for the other BL with respect to the horizontal position. Using the snapshot in 7.1 (top panel), it is apparent that the impacting region is qualitatively different than the wind sheared region and that it also has a smaller width than the ejecting region.

In order to connect these regions to the logarithmic profiles, the regions must be quantified. For this we use a local Richardson number, which has also been used in forced convection to identify upwelling plumes [220]. Here we use a local Richardson number of the form $Ri(x) = \frac{|\langle \theta(x) \rangle_t - \langle \theta(x) \rangle_{x,z,t}|}{\langle u_x(x)^2 \rangle_t}$. The horizontal x and vertical z coordinates are normalized by L . This quantity is evaluated at the edge of the temperature boundary layer $\lambda_\theta \equiv L/(2Nu)$, where $Nu = \sqrt{RaPr} \langle u_z \theta \rangle_{x,t} - \langle \partial_z \theta \rangle_{x,t}$. In our case $\langle \theta(x) \rangle_{x,z,t} = 1/2$. The Richardson number relates the potential energy with the kinetic energy, commonly used to express the importance of natural convection in relation to forced convection. Using the observation that plumes are predominantly emitted from the BL in regions of low shear, we can use a high Ri to indicate plume upwelling regions and a low Ri for the regions that are sheared by the large-scale wind. It must be noted that this does not provide a clear distinction between impacting and wind-shearing regions. However, this is unnecessary here, as we only compare ejecting regions with the other two.

7.3 Logarithmic regions

Figure 7.2 shows the respective boundary layer profile for each of the three regions, revealing a logarithmic like profile for the ejecting region. The profiles for the impacting and wind sheared regions are very similar to each other and do not show a clear logarithmic behavior. In addition, the horizontally averaged profile does not

show a logarithm either. This is expected considering the studied Ra, as this Ra is not in the so-called ultimate regime that has fully turbulent, logarithmic, boundary layers [35, 55, 65, 66]. In previous experiments [64] the profiles were fitted with the equation $\langle \theta \rangle_t = A \log(z) + B$ for a range of $z \in [0.01, 0.1]$. We use this equation but change the range to $z \in [0.02, 0.2]$ as it more accurately delimits the logarithmic region for this Ra. We connect the log profile to the thermal plume hotspots through R_i in figure 7.3. Here R_i , $-A$, P and the fit residual R are plotted as a function of x . The residual R is the Euclidean norm of the difference between the fit and the data. The quantity P is defined as $P = -|A|/R$ and signifies the "log-ness" of the profile. It is a *goodness of fit* parameter. R_i and Θ are evaluated at the edge of the thermal BL. All the plotted quantities are normalized by their maxima. The log amplitude $-A$ indicates the amplitude of the fitted log. This value is low in the sheared and impacting region and high in both the upwelling regions. A low residual indicates a good fit. It must be noted that fitting a constant value with a log gives a low residual like in the sheared and impacting regions. However, the log amplitude $-A$ reveals that in this regions there is a negligible log amplitude. The highest $-A$ is connected to a high residual, indicating that the log fit is not good. High amplitudes and low residuals, i.e. good log fits with strong log dependence, are found in the ejecting regions and it becomes clear that there is a strong correlation between the good and strong log profiles and R_i , indicating that the log profiles are connected to the plume hotspots and that these logarithmic profiles can be present without sidewalls. The value of P is high throughout the ejecting regions, but has distinct peaks near the edges of these regions.

The logarithmic profile can be tested using a logarithmic diagnostic function, which is commonly used in wall bounded turbulence [221]. The function in this case for temperature is $\Xi(z) = z \frac{\partial \langle \theta \rangle_t}{\partial z}$. For a logarithmic $\langle \theta \rangle(z)$ profile, this function is constant and can therefore be used to diagnose the logarithmic profile. Because of the required derivative, this function is difficult to converge in both experiments and numerics. In figure 7.4a the function is plotted separated for ejecting regions and the rest of the domain. The ejecting region is separated by conditioning on P . It appears that using $P > 0.4$ cleanly separates the profile into a logarithmic and a non-logarithmic part. The function $\Xi(z)$ is constant for approximately one decade for $P > 0.4$, while it is clearly not for $P \leq 0.4$.

In turbulent flows the temperature gradient hypothesis can be used to obtain a logarithmic profile for the temperature [214]. It states: $\langle u'_z \theta' \rangle_t \hat{=} -\kappa_{turb}(z) \frac{\partial \langle \theta \rangle_t}{\partial z}$, where $\kappa_{turb}(z)$ is the eddy diffusivity, which dominates the heat transfer in case of turbulence. The eddy diffusivity is approximated to depend linearly on the distance from the wall z . In that case, the term $\langle u'_z \theta' \rangle_t$ has to be constant throughout the logarithmic temperature layer, since $\frac{\partial \langle \theta \rangle_t}{\partial z} \sim z^{-1}$ as was shown in figure 7.4a. The conditioned $\langle u'_z \theta' \rangle_t$ is shown in figure 7.4b. This term is time-averaged and averaged over x con-

Figure 7.4: a) Logarithmic diagnostic function Ξ as a function of z for horizontal regions where P is smaller and larger than 0.4. This function is constant if $\langle \theta \rangle$ is logarithmic in z . This is the case in the one-decade log regime between $0.02 \leq z \leq 0.2$, delimited by the dashed black lines. The blue dashed line indicates the logarithmic fit from figure 7.2. b) $\langle u'_z \theta' \rangle_t$ as a function of z for horizontal regions where P is smaller and larger than 0.4.

ditioned on the value of P . For the non-logarithmic regions of $P \leq 0.5$, it can be seen that $\langle u'_z \theta' \rangle_t$ is not constant. This is expected for a non-logarithmic mean temperature profile. In case of a logarithmic profile with $\langle u'_z \theta' \rangle_t$ only depending on z , it is expected that $\langle u'_z \theta' \rangle_t$ is constant. However, this can hardly be distinguished in figure 7.4b for $P > 0.4$, even though the curvature of $\langle u'_z \theta' \rangle_t$ is much less than for $P \leq 0.4$. This observation is very similar to logarithmic profiles in channels [119], which indicates that also in systems where there is horizontal homogeneity this quantity is not exactly constant throughout the logarithmic layer. In addition, in both channel flow and here, the lower curvature of $\langle u'_z \theta' \rangle_t$ is in a region lower in z than the logarithmic layer. This offset seems to be stronger in RB flow, which might be due to the inherent horizontal dependence of the boundary layer profile in this flow. There is horizontal heat flux locally and the common BL approximation $|\partial \theta / \partial x| \ll |\partial \theta / \partial y|$ is not valid in the logarithmic regions. Between $z = 0.01$ and $z = 0.1$ these quantities are even of similar magnitude.

7.4 Discussion and Conclusion

The flow topology of Rayleigh-Bénard convection can be divided horizontally into three distinct regions, namely ejecting and impacting regions, where plumes are ejected from the corresponding boundary and impact from the opposite boundary, respectively. In between exists a wind-sheared region, where the large-scale wind shears the boundary layer and the flow is predominantly horizontal close to the plates. The profiles of the mean temperature differ strongly between these regions, which explains the radial dependence of the profiles found in cylindrical experiments [64, 217, 218]. In these experiments, the amplitude and the quality of the logarithmic fit to the data decreases from the sidewall to the central region of the domain. By removing the sidewalls completely, we have shown here that it is the presence of the thermal plumes that result in these profiles. Namely, in a low aspect ratio cylindrical setup, the thermal plumes move more closely to the sidewall than to the center of the cell. The mean log profiles are connected to the plume hotspots. This signifies that log profiles can and do locally exist in the classical regime and that in this regime the boundary layer profile is not laminar over its full range from certain Ra onwards. We argue that for the studied $Ra = 5 \times 10^{10}$ the ejecting region has on average a turbulent BL and both the sheared and impacting regions are laminar. The sheared region has a profile that closely resembles a laminar Pohlhausen profile [70, 86, 179, 189, 191] and the impacting region deviates slightly from this.

The presence of logarithmic profiles in the classical regime can be reconciled with the ultimate regime by arguing that as a function of Ra the relative size of the hotspot region grows until the full BL is a hotspot and thus has a logarithmic mean profile. Thermal plume related transitions have been seen before [222] and it is likely

that the transition to the ultimate regime can be triggered by thermal plumes and their local fluctuations instead of a large-scale shear. In future work we plan to study the width of the logarithmic region as a function of Rayleigh number to see if there is indeed a continuously growing turbulent boundary layer region up to the possible ultimate regime.

Comparison between two and three dimensional Rayleigh-Bénard convection*

Two-dimensional (2D) and three-dimensional (3D) Rayleigh-Bénard convection is compared using results from direct numerical simulations and previous experiments. The explored phase diagrams for both cases are reviewed. The differences and similarities between 2D and 3D are studied using $Nu(Ra)$ for $Pr = 4.38$ and $Pr = 0.7$ and $Nu(Pr)$ for Ra up to 10^8 . In the $Nu(Ra)$ scaling at higher Pr , 2D and 3D are very similar; differing only by a constant factor up to $Ra = 10^{10}$. In contrast, the difference is large at lower Pr , due to the strong roll state dependence of Nu in 2D. The behavior of $Nu(Pr)$ is similar in 2D and 3D at large Pr . However, it differs significantly around $Pr = 1$. The Reynolds number values are consistently higher in 2D and additionally converge at large Pr . Finally, the thermal boundary layer profiles are compared in 2D and 3D.

*Based on: E.P. van der Poel, R. J. A. M. Stevens and D. Lohse, *Comparison between two and three dimensional Rayleigh-Bénard convection*, J. Fluid Mech., **736**, 177–194 (2013) [86]

8.1 Introduction

Although all real-world applications of RB convection are three-dimensional (3D), two-dimensional (2D) simulations are used to better understand the physical mechanisms of 3D convection, as 2D simulations are substantially less CPU-intensive than 3D simulations. In addition, theoretical predictions for scalings in hard turbulent RB convection [26, 35, 55, 66, 68, 70, 98, 223] are based on 2D equations, namely the Prandtl equations for the boundary layer or use assumptions that apply to two dimensions as well as to three. This makes it an useful tool to validate theory, regardless of the similarity between 2D and 3D. Moreover, the quasi-2D character of the large-scale circulation (LSC) in both 2D and 3D flows hints towards a large similarity, in particular for integral quantities, between 2D and 3D in RB turbulence, in contrast to unbounded turbulence, where in three dimensions no such large-scale structures emerge.

Despite these similarities, there are significant differences between 2D and 3D convection. For example, the limited motion of the LSC in 2D convection increases the accumulation of energy in corner rolls leading to large-scale wind reversals [178] and high sensitivity of global output parameters on the roll state (§4). In 3D these phenomena are also observed [224], however the additional degree of freedom of the LSC attenuates the global effects of these phenomena. Furthermore, the intrinsic inverse energy cascade [197] of 2D turbulence is fundamentally different from the forward cascade of 3D turbulence. The effect of this difference at smaller scales on global properties is unfortunately unknown, as well the existence of an inverse cascade in 2D RB. However, one can argue that for RB flows with a large-scale roll the effect must be minor, as in 3D RB the self-amplifying local driving and global temperature gradient [87] result in a box-sized vortex, even without an inverse energy cascade. The large-scale dynamics are similar in 2D and 3D and therefore the main difference in global output between both systems is expected to come from the small scale dynamics.

