SHEARED RAYLEIGH-BÉNARD TURBULENCE

Alexander Georg Emanuel Blass

Sheared Rayleigh-Bénard Turbulence

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Volume rendering of a direct numerical simulation of sheared Rayleigh-Bénard turbulence, see figure 4.1.

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SHEARED RAYLEIGH-BÉNARD TURBULENCE

DISSERTATION

to obtain
the degree of doctor at the University of Twente,
on the authority of the rector magnificus,
Prof. Dr. T. T. M. Palstra,
on account of the decision of the graduation committee,
to be publicly defended
on Thursday, September 10th, 2020 at 16:45

by

Alexander Georg Emanuel Blass
Born on January 2nd, 1990
in Wiesbaden, Germany

This dissertation has been approved by the promotor:

Prof. Dr. rer. nat. D. Lohse

and

Prof. Dr. R. Verzicco

and the co-supervisor:

Dr. R. J. A. M. Stevens

To my parents, Erika and Heinrich.

In light of current events

The defense of this dissertation was originally scheduled for May 29th this year but had to be rescheduled due to the COVID-19 pandemic. Over the last few months, many people have been infected and countries had to shut down all non-essential activities. After the situation started to look slightly more stable, the university was able to offer me a new date for my defense. But as the near future is very unpredictable, even now while writing this paragraph it is uncertain if it will be possible to defend my dissertation as currently planned.

The pandemic has underlined the fateful importance for our future to enhance our knowledge about different turbulent flows and also their ability to spread virulent droplets. COVID-19 has made it evident to everyone that fundamental research is vital to better understand the world we live in. In the Physics of Fluids group at the University of Twente such state-of-the-art research is being conducted every day under the leadership of Professor Detlef Lohse, whose scientific qualifications are acknowledged worldwide and now are all the more in demand by our society. It was a great privilege for me to do research in this group.

*Alexander Blass
August 2020*

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Introduction

Preface

Dear reader, you have just started to read my dissertation on *Sheared Rayleigh-Bénard Turbulence* and I would like to thank you for your interest in my work as a PhD student at the University of Twente in the Netherlands. You might have heard of terms like *turbulence* or *thermal convection* before, but I would like to spend the next few pages on giving you an introduction to the very basic fundamental concepts, on which my doctoral work is based. In the spirit of text flow, I will abstain from adding literature references within the introduction. If you want to further broaden your knowledge after reading the following pages, I would like to offer you references to these works in literature: [1–27].

Now with no further ado, let's get into it.

Turbulence

When introducing turbulence, the chaotic behavior of interacting structures of larger and smaller scale, very often Leonardo da Vinci comes to mind. In his drawing of a jet of water entering a larger body of water (figure 1a), which is dated to the 16th century, one can already find a very detailed depiction of the many different length scales that make turbulent flow so intriguing and at the same time so hard to resolve. In the early 19th century, Japanese artist Katsushika Hokusai created a woodblock print of a large wave which is about to break over three fishing boats (figure 1b). While this may of course be an unfortunate situation for the fishermen, it is intriguing how much focus the artist laid on the wave crest and the formation of small-scale turbulent structures. It is fascinating how such a well known phenomenon like turbulence is still not fully understood. But more about the flow physics later in this chapter. The word turbulence very likely has its origin in the Latin word *turba*, which in

Figure 1: (a) Drawing of Leonardo da Vinci [1]. Many different length scales can be observed in this very detailed drawing of turbulent flow. (b) *The Great Wave off Kanagawa* by Katsushika Hokusai [2]. A great detail of different structure sizes can be observed at the crest of the great wave.

combination with the ending *-ulentus* basically stands for *full of disturbance*. Nowadays this is very easy to believe thinking of all the ‘disturbance’ that passengers have to endure during a turbulent flight, when the pilot instructs to fasten the seat belts to prevent getting catapulted out of the seat when the plane falls a few meters while passing through heavy clear air turbulence.

The first question that comes to mind when studying turbulence is: *How can it be defined*. Indeed it is not easy to find an exact definition. Many great minds of the last century have tried to solve what Richard Feynman called ‘the most important unsolved problem in classical physics’. Commonly, the study of turbulence is described as the analysis of flow patterns that appear random, non-deterministic and chaotic. Turbulent flow can be quantified by a dimensionless parameter which was introduced through the work of Osborne Reynolds (1842–1912) and now carries his name as the Reynolds number. It stands for the ratio of inertial forces and viscous forces. Here, an inertial force can be imagined analogous to the velocity of a mass and the concomitant viscous force as the resistance of the surrounding fluid against the motion of the mass. The flow is laminar if this ratio is small and becomes turbulent only once a certain critical value ($Re \gg 1$) is passed. The Reynolds number is defined as

$$Re = \frac{\text{inertial forcing}}{\text{viscous forcing}} = \frac{U_c L_c}{\nu}. \quad (1)$$

Here, U_c is a characteristic velocity, L_c a characteristic length and ν the viscosity of the fluid. The choice of typical scales depends on the specific problem at hand, but later in this introduction there will be some more specific examples.

The definition of turbulence might sound very abstract, but turbulence happens plenty in our daily life. For example when you open a faucet to its maximum, you will notice that the water, which originally was floating into your sink in a *laminar* flow state, now will make a more unsettled and chaotic impression, which can be described as *turbulent*. While your faucet might not necessarily have a larger impact to our life, turbulence also impacts us on a much larger scale. Air and maritime traffic are heavily impacted by turbulent flow structures in air and water as well, but let’s try to think even larger. Strong currents such as the North Atlantic Gyre (an ocean circulation in the Atlantic Ocean, which includes the Gulf Stream) play a major role to our climate system (figure 2a) and so does also the atmospheric circulation (figure 2b) and on an even larger scale, even the Sun’s atmosphere is highly turbulent (figure 2c).

Figure 2: Visualization of (a) ocean surface temperatures [8] and (b) aerosols in the air [10]. (c) Picture of the solar atmosphere [11] and (d) three-color composite picture of the Crab Nebula [12].

With today's technology it is possible to push forward into incredible new domains of imagination and push for a deeper understanding of life as we know it. Even the very turbulent Crab Nebula as part of the Taurus constellation, which was first discovered by John Bevis in 1731 at a distance of about 5,000–8,000 light years away from Earth, can be visualized showing its large-scale magnetic field and high-energy electrons getting ejected by a spinning neutron star