Previous work of Schmaltzl *et al.* (2004) [188] on the validity of the 2D approach to 3D RB convection concluded that for small Pr , 2D numerics are no longer a valid representation of 3D convection, due to the increasing energy in the toroidal component of the velocity in 3D flows at lower Pr [225]. The analysis was limited to a low Rayleigh number of 10^6 , which is in the laminar regime for most Pr , according to the coherence length criterion [38]. Furthermore, Schmaltzl *et al.* (2004) [188] used stress-free velocity boundary conditions on the lateral walls. Although this decreases computational requirement due to the absence of sidewall boundary layers, it complicates comparison to experiments where the boundary conditions are exhaustively no-slip. Now, eight years later, we are able to study the similarities and differences between 2D and 3D RB convection with no-slip boundary conditions at much higher Ra in the turbulent regime.

We explain the numerical methods used and provide resolution checks alongside the results. We show parameter spaces containing a comprehensive overview of available data points from 2D and 3D RB studies. A qualitative review is made using flow field snapshots of 2D and 3D flows at different Pr , illustrating the different regimes in Pr space and their proposed effect on the 2D/3D similarity. Moreover, the thermal boundary layer profiles obtained in the 2D and 3D simulations are compared with the 'flat-plate' Pohlhausen profile.

8.2 Explored parameter space

We first review the explored parameter space in both experiments and numerics. Figure 8.1 displays the 3D and 2D phase diagrams. The lines and numbers indicate the different regimes of the GL-theory based on a refit of the data (§1). Note that for the 2D plot the regimes resulting from the 3D fit are used. For the 3D plot, data points where Nu has been measured or numerically calculated have been included for aspect ratio $\Gamma = 1$ for no-slip velocity boundary conditions on all walls.

Unlike the 3D phase diagram in figure 8.1, multiple velocity boundary conditions are included in the 2D phase diagram. This increased variety in the boundary conditions employed presumably originates from the lack of 2D experiments; there is less willingness to mimic the no-slip experimental boundary conditions of experiments in 3D. In addition, the rectangular 2D geometry allows for more types of boundary conditions than the common cylindrical 3D setup as periodic sidewalls are not possible in this case.

Comparing the two phase diagrams, it becomes clear that the 3D parameter space has been explored more due to the availability of experiments and the closer resemblance to convection in nature. The 2D phase diagram is, apart from one experimental series, fully composed of numerical data. The highest $Ra = 10^{14}$ [228] is obtained for a flow without velocity boundary layers. Evaluating the grid resolution used and the saturating $Nu(Ra)$ data, we think that this simulation is underresolved and the heat flux was dominated by numerical diffusion. Discarding this point from the comparison and taking into account the fact that $Ra = 2 \cdot 10^{12}$ is the highest Rayleigh number obtained in three dimensions, it is apparent that the exploration of the parameter space in two dimensions is open for a large improvement.

8.3 Numerical simulations

We numerically solve the three-dimensional Navier-Stokes equations within the Boussinesq approximation. The 3D numerical scheme is described in detail in [37, 105, 128] and the 2D scheme in [177]. For this study we performed 3D simulations at $Ra = 10^8$ and $0.02 \leq Pr \leq 0.7$ in a $\Gamma = 1$ sample and 2D simulations in a $\Gamma = 1$ sample at

Figure 8.1: a) Phase diagram in the Ra - Pr plane for 3D studies. Here simulations and experiments are indicated by red squares and blue circles respectively. For more detail and references see §1. b) Phase diagram in Ra - Pr plane for two-dimensional studies. Note that the lines indicating the different GL regimes are taken from the 3D fit to assist the comparison of the two plots. The legend applies only to the 2D phase diagram. The data points are taken from studies where Nu has been measured in all aspect ratios and is from Refs. [174], [226], [227], [228], [229], [188], [41], [178], [230], §4 and this study. The different velocity boundary conditions used in these studies are indicated in the legend by NS (no-slip), SF (stress-free) and PD (periodic) in the format [plates-sidewall]. Note that '(exp.)' in the legend signifies that these data are taken from quasi two-dimensional experiments. The lines in both plots follow the Grossmann-Lohse theory [35, 66, 68, 70]: The upper solid line means $Re = Re_c$; the lower nearly parallel solid line corresponds to $\epsilon_{u,BL} = \epsilon_{u,bulk}$; the curved solid line is $\epsilon_{\theta,BL} = \epsilon_{\theta,bulk}$; and along the long-dashed line $\lambda_u = \lambda_\theta$, i.e., $2aNu = \sqrt{Re}$. The dotted line indicates where the laminar kinetic boundary layer is expected to become turbulent, based on a critical shear Reynolds number $Re_s^* = 1014$ of the kinetic boundary layer, with $a = 0.911$ (§1)

$Ra = 10^8$ with $0.065 \leq Pr \leq 55$, and with $Pr = 4.38$ and $10^7 \leq Ra \leq 10^{11}$ to complement some of our previous data sets [84, 182, 231].

To ensure adequate accuracy of the simulations, we compare the number of points we placed in the thermal boundary layer with the minimum number that should be placed inside the boundary layer [44]. For each Prandtl number this criterion is satisfied for the highest resolution simulation and/or checked with resolution checks. Once a simulation is properly resolved there is no dependence on the grid resolution as the grid-dependent errors diminish. This is a strict resolution criterium as it is sensitive to the resolution in the entire domain and not just in the boundary layers. Apart from the boundary layer the azimuthal resolution close to the sidewall has to be chosen properly in cylindrical domains. The only way to check this is to perform the same simulations on different resolutions and compare the results [94]. In order to check this we have performed the simulation for several Prandtl numbers, specifically the lowest and highest Pr , with different resolutions, and we find good agreement between the results obtained at different resolutions. We compared the average length scale in the flow with the largest grid scaling and the time convergence of the results.

8.4 Flow topology

Figures 8.2, 8.3, and 8.4 show flow field snapshots of the complete 2D field, a vertical cross-section and a horizontal cross-section of the 3D cylinder, respectively. The top row of the panels depicts the temperature field and the bottom row depicts the vertical velocity field. The left, center, and right column are for $Pr = 0.045$, $Pr = 0.7$ and $Pr = 55$, respectively. In the 3D panels it becomes apparent that the temperature structures become more localized at $Pr = 55$, as is expected for high Pr flows. At high Pr there is hardly any LSC and the flow is plume-dominated [128]. This is reflected in 2D, for which the panels of both the temperature and velocity look very similar to those for three dimensions, in agreement with Schmaltzl *et al.* (2004) [188], who concluded that 2D and 3D cases are similar at high Pr due to the vanishing toroidal component of the velocity. Another interpretation of the similarity of the flow topology at high Pr can be made using the plume topology, since at high Pr the flow is plume-dominated. In two dimensions it can be seen that for increasing Pr , the plumes change from roll-up type to sheet-like and finally to the mushroom type. The roll-up type plumes are vortices that become buoyant by extracting thermal energy from the boundary layer. These can be seen in figure 8.2 for $Pr = 0.045$. The sheet-like plumes are elongated boundary layers stretching upwards and can be found for moderate Pr . For high Pr the flow is dominated by mushroom-shaped plumes. One can imagine that 3D mushroom type plumes can be reduced to two dimensions through axisymmetry, while the other types do not possess symmetry that translates from two to three dimensions without violating the divergence-free condition imposed on the velocity field and/or the no-

Figure 8.2: Temperature (top panels) and vertical velocity (bottom panels) of a 2D $\Gamma = 1$ cell at $Ra = 10^8$. The panels from left to right are for $Pr = 0.045$, $Pr = 0.7$, and $Pr = 55$. Red and blue indicate hot and cold fluid, respectively, for the temperature snapshots. For the velocity, red and blue indicate upward and downward moving fluid, respectively. The temperature colormap is the same for all temperature snapshots in figures 8.2, 8.3 and 8.4 and ranges between $0.4 \leq \theta \leq 0.6$.

Figure 8.3: Temperature (top panels) and vertical velocity (bottom panels) at a vertical plane of a 3D cylindrical $\Gamma = 1$ sample at $Ra = 10^8$. The panels from left to right are for $Pr = 0.045$, $Pr = 0.7$, and $Pr = 55$. Same color coding as in figure 8.2. The azimuthal orientation of these vertical cross-sections can be seen in figure 8.4

Figure 8.4: Temperature (top panels) and vertical velocity (bottom panels) at the horizontal midplane of a $\Gamma = 1$ cell at $Ra = 10^8$. The black lines indicate the azimuthal orientation of the corresponding vertical cross-sections found in figure 8.3. The panels from left to right are for $Pr = 0.045$, $Pr = 0.7$, and $Pr = 55$. Note that the velocity scales are visibly smaller than the temperature scales for the small Pr number case, while the temperature scales are smaller than the velocity scales for the high Pr number case.

slip boundary conditions. For example, the 3D analogue of a roll-up plume would be a cylinder.

The visual differences emerge at $Pr < 1$. At $Pr = 0.7$ a pronounced LSC with corner rolls can be seen in two dimensions in figure 8.3. In three dimensions, the LSC is less pronounced and the corner rolls are much smaller. These differences might be due to the absence of a preferential azimuthal orientation of the LSC in three dimensions [90, 232, 233]. The azimuthal orientation of the vertical cross-sections displayed here is selected to obtain the clearest depiction of the LSC. In addition, it can be seen that in three dimensions, thermal plumes are emitted from the horizontal center of the boundary layer and move through the bulk, in contrast to the 2D case. This is because in three dimensions the LSC cannot fully enclose the flow and limit the movement of plumes.

A clear difference between the 2D and 3D cases can be found at $Pr = 0.045$. In particular, the vertical velocity snapshots reveal a drastically different structure. The 2D field has locally very small velocity structures similar to the 3D field. However, even though both 2D and 3D appear to have a large-scale circulation, the average velocity scale in three dimensions is much smaller than in two dimensions. It was previously concluded that for $Pr = 0.1$ and $Ra = 10^8$ the LSC is driven by buoyancy forces more than by small scale turbulent fluctuations in both 2D and 3D [229]. While the small scales do appear to have merged with the LSC in 2D, they are possibly not the dominant contribution to the driving of the LSC.

8.5 Nusselt number

In this section we will first compare the Rayleigh number scaling of the Nusselt number obtained in 2D and 3D simulations before we compare the Prandtl number dependence in detail.

8.5.1 Rayleigh number dependence

In figure 8.5a the compensated Nusselt number $Nu/Ra^{1/3}$ as a function of Ra for $Pr = 4.38$ and $\Gamma = 1$ is displayed. The data is taken from 3D experimental results of Refs. [79, 95], 3D numerics of Refs. [39, 96, 97] and 2D numerics of this research. Both the uncorrected and corrected experimental data are depicted. The corrected data is compensated for finite plate conductivity: see [87]. In these and forthcoming figures, the 2D data are represented by triangles with varying orientations and the 3D data by other symbols. For reference, the refitted GL prediction for 3D is included. As the 3D data and GL theory display near-equal results for the evaluated Ra range, the latter can be used as a guide in comparing the 2D $Nu(Ra)$ data with 3D data by rescaling with a constant factor of 0.78. For 3D and 2D the scaling of $Nu(Ra)$

agrees very well for $10^7 \leq Ra \leq 10^{10}$. At higher Ra the 2D points are smaller than the rescaled 3D GL prediction. This indicates that for $Ra > 10^{10}$ the 2D scaling differs from the 3D scaling since the 3D data do follow this scaling. An analysis of the roll states of $Ra = 4.64 \cdot 10^9$ and $Ra = 10^{10}$ reveals that there is a substantial change in flow state between these Rayleigh numbers, which might be connected to the discrepancy in scaling. At $Ra = 4.64 \cdot 10^9$, the flow is in a single roll state similar to the state depicted for $Pr = 0.7$ and $Ra = 10^8$ in figure 8.2 while at $Ra = 10^{10}$ the roll state has become uncondensed. Here, the term uncondensed signifies that there is no energy pile-up at a scale close to system size and thus there is no LSC. The largest scale in the flow consists of two mobile and orbiting smaller rolls. That Nu is (counter-intuitively) lower for this broken LSC has been observed in §5 for $Pr = 0.7$ and $Ra = 10^9$ and we believe that this is due to the increased path length of the thermal plumes before they can deliver the heat to the opposite plate. For a large-scale circulation the plumes move directly from their original boundary layer to the opposite boundary layer, while otherwise the plumes move less directly to the opposite boundary layer, interacting with the multiple rolls composing the bulk. Now, not only the absolute Nu but also the scaling between Nu and Ra appears to be lower for this roll state. Extrapolating towards higher Ra , one expects that the scaling will change subsequently when these orbiting rolls are replaced by a more complex roll state with even smaller scales. Eventually, the fluctuations will become too large and the scales too small for the existence of a coherent roll state that can affect integral quantities. In §5 we showed that the scaling of Nusselt can change locally in 2D RB convection and can recover to the expected 3D scaling for higher Ra ; see also the $\Gamma = 1/2$ results.

In three dimensions no such transition in an integral quantity exists, since the LSC does not fully enclose the system. This gives the thermal plumes more freedom to move from one boundary layer to another. Therefore, the difference in Nu between a system with a single roll state and one with a broken single roll state is expected to be small and more gradual than in two dimensions, where the system can jump between these states, affecting Nu (§5) and its scaling.

The difference between the 2D and 3D cases is expected to be larger for lower Pr due to the larger toroidal component of the velocity. In addition, it is known (§4) that the integral quantities and flow state in 2D have a stronger dependence on the aspect ratio Γ than in three dimensions [172]. This is emphasized by the increased effect of the flow state on Nu for low Pr due to the thermal boundary layer being exposed to the bulk flow (§4). For low Pr , the bulk flow directly extracts heat from the thermal boundary layer, and therefore the flow state of the bulk has a large effect on Nu . We therefore include a comparison for $Pr = 0.7$ and $\Gamma = 0.5$, where we expect a substantial difference. The result is displayed in figure 8.5b. Although the average scaling exponent appears to be similar, the 2D data reveal much more structure than

Figure 8.5: a) Nu versus Ra scaling for water ($Pr = 4.38$) in a $\Gamma = 1$ sample. The simulation result for 2D RB is indicated by the blue upward-pointing triangles. The 3D experimental results from [79, 95] are indicated by circles and squares, respectively. Here the open symbols indicate uncorrected data, while the filled symbols indicate corrected data. The numerical results from [39, 97], and [96] ($Pr = 5.4$) are indicated by the purple stars, blue asterisks and olive diamonds, respectively. The black solid line indicates the GL prediction and the red dashed line indicates the GL prediction multiplied by a constant value A of 0.78. The rest of the points are 3D experimental and numerical data. b) Nu vs Ra for $Pr = 0.7$ in a $\Gamma = 0.5$ sample. The 2D data are indicated by the yellow rightward-pointing triangles. The stars [99], asterisks [30], diamonds [100] and circles [29, 101] indicate experimental data and the squares results from numerical simulations [31, 94]. The refitted GL theory is indicated by the black line.

for three dimensions. This is caused by multi-stability of different flow states and the large difference in Nu between these flow states. By increasing Ra , the system is successively in a triple roll state, an unstable triple roll state and back to a triple roll state, passing through an unstable region until the roll state breaks up. These roll states strongly affect the resulting Nu . This effect is expected to decrease as the LSC loses its strength (§5) and the length scales become smaller at higher Ra .

8.5.2 Prandtl number dependence

The main conclusion from Schmalzl *et al.* (2004) [188] was that the agreement of global quantities between 2D and 3D depends on Pr . More specifically, they conclude that for lower Pr the 2D output increasingly deviates from 3D. We repeat their measurements in 2D for $Ra = 10^6$ and supplement it with a series for $Ra = 10^8$, albeit with a no-slip boundary condition on the sidewalls in contrast with their stress-free sidewall boundary condition. In figure 8.6a it can be seen that numerical simulations for low Pr become increasingly demanding in terms of resolution. Here the results for the $Ra = 10^8$ runs are depicted, with symbols indicating the numerical resolution

Figure 8.6: Nu as function of Pr. a) The Nusselt number obtained in numerical simulation performed on different grids for $Ra = 10^8$. The legend indicates the number of grid-points in the vertical and horizontal direction for two dimensions and in the azimuthal, radial, and axial direction for three dimensions. b) Comparison of the Pr number dependence on Nu in two and three dimensions. Here the green downward-pointing and cyan upward-pointing triangles indicate the results from 2D RB simulations at $Ra = 10^8$ and $Ra = 10^6$, respectively. For three dimensions this is indicated by the blue squares and black circles, respectively. The $Ra = 10^6$ data are from [105]. In both panel the solid lines give the prediction of the GL theory.

used. Figure 8.6b shows $Nu(Pr)$ for Ra for 10^6 and 10^8 . The solid lines are the refitted theoretical GL predictions for the different Ra corresponding to the experimental and numerical data. First, we observe that the numerical results for 2D (green triangles) and 3D (black dots) at $Ra = 10^6$ display no qualitative similarity, except for the Pr independence of Nu at higher Pr. Furthermore, in 2D multiple states are observed around $Pr = 1$, where the outlying points are caused by the double roll state of the system as opposed to the single roll state corresponding to the other data points. It is likely that the single roll state is stable as well, which would display a Nu similar to the surrounding Pr data (§4). However, this has not been checked. The discrepancy that [188] did not observe these multiple states might be due to multi-stability or caused by their free-slip sidewall boundary condition. For $Ra = 10^8$ the 2D and 3D cases seem to converge for high Pr. The largest difference is seen at intermediate Pr, which is reflected in the flow topology, see section 8.4. Here the strong LSC results in a substantial difference in Nu between the 2D and 3D cases. At low Pr, unlike for $Ra = 10^6$, the 2D and 3D Nu are matching. However, the number of data points is too low to make a strong conclusion given this surprising low Pr behavior.

Figure 8.7: The compensated Reynolds number based on the root-mean-square vertical velocity Re_3^{RMS} for 2D (rightward-pointing triangles) and 3D (squares): a) Re_3^{RMS} as a function of Ra for $Pr = 0.7$ and $\Gamma = 0.5$. b) Re_3^{RMS} as a function of Pr for $Ra = 10^8$ and $\Gamma = 1$. The legend in b) applies to both plots. Corresponding Nu comparison can be found in figures 8.5b and 8.6b for a) and b), respectively.

8.6 Reynolds number

Figure 8.7 shows the comparison for the compensated Reynolds number based on the root-mean-square vertical velocity $Re_3^{RMS} = u_3^{RMS} L / \nu$ as a function of both Ra and Pr . The data in figure 8.7a correspond to the low $Pr = 0.7$ and low $\Gamma = 0.5$ parameters, where we expect a large difference. This is confirmed for Nu in figure 8.5b and appears to be the same for Re_3^{RMS} . A similar difference in structure between the 2D and 3D cases can be seen, with no noticeable convergence at the highest Ra evaluated. Re_3^{RMS} can be seen to locally scale larger than $Ra^{1/2}$ for 2D, which highlights the roll state dependence of integral quantities in two dimensions. The comparison of Re_3^{RMS} as a function of Pr in figure 8.7b reveals a picture to that seen by Schmalzl *et al.* (2004) [188] for $Ra = 10^6$: the Reynolds number for two dimensions converges to the 3D value at high Pr . In both cases the 2D Re_3^{RMS} is higher than in 3D, while in contrast Nu is lower in 2D compared to 3D. The inverse energy cascade in two dimensions is possibly causing a stronger LSC than in three dimensions. However, up to now there have been no studies on the existence of the inverse energy cascade in 2D RB and therefore this remains uncertain. It could also be that in two dimensions, all emitted plumes drive the LSC, while in three dimensions not all plumes follow the motion of the LSC. This can result in a lower Nu due to plumes being dragged down by the LSC before releasing most of their thermal energy at the boundary opposite to the plumes' origin. In this situation Re_3^{RMS} can be higher in two dimensions while Nu is lower.

8.7 Boundary layer profile

The boundary layer profile is a fundamental ingredient in most theoretical studies on the scaling of Nu and Re . In the 'classical' regime, where the boundary layer is assumed to be laminar, a reference analytical solution for the situation of a flow over a infinitely long plate is provided by Pohlhausen (1921) [234], which is based on the Prandtl-Blasius (PB) boundary layer approximation. The purpose of this section is to compare the 2D and 3D boundary layer profiles, with the Pohlhausen profile included for reference. For a laminar boundary layer, it is assumed that for $Pr \approx 1$ both the velocity and temperature have a similar profile. This allows us to use the temperature boundary layer profile that is relatively easy to extract, for comparison. It is known that the time-averaged and instantaneous laminar boundary layers at the center of a large-scale roll in both 2D and 3D RB flow are well approximated by the Pohlhausen profile when dynamically rescaled [179, 189, 191]. This is despite the fact that the instantaneous flow in RB is only in rare cases locally parallel to the plates, in contrast to the PB assumptions of a completely parallel flow. The resulting deviations have been studied in detail for several cases [43, 215, 216]. The vertical velocity gradient is nonzero due to the LSC, plume emission and corner rolls. As this effect is minimal at the center of a roll for most control parameters, the temperature profile is measured in the center of the cell; $r = 0$ for 3D and $x = D/2$ for 2D in a $\Gamma = 1$ cell. It was shown by [179] that the lateral dependence is strong. In figure 8.8 the time-averaged temperature profiles for two and three dimensions for identical $Pr = 4.38$ and the Pohlhausen solution are shown. The Ra number is varied to match Nu in two and three dimensions to obtain an equal temperature boundary layer thickness $\lambda_\theta \approx 1/(2Nu)$ and similar local flow conditions induced by the heat flux. The profiles are measured in the laboratory frame in order to reveal the differences, as both the 2D and 3D profiles match the Pohlhausen profile when measured in the dynamical frame.

It can be seen that neither the 2D and 3D profiles in figure 8.8 match the Pohlhausen profile well in the laboratory frame. The agreement of the 3D profile is worse than that of the 2D profile. This is most likely due to a combination of several causes. The PB theory is a 2D theory and, because of the more complex dynamics of the LSC in three dimensions compared to two dimensions, the velocity field cannot be considered constantly parallel to the horizontal plates, even at $r = 0$. Furthermore, increased plume activity in the bulk indicates that more plumes are emitted at the center of the 3D cell due the increased degrees of freedom and LSC cessations. This results in the 3D profile being lower than 2D throughout the boundary layer, as an increased amount of thermal energy is taken by plumes.

Figure 8.8: a) Thermal boundary layer profile for two dimensions (red triangles) and three dimensions (blue dots) compared to the Pohlhausen solution (black line) of the Prandtl-Blasius laminar boundary layer approximation. The 2D and 3D cases used for the profiles have identical $Pr = 4.38$ and Ra is varied to obtain an approximately equal Nu . For three dimensions $Ra = 10^8$ and $Nu = 33.11$ and for two dimensions $Ra = 2.25 \cdot 10^8$ and $Nu = 33.26$. b) A close-up of a).

8.8 Conclusion

The comparability of 2D and 3D Rayleigh-Bénard convection can in most cases be explained using the coherent structures present in the flow. At high Pr , the regime dominated by mushroom-type plumes, similar 2D and 3D behavior is observed, as expected. However, the LSC in two dimensions has a largely different effect on heat transport compared to three dimensions. In two dimensions the LSC covers the full system, causing the plume movement to be dominated by the LSC, resulting in a significant discrepancy in this regime. The Ra and Pr scaling of the integral quantities in two and three dimensions are similar in some parameter regions. For $Ra = 10^8$, Nu appears similar for low and high Pr while it is substantially different for $Pr \approx 1$. The similarity at low Pr is surprising as Schmaltzl *et al.* (2004) [188] concluded, albeit for $Ra = 10^6$, that here the 2D and 3D cases become incomparable. For $Pr = 4.3$ the $Nu(Ra)$ scaling is nearly identical with only a constant factor between them up to $Ra = 10^{10}$. The temperature boundary layer profiles of both 2D and 3D, obtained in the lab frame, differ from the Pohlhausen profile and from each other. As expected, the 2D boundary layer is closer to the Pohlhausen profile.

It is not difficult to find parameters for which there is a large difference between two and three dimensions. At low aspect ratios the flow states in two dimensions vary more strongly than in three dimensions and have a larger effect on Nu and Re , in particular for $Pr < 1$ (§4). This is reflected in the $Nu(Ra)$ analysis at $\Gamma = 0.5$, where the 3D scaling is smooth and the 2D scaling is very structured. Less expected is the deviation at $Pr = 4.3$ for $Ra > 10^{10}$, which concurs with a change in flow state in

two dimensions. At this Ra the LSC breaks up and one would expect more similarity since the 3D LSC differs strongly from the 2D LSC in that it does not limit the movement of plumes as much. Adding to the question is the discrepancy in $Nu(Ra)$ around $Pr = 1$. Here, the flow state is a large-scale circulation resulting in decreased similarity, in contrast to the increased similarity in the $Nu(Ra)$ scaling.

A remarkable difference is found for Re_3^{RMS} , which is in contrast to Nu , higher in two dimensions than in three. This can be attributed to the strong LSC in two dimensions, dragging thermal plumes back towards their originating plates before they can release their thermal energy.

8.9 Details of numerical simulations

Table 8.1 and 8.2 summarize the details of the 3D and 2D simulations that are presented in this study. The data are presented in a similar way as in table 1 of [94]. The tables indicate the grid resolution used for the different Pr number cases and compare the resolution used in the boundary layer with the criterion given in equation (42) of [44]. The resolution over the whole domain is compared by using equation (2.5) and (2.6) of [94] and using $h = \max(\Delta x, \Delta y, \Delta z)$ or $h = \max(\Delta r, \Gamma L / 2\Delta\phi, \Delta z)$ in a cylindrical domain. Note that for high Pr number regime equation (2.6) of [94] is more restrictive than the criterion given in equation (37) of [44]. The current results seem to indicate that the criterion of [44] is sufficient to ensure convergence of the Nusselt number for the high Pr number cases.

In table 8.1 it can be seen that the number of gridpoints in the thermal boundary layer is no more than given by the criterion. However, the resolution tests show that the simulation is well resolved. In addition, the new parameter value $a = 0.911$ is used in the determination of this criterion, while numerical tests [44] indicate that the minimum number of gridpoints required in the boundary layer is closer to the value obtained by using the old $a = 0.482$. It can be seen in the table that the boundary layers are underresolved for low Pr according to the [44] criterion. However, the agreement of Nu for identical parameters and different grid resolutions, indicate that at least for integral quantities the resolution is sufficient and that the criterion is possible too strict for low Pr .

Table 8.1: Details of 3D simulations at $Ra = 10^8$. Columns from left to right: Pr number; the resolution in azimuthal, radial, and axial direction, $N_\theta \times N_r \times N_z$; the number of points in the thermal boundary layer used in the simulation; the minimum number of points that should be used in the thermal boundary layer according to the criteria of [44]; average length scale in the flow compared to the largest grid length used in the grid; Nu_f , i.e. the Nusselt number over the whole simulation length, omitting the initialization period; Nu_h , the Nusselt number over the last half of the simulation time considered; τ_f , the simulation time in free-fall time units after the initialization period of 30 to 200 τ_f . Note that the bold cases indicate Pr number for which the effect of the numerical resolution has been tested.

Pr	$N_\theta \times N_r \times N_z$	N_{BL}	N_{BL}^{min}	$\frac{\max(\delta_z, \delta_\phi, \delta_r)}{\eta}$	Nu_f	Nu_h	τ_f
55.00 [84]	384 × 192 × 384	15	8	1.68	32.00	32.00	600
55.00 [84]	256 × 128 × 256	23	8	2.52	32.25	32.20	750
30.00 [84]	256 × 128 × 256	15	8	2.17	32.31	32.40	600
20.00 [84]	256 × 128 × 256	15	8	1.97	32.54	32.56	400
15.00 [231]	256 × 128 × 256	15	8	1.83	32.36	32.60	400
10.00 [231]	256 × 128 × 256	15	8	1.65	32.42	32.53	400
6.400 [84]	384 × 192 × 384	23	8	0.99	32.59	32.42	400
6.400 [231]	256 × 128 × 256	15	8	1.48	32.95	33.00	200
4.380 [231]	256 × 128 × 256	15	8	1.35	33.15	32.91	400
3.050 [231]	256 × 128 × 256	15	8	1.24	33.48	33.45	400
1.500 [231]	256 × 128 × 256	15	8	1.03	33.13	33.13	400
0.700 [84]	512 × 128 × 256	12	9	0.58	31.71	31.79	302
0.700 [231]	256 × 128 × 256	15	9	1.11	31.94	31.88	400
0.450	512 × 128 × 256	12	12	0.73	31.13	31.22	259
0.300	512 × 128 × 256	13	15	0.88	30.00	30.03	341
0.200	1024 × 256 × 512	27	18	0.53	28.40	28.64	151
0.200	512 × 128 × 256	13	18	1.07	28.73	28.68	377
0.140	1024 × 256 × 512	28	22	0.63	27.27	27.37	135
0.100	1024 × 256 × 512	29	27	0.74	25.93	25.84	123
0.065	1024 × 256 × 512	30	35	0.90	24.07	23.64	126
0.045	1024 × 256 × 512	33	45	1.05	22.38	22.26	100
0.030	1024 × 256 × 512	39	57	1.35	20.31	20.04	56
0.030	512 × 128 × 256	18	57	2.55	20.20	20.48	447
0.020	1024 × 256 × 512	44	76	1.61	18.90	19.46	78
0.020	512 × 128 × 256	19	76	3.04	18.82	18.59	414

Table 8.2: Details of 2D simulations at $Ra = 10^8$. Columns from left to right: Pr number; the resolution in horizontal and vertical direction, $N_x \times N_y$; number of points in the thermal boundary layer used in the simulation; minimum number of points that should be used in the thermal boundary layer according to the criteria of [44]; average length scale in the flow compared to the largest grid length used in the grid; τ_f , the simulation time in free-fall time units after the initialization period of 30 to 3000 τ_f . Note that the bold cases indicate Pr number for which the effect of the numerical resolution has been tested.

Pr	$N_x \times N_y$	N_{BL}	N_{BL}^{min}	$\frac{\max(\delta_x, \delta_y)}{\eta}$	Nu_f	Nu_h	τ_f
55.00	512 $\times$ 256	16	7	1.27	27.83	27.86	50000
55.00	256 $\times$ 128	8	7	2.38	27.76	27.75	50000
30.00	256 $\times$ 128	8	7	2.38	27.50	27.51	40000
20.00	256 $\times$ 128	8	7	2.38	27.44	27.44	30000
10.00	256 $\times$ 128	8	7	2.37	27.25	27.26	20000
6.400	512 $\times$ 256	16	7	1.26	26.99	26.99	10000
6.400	256 $\times$ 128	8	7	2.36	26.79	26.79	20000
4.380	256 $\times$ 128	8	7	2.33	25.51	25.47	30000
3.000	256 $\times$ 128	8	7	2.32	25.07	25.05	10000
1.500	256 $\times$ 128	8	7	2.31	24.83	24.82	10000
1.000	512 $\times$ 256	8	7	2.32	25.17	25.16	10000
0.700	1024 $\times$ 512	30	8	0.78	25.22	25.10	8000
0.700	512 $\times$ 256	15	8	1.48	25.14	25.16	8000
0.450	1024 $\times$ 512	34	11	0.96	24.78	24.59	2000
0.300	1024 $\times$ 512	37	13	1.18	25.25	25.09	2000
0.200	1024 $\times$ 512	34	17	1.43	25.73	25.40	1500
0.100	2048 $\times$ 1024	76	26	1.01	23.63	23.18	200
0.100	1024 $\times$ 512	36	26	1.97	23.32	23.03	1000
0.065	2048 $\times$ 1024	82	34	1.23	21.76	22.07	200
0.045	2048 $\times$ 1024	102	43	1.46	20.52	20.95	80

Plume emission statistics in turbulent Rayleigh-Bénard convection*

Direct numerical simulations of turbulent thermal convection in a $Pr = 0.7$ fluid up to $Ra = 10^{12}$ are used to study the statistics of thermal plumes. At various vertical locations in a cylindrical setup with aspect ratio $\Gamma = \text{width}/\text{height} = 1/3$, plumes are identified and their properties extracted. It is found that plumes are much less likely to be emitted from plate regions with large wind shear. Close to the plates, the plumes have a unimodal log-normal distribution, whereas at more central locations the distribution becomes weakly bimodal, which can be traced back to clustering of the plumes and influence of the large-scale circulation. The number of hot plumes decreases with height. The width of the plumes scales with Ra approximately as Nu^{-1} , indicating that it is determined by the thermal boundary layer thickness.

*Based on: E.P. van der Poel, R. Verzicco, S. Grossmann, D. Lohse, *Plume emission statistics in turbulent Rayleigh-Bénard convection*, J. Fluid Mech. **772** 5–15 (2015) [32]

Figure 9.1: Sketch of a confined Rayleigh-Bénard system with $\Gamma \approx 1$. A large-scale circulation and plumes paths are indicated, as well as the distinction of the three different horizontal boundary regions: impacting, wind-shearing and ejecting. The corner rolls are not drawn.

9.1 Introduction

RB convection features ubiquitous coherent structures, which continue to survive in strong turbulence. The most prevalent structures are thermal plumes and large-scale circulation (LSC). The thermal plumes and LSC are intrinsically coupled [70], as thermal plumes cluster to form a LSC [138, 235] and fragment in the bulk [236]. In addition, both thermal and shear instabilities can result in the emission of buoyant fluid parcels, as was shown by [237], who distinguished between plumes and puffs. Here, this distinction is not made, and all buoyant parcels are classified as plumes, irrespective of the mechanism behind their origin. Ref. [238] divided the plumes into "sheet" or "line" plumes that are of elongated shape and into circular "mushroom" plumes. They showed that the plumes are predominantly sheetlike close to the plates and mushroom-like higher in the system. Eventually the numbers of both types of plumes are shown to decrease with height. We will connect this phenomenon to the clustering of plumes by using a plume identification criterion and image segmentation.

The concept of thermal plumes has been used to directly and indirectly derive scaling laws for the heat flux [70, 98]. This is because the contribution of thermal plumes to the total heat flux, relative to that of the LSC, is substantial [239]. It is generally assumed that thermal plumes have a characteristic width equal to that of

the thermal boundary layer, which stems from the understanding that thermal plumes are detached thermal boundary layers. This assumption is used [70, 98] to derive scaling laws for the heat flux through the system. We attempt to extract the plume width and thereby substantiate this assumption.

The dynamics of plumes is complex. Plumes move not only vertically, but also horizontally, being advected by the LSC [240]. In addition, the dynamics of the LSC is highly nontrivial [87, 178, 207], affecting the collective motion of the thermal plumes through an opposing pressure gradient. This complicates the simple (two-dimensional) picture of a stationary LSC with thermal plumes moving alongside it [241] (see figure 9.1), as it was shown that plumes are found in the center of the cell and even throughout the entire volume [82, 242]. Recently, it was found in a Taylor-Couette (TC) flow that the boundary layer transition from laminar to turbulent occurs in plume ejecting locations at lower driving than in the wind-sheared region [60]. It was shown by Eckhardt, Grossmann and Lohse (2007) [243] that RB is analogous to TC, which raises the question of whether this phenomenon can also be observed in RB. Because the driving in RB is less efficient than in TC, turbulent boundary layers, such as those seen in RB [64], are difficult to observe due to the required high Ra and long averaging time. This prevents a study in RB convection comparable to the TC flow study [60]. However, it is possible to study the connection between wind shear and plume ejection and hence gain insights into how shear is related to thermal plumes and in turn to boundary layer turbulence. The turbulent boundary layer in RB is an important ingredient in expected heat flux scaling arguments for the ultimate regime [54, 55].

9.2 Method

Direct numerical simulations (DNS) of the Boussinesq equations were performed using a second-order staggered finite difference scheme [105, 128] that is energy conserving. The boundary conditions chosen are no-slip on all walls for the velocity, adiabatic on the sidewall and isothermal on the horizontal plates for temperature. The numerical setup has a Prandtl number $Pr = 0.7$ and aspect ratio $\Gamma = 1/3$. In addition, for fixed Ra a low aspect ratio domain is computationally less demanding than a large aspect ratio domain due to the smaller volume. The used resolutions are up to $1536 \times 512 \times 2048$ for Rayleigh number $Ra = 10^{12}$ with clustering of grid points near the boundaries similar to the previous high Ra DNS of [31]. Horizontal cross-sections of $u_{r,\phi,z}(r, \phi)$ and $\theta(r, \phi)$ are used that have a time interval of 0.5 free fall time. This interval is tested for statistical independence and shown to be sufficient. The number of cross-sections required for statistical convergence is approximately 100.

Figure 9.2 shows the compensated Nu as a function of Ra compared with previous

Figure 9.2: Compensated Nusselt number $Nu/Ra^{1/3}$ as a function of Ra . The blue squares indicate DNS data for $\Gamma = 1/2$ [31]; the data used in this chapter for $\Gamma = 1/3$ is represented by the orange triangles. The solid black line is the result of the Grossmann-Lohse fit for $Pr = 0.7$ from §1

results at $\Gamma = 1/2$. It is apparent that the heat fluxes for $\Gamma = 1/3$ and $\Gamma = 1/2$ are within the error bars of the data. In addition, no transition in the $Nu(Ra)$ scaling towards the steeper scaling (the so-called ultimate regime) is observed and the system can be considered to be in the classical regime, i.e., the boundary layers are not yet turbulent, consistent with the theoretical expectation at $Ra \leq 10^{12}$ [35, 55, 65, 66].

Various methods for detecting plumes have been used previously [242]. We define a thermal plume as the set of coordinates P , where $\theta(r, \phi) - \langle \theta \rangle_{r, \phi} > c\theta_{RMS}$ and $\sqrt{RaPr} u_z(r, \phi)\theta(r, \phi) > cNu$, as [206] did in their study on confined RB convection. This criterion selects coordinates based on a high temperature anomaly and an excess of convective heat flux. Only hot plumes in the lower half of the domain are considered. The empirical constant c was chosen to be 0.8 in [206], but here we take $c = 1.2$ to better separate the plumes from the background and emphasize their core structure. In addition, this choice of c matches the absolute value of the plume with the thermal boundary layer thickness, as will become apparent later on. A similar threshold based only on $u_z\theta$ was used previously [82], where they found no qualitative differences in their results when the threshold was varied by two orders of magnitude. Along the lines of what was already shown there, quantitatively our results do depend on the value of threshold c . In figures 9.3(g)-9.3(i) the results of applying this criterion to the temperature snapshots shown in figures 9.3(d)-9.3(f) are depicted. It should be noted that this method of extracting thermal plume information limits the analysis to treating the plume as a two-dimensional entity, although in reality it is three-dimensional.

Figure 9.3: a) Temperature field snapshot for $Ra = 10^{11}$ at a) $z/L = 0.004$, b) $z/L = 0.04$ and c) $z/L = 0.2$. Hot and cold are indicated by red and blue, respectively. The colormaps are displayed above the corresponding snapshots. Plume detection P corresponding to the temperature field snapshot in (a)-(c) at d) $z/L = 0.004$, e) $z/L = 0.04$ and f) $z/L = 0.2$, where white indicates a plume.

Figure 9.4: a) Probability density functions of the plume areas A_P (normalized by the total area) at different vertical locations z indicated in the legend for $Ra = 10^{11}$. The solid line is a log-normal fit to the data at $z/L = 0.002$. The gray dashed line indicates the characteristic plume area A_c . b) Most probable value Mo of the PDFs at all the measured z . The blue dashed line indicates the mean thermal boundary layer thickness $\lambda_\theta = 1/(2Nu)$.

9.3 Plume size as a function of vertical position

Previous studies have revealed a log-normal distribution for the area of the plume [238], for the length of the plumes [236] and for the spacing between the plumes [244]. These results suggest that the three quantities are intrinsically related to each other. The log-normal distribution suggests a fragmentation process that can be dealt with by the central limit theorem. The physical mechanism resulting in this distribution is that the fluctuations, acting on all scales, fragment the plumes [245]. When modeling this process, the fragmentations are iterated, and a new sample is drawn from some distribution at each individual fragmentation. After many of these iterations, in each of which the plume area is always subdivided, a log-normal distribution results. We use the data at $Ra = 10^{11}$ to analyze the resulting plume area distribution as a function of z , because this gives the optimum available Ra with respect to minimum sidewall influence and the amount of statistics collected.

In figure 9.4(a) we plot the probability density functions (PDF) of the plume areas at three vertical locations for $Ra = 10^{11}$. Closest to the plate, the distribution is unimodal and log-normal, which is illustrated by the quite accurate Gaussian fit to the data in the semi-log plot. Higher in the cell, the distribution becomes weakly bimodal. We interpret the second mode, indicating a larger plume area, as a reflection of plume clustering which is a signature of the LSC, as the large-scale roll contains clusters of hot plumes in its upwelling region. The small area peaks indicate the

Figure 9.5: a) The number of hot plumes N_p as a function of height z/L for $Ra \in \{10^{10}, 10^{11}, 10^{12}\}$. The error bars increase with increasing height z/L but are removed for the last data points for clarity. b) N'_p as a function of z/λ_θ , where N'_p is the number of plumes normalized with N_p at $z/\lambda_\theta = 4.5$.

existence of fragmented smaller plumes traversing the bulk. This view is supported by the data displayed in figure 9.4(b), where the most probable area is plotted as a function of the vertical location z . For all z , the most probable area is characterized by the smaller plumes, as in all of these bimodal distributions at $Ra = 10^{11}$ the right peak is considerably smaller than the left one. In figure 9.4(b) the thermal boundary layer thickness λ_θ based on the time- and volume-averaged Nu is shown. It can be seen that for this $Ra = 10^{11}$ there is a region, extending much beyond λ_θ , where the most probable area is nearly constant. Beyond that region, the area of the small plumes decreases with height, a reflection of the fact that thermal plumes dissipate most of their energy near the plates [246] and are weakened through molecular and turbulent diffusion while moving towards the bulk of the flow higher in the cell [247]. The small plumes either become smaller or cluster to become part of the LSC, thus driving it.

The clustering is further highlighted by the behavior of the plume number N_p as a function of height z , plotted in figure 9.5(a). It can be seen that N_p decreases strongly with z in the bulk, indicating the clustering and dissipation of plumes. In addition, there appears to be a region close to the lower boundary where N_p is approximately constant. The vertical extent of this region decreases with Ra , which signifies the relation of this region to the boundary layer thickness. Close to the upper boundary, N_p displays a steep drop-off, the location of which depends on Ra : The hot plumes travel further in the vertical direction for higher Ra . In figure 9.5(b), the normalized N'_p is plotted as function of z/λ_θ . Here N'_p is the number of plumes normalized by N_p at $z/\lambda_\theta = 4.5$. The profiles for $Ra = 10^{11}$ and $Ra = 10^{12}$ look strikingly similar, hinting at a universal profile for high Ra .

Figure 9.6: a) Thermal boundary layer thickness $\lambda_\theta/L = 1/(2Nu)$ and plume thickness W_P as defined in the text as functions of Ra . Thick solid black line indicates $Ra^{-0.31}$. This exponent is obtained from a fit to the λ_θ points. b) The mean plume area inside the sliding window conditioned on the shear velocity outside the plume $\langle A_{P \cap C} | u_{C \setminus P} \rangle$ for two Ra .

9.4 Scaling of the plume width with Ra

One could think of two parameters that determine the area of a plume. Close to the plates and thus for line plumes, the length of the plumes should be determined by the domain width $D = L\Gamma$, while their thickness is determined by the width λ_θ of the thermal boundary layer, characterized by $\lambda_\theta = L/(2Nu)$. The resulting characteristic nondimensional plume area is then $A_c = \frac{L\Gamma}{2Nu}$. Illustratively, A_c is the area of a plume that is as long as the diameter of the cell and as wide as the thermal boundary layer. This characteristic plume area is indicated in figure 9.4(a). It can be seen that most of the plume areas are smaller than A_c ; either be the plume length, the plume width or both can differ from the dimensional expectation. Conceptually, the line plumes can be understood as detached thermal boundary layers of similar width; cf. [35]. This has also been observed by [248] using a different method. We expect that the observation that A_c approximately separates the two distributions at higher z/L is coincidental, as the assumptions associated with the definition of A_c are not applicable to plumes at this height.

As the absolute value of a quantity obtained from any thermal plume identification depends on the threshold, we compare the *scaling* of the width with the *scaling* of Nu . To be more precise, we compare the plume width with the thermal boundary layer thickness λ_θ , which scales approximately as $\lambda_\theta/L \sim Ra^{-0.31}$ for the data points $Ra \in \{10^9, 10^{10}, 10^{11}\}$. The data for $Ra = 10^{12}$ is not used in this analysis due to lack of statistical convergence.

The data at $z/L = 0.002$ are inside (for $Ra = 10^9$ and $Ra = 10^{10}$) or on the edge

(for $Ra = 10^{11}$) of the thermal boundary layer. It is non-trivial to extract the width of the plumes from the results of the plume detection method used, as displayed in figure 9.3(g). We obtain the average plume width W_P by defining $\mathcal{D}$ as a so-called distance transform on P and $\mathcal{T}$ as a so-called thinning operation on P . These are defined as follows. For every plume element, the distance transform $\mathcal{D}$ gives the Euclidean distance to the closest non-plume element (figure 9.7(b)); the thinning operation $\mathcal{T}$ reduces P to minimally connected lines (figure 9.7(a)). These minimally connected lines are set to 1 and the rest of $\mathcal{T}$ is set to zero. The resulting set characterizes the 'backbone' of the plume. The plume width is obtained from $W_P = 2 \langle \frac{\mathcal{D}:\mathcal{T}}{\mathcal{T}:\mathcal{T}} \rangle_t$, where $\mathcal{D}:\mathcal{T}$ denotes the componentwise inner product of $\mathcal{D}$ and $\mathcal{T}$, namely $\sum_{i,j} \mathcal{D}_{ij} \mathcal{T}_{ij}$ with the sum $\sum_{i,j}$ taken over all points of the set P . An alternative approach that gives identical results involves iterating over all the coordinates in $\mathcal{T}$ and time-averaging the minimum distance to the edge of a plume in P , which is more intuitive but much slower computationally.

The data are obtained at absolute vertical positions, constant for each Ra value. Consequently, the vertical position relative to the boundary layer thickness varies, as the boundary layer thickness decreases with Ra . In figure 9.4(b) we see that the most probable plume area can be approximated as being constant between $z/L = 10^{-3}$ and 10^{-2} , revealing insensitivity to the vertical position over a substantial range. However, this insensitivity is only for the plume area and not for the plume width. Therefore, performing the analysis at a fixed vertical position introduces an uncertainty that is added to the data. The uncertainty is obtained from the variation of the plume width between $z/L = 0.002$ and 0.004 and is included in the error bar on each data point in figure 9.6(a), where the results of the plume width quantification are shown. The results demonstrate that the scaling of W_P is similar to the scaling of λ_θ . We emphasize that the close similarity of the absolute values is incidental, as the absolute value of W_P depends on c . On the other hand, this shows that $c = 1.2$ is a reasonable value for c . The scaling of W_P agrees approximately with that of λ_θ , which shows that the method used for plume identification provides the expected results and that it is the length of the plumes that gives rise to the deviations from A_c as a characteristic plume area.

9.5 Relation between wind shear and plume emission

The boundary layer of RB convection can conceptually be divided into three regions, namely the *ejecting*, *wind-shearing* and *impacting* regions, as was shown for TC flow [60], which has similar topology. We refer to figure 9.1 for an indication of these regions in RB convection. In the ejecting region, the plumes are emitted from the corresponding boundary layer, whereas in the impacting regions, the descending current and thermal plumes originating from the opposite boundary impact the

Figure 9.7: a) Thinning operation $\mathcal{T}$ indicated by the thin red lines on an arbitrary subset of the domain at $z/L = 0.004$. $\mathcal{T}$ is drawn on P for clarity. We emphasize that $\mathcal{T}$ equals 1 on the red line and 0 elsewhere. b) Distance function $\mathcal{D}$ on the same subset as in (a). The darkness inside the plumes reflects the distance of the location to the edge of the plume in units of λ_θ .

boundary layer under consideration. Between these two regions is the wind-shearing region, where the large-scale wind shear is high and the velocity is predominantly horizontal. In TC flow, Ref. [60] used this classification to rationalize the different boundary layer profiles found in each of these regions. As the ejecting region is defined by the emission of a large number of thermal plumes and the wind-shearing region is defined by the high shear, this classification implies that regions of high shear emit fewer plumes than regions with low shear. This is opposite to what is observed in pressure-driven flows, where it is the high shear that results in bursts of momentum, concentration or temperature being emitted from the boundary layer into the bulk. This effect of plume emission being anticorrelated with large shear will now be quantified using our numerical data. A circle C with diameter $D_c = 0.05 \cdot L\Gamma$ is used as a non-overlapping sliding window in which the mean shear velocity outside a plume $u_{C \setminus P} = \langle \sqrt{u_\phi^2 + u_r^2} \rangle_{C \setminus P}$ and the plume area in that circle, $A_{P \cap C}$, are calculated. The velocity and area are normalized with the free-fall velocity and total area, respectively. For the shear velocity, only the area in the circle outside of the plume is considered, to avoid the contribution that the plume makes to the shear. We focus on the effect of the large-scale flow on the plumes by considering only the shear outside of a plume in the circle average. One of the contributions is the horizontal inflow near the boundary due to continuity. Conditioning $A_{P \cap C}$ on $u_{C \setminus P}$ gives $\langle A_{P \cap C} | u_{C \setminus P} \rangle$ averaged over r , ϕ and t , a quantity that can be used to quantify and study the effect of shear on plume emission. We find that only the amplitude of $\langle A_{P \cap C} | u_{C \setminus P} \rangle$ depends on D_c ; in contrast, the trend does not, as long as $1 \gg D_c/\Gamma \gg 1/(2\text{Nu})$. The analysis is performed on the data at $z/L = 0.002$, which is inside or on the edge of

the viscous boundary layer for the studied $Ra = 10^{10}$ and 10^{11} . At this height, the horizontal velocity can be interpreted as being proportional to the vertical gradient of horizontal velocity, averaged over $0 \leq z/L \leq 0.002$. In figure 9.6(b), the quantity $\langle A_{P \cap C} | u_{C \setminus P} \rangle$ is plotted for these two values of Ra . The trend is clear: Regions of the boundary layer where the large-scale shear is high emit fewer plumes than regions where the shear is low. We emphasize that this analysis only accounts for the emitted plumes; plumes originating from the opposing plate that impact the boundary layer may display different behavior, although we expect the behavior to be similar.

9.6 Summary

In summary, we have studied three-dimensional thermal plumes using their cross-sections with horizontal planes at different heights in a cylindrical RB system. We have shown that the log-normal distribution of the thermal plume areas becomes weakly bimodal at higher vertical locations. This observation, together with the decline in the number of plumes, shows that there is clustering of plumes not only during a transient [138], but also in a statistically stationary state. In addition, the weakly bimodal distribution indicates that plumes either cluster or lose energy while traversing the system. Both these mechanisms result in the number of plumes decreasing with increasing vertical position, an observation noted here and previously [238]. As was used in scaling law derivations [70, 98], the assumption that the width of the plumes close to the plates is determined by the thermal boundary layer thickness is shown to be reasonable. The length of the plumes is not simply determined by the domain size; it originates from the flow structure and from the instability mechanism [236]. The plumes are more likely to be emitted in regions of low shear, an observation used [60] in TC flow to study the transition into turbulence of the boundary layers. The turbulent boundary layer is an important ingredient in the asymptotic scaling laws [54, 55], and our finding supports the classification of different horizontal regions of the boundary layer into ejecting, wind-shearing and impacting regions in RB convection as well. It provides an argument for conceptually dividing the RB cell not only vertically into bulk and boundary layer regions, but also horizontally into the aforementioned three regions. The existence of different boundary layer properties in these regions and their relative sizes can play an important role in understanding the transition to the ultimate regime in RB convection.

Conclusion

The structures, boundary layers and thermal plumes in turbulent Rayleigh-Bénard convection have been numerically studied. In §1 the fitting coefficients for the unifying Grossmann-Lohse theory have been updated using novel data from experiments. The previous coefficients, from 2001 [66], were outdated as new and well established $Nu(Ra,Pr)$ data points have become available. The GL model is an intuitive model, useful for explaining several features of RB convection and successful in predicting large regions of $Nu(Ra,Pr)$ parameter space. As the output Reynolds number of numerics and experiments is arbitrarily defined, an extra $Re(Ra,Pr)$ data point is required for the fit in addition to the four $Nu(Ra,Pr)$ data points already required for the fitting coefficients. Since Re can depend on the definition and the aspect ratio, the transformation properties of the GL equations are discussed in order to show how the GL coefficients can easily be adapted to new Reynolds number data while keeping $Nu(Ra,Pr)$ unchanged. Evaluating the resulting $Nu(Ra,Pr)$ space, it becomes apparent that there is good agreement with most numerical and experimental results. However, more effort is required to improve the predictions at high Pr [148](§1). Inherent to the assumption of the theory that the boundary layer is laminar, separate scaling laws are derived for the ultimate regime [55] and due to the scarcity and quality of data in this unconfirmed regime, they cannot be tested yet.

In order to provide numerical data at high Rayleigh numbers, a novel parallelization of our second-order finite difference scheme [37] has been developed and described in §2. The parallelization consists of a two-dimensional domain decomposition, in contrast with the previous one-dimensional decomposition. The 2D decomposition performs better, as the amount of distributed memory processes are divided over two dimensions instead of only one. This allows for the use of more distributed memory processes before shared memory processes become necessary, increasing performance and versatility. Furthermore, the topology of modern computer clusters can more optimally be utilized with this decomposition, resulting in a communication speedup. Not only the domain composition has been improved, but also the previously implicit time-integration of the viscous terms has been made explicit. This specializes the code for high Ra flows, losing convenience at low Ra . However, efficient and scalable codes are nearly exclusively used for high Ra flows, making manual determination of the maximum timestep at low Ra a negligible problem. The profit of making the integration explicit is that it is local in space. This prevents expensive domain transposes required for non-local integration. These measures, together with several serial optimizations have results in a typical speedup compared to the one-dimensional implicit scheme of a factor of at least 7. In addition, the scaling of the

code has been shown up to 64K cores, with realistic prospects to reach an even higher number.

This scheme is extended in §3 by decoupling the sizes of the grids used for the momentum and scalar fields. High Pr number flows contain, by definition, sharper gradients in the temperature field than in the velocity field [44](§3). Sharp gradients require higher resolution and in case the velocity and temperature have equal resolution, the velocity field will be overresolved. This is wasteful computationally, since imposing continuity on the velocity is the most computationally expensive step in most numerical codes. For high Pr simulations it is immediately apparent that solving the velocity and temperature on different grids, with different resolutions, will result in an increase in computational efficiency. However, it has been shown in this thesis that even for Pr is unity RB convection, the gradients of the temperature field are also sharper. A numerical procedure to simulate low diffusivity scalar turbulence is presented. The method consists of using a grid for the advected scalar with a higher spatial resolution than that of the momentum. A multiple resolution approach is used also in the time integration in order to maintain the stability of the scalars on the finer grid. The method is the more advantageous the less diffusive the scalar is with respect to momentum, i.e. particularly well suited for large Prandtl or Schmidt numbers. But even in the case of equal diffusivities the present procedure gives CPU time and memory occupation savings.

In §4 the aspect ratio dependence of the heat transfer in turbulent two-dimensional Rayleigh-Bénard convection is numerically studied in the regime $0.4 \leq \Gamma \leq 1.25$ for Rayleigh numbers $10^7 \leq Ra \leq 10^9$ and Prandtl numbers $Pr = 0.7$ (gas) and 4.3 (water). $Nu(\Gamma)$ shows a very rich structure with sudden jumps and sharp transitions. We connect these structures to the way the flow organizes itself in the sample and explain why the aspect ratio dependence of Nu is more pronounced for small Pr. Even for fixed Γ different states, with different resulting Nu , can exist despite turbulence, between which the flow can or cannot switch. This is in line with what is observed in other closed turbulent systems [46–50]. In case flow cannot switch, the heat transfer thus depends on the initial conditions. This study is extended in §5, where we consider small aspect ratio cells. At high Ra numbers we find a sharp transition from a low Ra number branch towards a high Ra number branch, due to changes in the flow structure. Subsequently, we show that the influence of the aspect ratio on the heat transport decreases with increasing aspect ratio, although even at very large aspect ratio of $\Gamma \approx 10$ variations up to 2.5% in the heat transport as a function of Γ are observed. Finally, we observe long-lived transients up to at least $Ra = 10^9$, as in certain aspect ratio cells we observe different flow states that are stable for thousands of turnover times. To facilitate this study, an efficient algorithm to store flow state information is developed and presented here.

The effect of various velocity boundary condition on two-dimensional Rayleigh-

Bénard convection is studied and presented in §6. Combinations of no-slip, stress-free and periodic boundary conditions are used on both the sidewalls and the horizontal plates. For the studied Rayleigh numbers Ra between 10^8 and 10^{11} the heat transport is lower for $\Gamma = 0.33$ than for $\Gamma = 1$ in case of no-slip sidewalls. This is, surprisingly, the opposite for stress-free sidewalls, where the heat transport increases for a lower aspect ratio. In wider cells the aspect ratio dependence is observed to disappear for $Ra \geq 10^{10}$. Two distinct flow types with very different dynamics can be seen, mostly dependent on the plate velocity boundary condition, namely roll-like flow and horizontal zonal flow, which have a substantial effect on the dynamics and heat transport in the system [52, 53]. The predominantly horizontal zonal flow suppresses heat flux and is observed for stress-free and asymmetric plates. Low aspect ratio periodic sidewall simulations with a no-slip boundary condition on the plates also exhibit zonal flow. In all the other cases, the flow is roll-like. In two-dimensional Rayleigh-Bénard convection, the velocity boundary conditions thus have large implications on both roll-like and zonal flow that have to be taken into consideration before the boundary conditions are imposed, in sharp contrast with the temperature boundary conditions [41].

Two-dimensional simulations of Rayleigh-Bénard convection at $Ra = 5 \times 10^{10}$ have been used in §7 to show that vertical logarithmic mean temperature profiles can be observed in regions of the boundary layer where thermal plumes are emitted. The profile is logarithmic only in these regions and not in the rest of the boundary layer where it is sheared by the large-scale wind and impacted by plumes. In addition, the logarithmic behavior is not visible in the horizontal average. The findings reveal that the temperature profiles are strongly connected to thermal plume emission and support a perception that parts of the boundary layer can be turbulent, while others are not. The transition to the ultimate regime, in which the boundary layers are considered to be fully turbulent, can therefore be understood as a gradual increases in fraction of the plume-emitting ('turbulent') regions of the boundary layer.

Predominantly two-dimensional simulations were used up to now. To judge the validity of directly extrapolating these results to three-dimensional RB, two-dimensional and three-dimensional Rayleigh-Bénard convection is compared in §8 using results from direct numerical simulations and previous experiments. The explored phase diagrams for both cases are reviewed. The differences and similarities between 2D and 3D are studied using $Nu(Ra)$ for $Pr = 4.38$ and $Pr = 0.7$ and $Nu(Pr)$ for Ra up to 10^8 . In the $Nu(Ra)$ scaling at higher Pr , 2D and 3D are very similar; differing only by a constant factor up to $Ra = 10^{10}$. In contrast, the difference is large at lower Pr , due to the strong roll state dependence of Nu in 2D. The behavior of $Nu(Pr)$ is similar in 2D and 3D at large Pr . However, it differs significantly around $Pr = 1$. The Reynolds number values are consistently higher in 2D and additionally converge at large Pr . Finally, the thermal boundary layer profiles are compared in 2D

and 3D.

Direct numerical simulations of turbulent thermal convection in a $Pr = 0.7$ fluid up to $Ra = 10^{12}$ are used to study the statistics of thermal plumes in §9. At various vertical locations in a cylindrical setup with aspect ratio $\Gamma = \text{width}/\text{height} = 1/3$, plumes are identified and their properties extracted. It is found that plumes are much less likely to be emitted from plate regions with large wind shear. Close to the plates, the plumes have a unimodal log-normal distribution, whereas at more central locations the distribution becomes weakly bimodal, which can be traced back to clustering of the plumes and influence of the large-scale circulation. The number of hot plumes decreases with height. The width of the plumes scales with Ra approximately as Nu^{-1} , indicating that it is determined by the thermal boundary layer thickness.

The GL-theory, updated for RB in §1, has shown good agreement for almost all cases. Only for high Pr flows, a significant deviation from experimental data can be distinguished. This regime requires more attention, since applications in e.g. double diffusive convection, for which the GL-theory can also be used [148], are mostly at high Pr . Furthermore, the GL-theory is utilized in an increasing number of systems. Not only for RB and DDC, but also for vertical natural convection GL-theory can be used [249]. The problem might be due to the assumption of a large-scale wind that is not present for high Pr . This is currently remedied by using $Re = 1$ in the GL-model. However, this is apparently not sufficient. A remaining question regarding GL-theory is in relation to the logarithmic profiles found in §7 in the classical regime and the deviations from a laminar profile previously observed [43, 215, 216]. Since the contribution to the global dissipation rates are modeled distinctively to bulk and boundary layer contributions, with their respective scalings obtained from homogeneous isotropic turbulence and laminar Prandtl-Blasius theory [35, 70, 88, 212, 213], it remains unknown why the GL-theory works so well. Even though the boundary layer deviates strongly from the PB profile in regions with high heat flux and substantial parts of the bulk are not homogeneous, the GL-theory can predict $Nu(Ra, Pr)$ in the classical regime. A possible answer is that the contribution of the logarithmic boundary layer in the plume ejecting regions to the total dissipation can still be broken into the contributions of a HIT bulk and a laminar BL. The GL-theory incorporates this simply in the fitting coefficients.

The development of the numerical code presented in §2 and §3 will be continued. The code is open-sourced, which allows the contribution of not only our developer, but the entire bounded fluid dynamics community. The scaling of the code is sufficient for contemporary compute clusters, and will remain so for at least the next three years. By then, it is estimated that an increase in CPU to memory bandwidth, a decrease in communication time and/or utilization of GPUs is required to prepare for future compute clusters. Currently, various modules are implemented on the base, single-phase, scheme. The multiple resolution scheme, immersed boundary methods

and multiphase models are being implemented by virtue of the flexibility of the code.

Improved numerical methods are required to reach the arguably elusive ultimate regime in RB. In the analogous system of TC [243], the ultimate regime has been confirmed by reaching it experimentally and numerically [60, 250]. The reason why it is more difficult in RB is that the driving is less efficient. In RB the system is driven indirectly by accelerating thermal plumes, while in TC the driving is directly into the boundary layer. A more elaborate study could reveal that the logarithmic profiles in plume ejecting regions of the boundary layer are sign of the ultimate regime. It is expected that the horizontal extent of these regions grow until the ultimate regime is reached, in which the complete boundary layer is turbulent. One may wonder how this 'plume-driven' perspective on the ultimate regime is reconciled with the 'shear-driven' perspective [35], in which it is assumed that the boundary layer transitions to a turbulent one once the large-scale shear exceeds a threshold shear Reynolds number.

The work on multiple stable states, with or without an effect on global properties, has been collectively continued in other bounded systems. Recently, they have been observed in highly turbulent Taylor-Couette flow [251]. Without a doubt, they have a profound effect on our perspective on turbulence in bounded systems and their existence is surprising. However, great care must be taken when using the ambiguous statement of 'multiple turbulent states'. It can be interpreted that there are multiple states of turbulence, more specifically HIT, which is completely unsupported. A better formulation is 'multiple states despite turbulence', which is closer to the actual observation. Surprisingly there are multiple states, regardless of the strong fluctuations in the system.

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Summary

A numerical study of the structures, boundary layers and thermal plumes in Rayleigh-Bénard convection, a fluid heated from below and cooled from above, is presented. The concepts of RB convection are explained using the GL-theory. Its fitting coefficients, used to obtain a $Nu(Ra, Pr)$ prediction, have been updated using novel experimental data. Here, Nu is the heat flux, Ra the driving of the system and Pr a property of the fluid. It is shown that the new fitting coefficients provide accurate predictions in large regions of the parameter space. A novel parallelization of the numerical scheme used is developed and described. It comprises a two-dimensional domain decomposition and uses an explicit time-integration of the viscous terms to obtain a shown scaling of up to 64000 cores. The code has been open-sourced and is currently actively extended and optimized by several developers. One of the available modules is using different resolutions for the momentum and temperature fields. This is shown to be beneficial not only for high Pr fluids, but also for Pr unity fluids sharper gradients are found in the temperature field as compared to the momentum field. As using multiple resolutions prevents overresolving the momentum field to capture the sharp gradients in the temperature, huge savings in computational effort can be obtained. In order to efficiently scan parameter space, two-dimensional RB simulations have been used to study the effect of flow structures on the heat flux. It has been found that different states, which exist despite strong turbulence, can result in different global properties such as the heat flux. This has been shown for low aspect ratios, where the roll states are vertically stacked, and for high aspect ratio, where the rolls are horizontally arranged. In both cases, jumps in the heat flux coincide with a change in the number of rolls in the system. In addition, more complex roll states that do not fill the complete system are found to exist and affect the heat flux. These phenomena are only found for RB systems that are bounded horizontally, prompting a study of the effect of the velocity boundary conditions on RB convection. This study revealed that unlike the temperature boundary conditions, the velocity boundary conditions have a profound effect on the flow topology and the heat flux. In addition to large differences in absolute heat flux, zonal flows can emerge that completely suppress the heat flux for extended periods of time. The common perspective is that RB convection is horizontally homogeneous. This has been used in numerous scaling theories, where the boundary layer is considered to be either laminar or turbulent. It has been shown in two-dimensional RB convection, that the boundary layer shows features of both a laminar and a turbulent profile in the classical regime, depending on the ejection of plumes. Ejecting thermal plumes can result in a locally turbulent boundary layer. This observation provides hints on the transition to the ultimate regime of RB con-

vection. It can be conjectured that this region of turbulence can grow until it fully covers the horizontal extent of the system. It is at this point that the ultimate regime is reached. A comparison of two -and three-dimensional RB convection has revealed for which parameters 2D RB can be used directly as a model for 3D RB. It is at low Pr where the largest differences occur. In a cylindrical domain at high Ra , the statistics of plume emission have been studied using image analysis, where it has become apparent that the location of plume emission is dependent on the large-scale wind and that the plumes cluster while traversing the system.

Samenvatting

In deze thesis is een numeriek onderzoek naar de structuren, grenslagen en thermische pluimen in Rayleigh-Bénard (RB) convectie, een fluïdum verwarmd van onder en gekoeld van boven, gepresenteerd. De concepten van RB convectie zijn uitgelegd met gebruik van de Grossman-Lohse theorie. De fit coëfficiënten, die gebruikt worden in een $Nu(Ra, Pr)$ voorspellingen, zijn vernieuwd op basis van nieuwe experimentele data. Hier is Nu de warmteoverdracht, Ra de aandrijving van het systeem en Pr een eigenschap van het fluïdum. Het is gebleken dat de nieuwe coëfficiënten een nauwkeurige voorspelling geven in grote delen van de parameter ruimte. Een gemoderniseerde versie van de parallellisatie van het numerieke model is ontwikkeld en beschreven. Deze bestaat uit een tweedimensionale domein verdeling en gebruikt een expliciete tijds-integratie van de viskeuze termen om een schaling tot 64000 processoren te bereiken. De code is openbaar gemaakt en wordt momenteel actief ontwikkeld en geoptimaliseerd door verschillende ontwikkelaars. Eén van de mogelijke modules is het gebruik van verschillende resoluties voor het snelheids- en temperatuursveld. Het is aangetoond dat dit voordelig is voor niet alleen hoge Pr vloeistoffen, maar ook voor vloeistoffen met $Pr = 1$, waar temperatuursgradiënten gevonden zijn die steiler zijn dan de snelheidsgradiënten. Grote besparingen in computationele inspanning kunnen behaald worden, omdat het gebruik van meerdere resoluties het teveel oplossen van het snelheidsveld voorkomt. Tweedimensionale simulaties, waarmee de parameter ruimte efficiënt gescand kan worden, zijn gebruikt voor het onderzoeken van het effect van stromingsstructuren op de warmteoverdracht. Verschillende toestanden bestaan ondanks sterke turbulentie die verschillende globale eigenschappen, zoals de warmteoverdracht, tot gevolg hebben. Deze zijn gevonden voor lage aspectverhoudingen, waar de roltoestanden verticaal gestapeld zijn, en voor hoge aspectverhoudingen, waar de rollen horizontaal uitgelijnd zijn. Sprongen in de warmteoverdracht die samenvallen met een verandering in het aantal rollen zijn waargenomen in beide gebieden. Ook zijn er complexere roltoestanden gevonden die niet het hele systeem vullen maar wel een invloed hebben op de warmteoverdracht. Deze verschijnselen zijn alleen gevonden voor RB systemen die horizontaal begrenst zijn; een observatie die geleid heeft naar een onderzoek naar het effect van de snelheidsrandvoorwaarden op RB convectie. Dit onderzoek heeft onthuld dat, anders dan de temperatuursrandvoorwaarden, de snelheidsrandvoorwaarden een diepgaand effect hebben op de stromingstopologie en de warmteoverdracht. Naast grote verschillen in warmteoverdracht, kunnen er ook zonale stromingen ontstaan die de warmteoverdracht voor lange periodes volledig kunnen onderdrukken. Een veel voorkomende kijk is dat RB convectie homogeen is in horizontale richting. Dit is gebruikt in vele

schalingstheorieën, waar wordt aangenomen dat de grenslaag of laminair of turbulent is. Het is echter aangetoond in tweedimensionale RB convectie dat de grenslaag beide laminaire en turbulente kenmerken heeft in het klassieke regime, afhankelijk van de emissie van thermische pluimen. Op de locaties van pluimen kan er een lokale turbulente grenslaag aanwezig zijn. Deze observatie geeft informatie over de transitie naar het ultieme regime in RB convectie. Een conjectuur is dat de breedte van het domein van de turbulente grenslaag groeit totdat het de volledige horizontale breedte van het systeem beslaat. Op dit punt zal dan het ultieme regime bereikt zijn. Een vergelijking van twee -en driedimensionale Rb convectie heeft onthuld voor welke parameters 2D RB gebruikt kan worden als model voor 3D RB. Voor lage Pr zijn de grootste verschillen aanwezig. In een cilindrisch systeem bij hoge Ra zijn de statistieken van de pluimemissie onderzocht met gebruik van beeldanalyse, waar het duidelijk is geworden dat de locatie van pluimemissie afhankelijk is van de wind op grote schaal en dat de pluimen clusteren terwijl ze door het systeem bewegen.

Scientific output

Publications in refereed journals

- E.P. van der Poel, R.J.A.M. Stevens, D. Lohse. *Connecting flow structures and heat flux in turbulent Rayleigh-Bénard convection* Physical Review E Rapid Communication, **84**, (4) 045303. (2011) – see §4.
- E.P. van der Poel, K. Sugiyama, R.J.A.M. Stevens, D. Lohse. *Flow states in two-dimensional Rayleigh-Bénard convection as a function of aspect ratio and Rayleigh number* Physics of Fluids, **24**, (8) 085104. (2012) – see §5.
- R.J.A.M. Stevens, E.P. van der Poel, S. Grossmann, D. Lohse. *The unifying theory of scaling in thermal convection: The updated prefactors* Journal of Fluid Mechanics, **736**, 177–194. (2013) – see §1.
- E.P. van der Poel, R. J. A. M. Stevens and D. Lohse. *Comparison between two and three dimensional Rayleigh-Bénard convection* Journal of Fluid Mechanics, **736**, 177–194. (2013) – see §8.
- R. Ostilla-Mónico, E. P. van der Poel, R. Verzicco, S. Grossmann, D. Lohse. *Boundary layer dynamics at the transition between the classical and the ultimate regime of Taylor-Couette flow.* Physics of Fluids, **26**, 015114. (2014).
- R. Ostilla-Mónico, E. P. van der Poel, R. Verzicco, S. Grossmann, D. Lohse. *Exploring the phase diagram of fully turbulent Taylor-Couette flow.* Journal of Fluid Mechanics, **761**, 1–26. (2014).
- E. P. van der Poel, R. Ostilla-Mónico, R. Verzicco, D. Lohse. *Effect of velocity boundary conditions on the heat transfer and flow topology in two-dimensional Rayleigh-Bénard convection.* Physical Review E, **90**, 013017. (2014) – see §6.
- Y. Yang, E. P. van der Poel, R. Ostilla-Mónico, C. Sun, R. Verzicco, S. Grossmann, D. Lohse. *Salinity transfer in bounded double diffusive convection* Journal of Fluid Mechanics **768**, 476–491. (2015)
- E.P. van der Poel, R. Verzicco, S. Grossmann, D. Lohse. *Plume emission statistics in turbulent Rayleigh-Bénard convection* Journal of Fluid Mechanics **772**, 5–15. (2015) – see §9.

- E. P. van der Poel, R. Ostilla-Mónico, J. Donners and R. Verzicco. *A pencil distributed code for strongly turbulent wall-bounded flows* Computers and Fluids, **116**, 10–16. (2015) – see §2.

Publications under review

- R. Ostilla-Mónico, E. P. van der Poel, R. P. J. Kunnen, R. Verzicco, D. Lohse. *Geostrophic convective turbulence: The effect of boundary layers*.
- Y. Yang, R. Ostilla-Mónico, E. P. van der Poel, D. Lohse and R. Verzicco *A multiple-resolution strategy for Direct Numerical Simulation of scalar turbulence*. – see §3.
- E.P. van der Poel, R. Ostilla-Mónico, R. Verzicco, S. Grossmann, D. Lohse, *Logarithmic mean temperature profiles and their connection to plume emissions in turbulent Rayleigh-Bénard convection*. – see §7.

Contributed talks

- *2D Rayleigh-Bénard aspect-ratio dependencies*. Drop meeting, Delft NL, 2011.
- *Connecting flow structures and heat flux in turbulent Rayleigh-Bénard convection*. APS DFD, Baltimore USA, 2011.
- *Multiple states in 2D Rayleigh-Bénard convection*. PoF seminar, Enschede NL, 2012.
- *Connecting flow structures and heat flux in turbulent Rayleigh-Bénard convection*. PoF seminar, Enschede NL, 2012.
- *Multiple states in 2D Rayleigh-Bénard convection*. JMBC turbulence meeting, Groningen NL, 2012.
- *Comparison between 2D and 3D Rayleigh-Bénard convection*. DROP meeting, Eindhoven NL, 2012.
- *Comparison between 2D and 3D Rayleigh-Bénard convection*. APS DFD, San Diego USA, 2012.
- *Temperature log-layers in the classical regime*. RBC, Hong-Kong CH, 2012.
- *Simulations of turbulent closed systems*. SURFsara Superday, Amsterdam NL, 2012.
- *Why did we win the Wim Nieuwpoort award?* PoF Journal Club, Enschede NL, 2013.

- *Rayleigh-Bénard simulations at high Ra.* SIAM GS, Padova IT, 2013 *invited*.
- *Rayleigh-Bénard simulations at high Ra.* APS DFD, Pittsburgh USA, 2013.
- *Large scale DNS of Rayleigh-Bénard convection.* RB meeting, Münster DE, 2014 *invited*.
- *Plume morphology in Rayleigh-Bénard convection.* Burgersday, Delft NL, 2014.
- *Plume emission statistics in Rayleigh-Bénard convection.* APS DFD, San Francisco USA, 2014.

Poster sessions

- ETC13 2011. Erwin P. van der Poel, Richard J.A.M. Stevens, D. Lohse. *Connecting flow structures and heat flux in turbulent Rayleigh-Bénard convection.*
- Physics@FOM 2012. Erwin P. van der Poel, Rodolfo Ostilla Mnico, Roberto Verzicco, Siegfried Grossmann, Detlef Lohse. *Ultimate Rayleigh-Bénard and Taylor-Couette turbulence.*
- Physics@FOM 2013. Erwin P. van der Poel, Rodolfo Ostilla Mnico, Roberto Verzicco, Siegfried Grossmann, Detlef Lohse. *Ultimate Rayleigh-Bénard and Taylor-Couette turbulence.*
- MESA+ day 2013. Erwin P. van der Poel, Rodolfo Ostilla Mnico, Roberto Verzicco, Siegfried Grossmann, Detlef Lohse. *Ultimate Rayleigh-Bénard and Taylor-Couette turbulence.*
- Physics@FOM 2014. Erwin P. van der Poel, Rodolfo Ostilla Mnico, Roberto Verzicco, Siegfried Grossmann, Detlef Lohse. *Ultimate Rayleigh-Bénard and Taylor-Couette turbulence.*
- Physics@FOM 2014. Yantao Yang, Erwin P. van der Poel, Rodolfo Ostilla Mnico, Roberto Verzicco, Siegfried Grossmann, Detlef Lohse. *Salinity transfer in double-diffusive convection.*
- Physics@FOM 2015. Vamsi Spandan Arza, Yantao Yang, Erwin P. van der Poel, Rodolfo Ostilla Mnico, John Donners, Detlef Lohse, Roberto Verzicco. *A multipurpose and versatile tool for turbulence simulations.*

Supervised MSc projects

- Dennis Bakhuis, *Effects of boundary variations on Rayleigh-Bénard convection*.
- Matthijs Neut, *Spherical body orientation extraction and Rayleigh-Bénard convection*.

Other

- Wim Nieuwpoort award 2012 for most efficient use of High Performance Computing in the Netherlands.
- Refereed 15 manuscripts for the Journal of Fluid Mechanics.
- Produced visualizations featured at FLOW 2014, APS 2014, SC 2013, PRACE 2014, 'Het Klokhuis' and the VisIt gallery.
- Teaching assistant for the master course on Turbulence twice.

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About the author

Erwin Paul van der Poel was born in Lisse, The Netherlands, on April 15, 1986. He moved to Haaksbergen after elementary school and attended ‘Het Assink Lyceum’ where he received his high school diploma. He received his bachelor degree in Applied Physics in 2009 at the Saxion University of Applied Sciences, where he did his internship at PANalytical B.V. in Almelo and graduated at the TCCB group at the University of Twente. Afterwards, he co-founded the company Immend for which he has been working continuously. In 2011, he obtained his master degree with honors working on turbulent Rayleigh-Bénard convection in the Physics of Fluids group. This work was continued during his PhD under the supervision of Prof. Detlef Lohse and Prof. Roberto Verzicco.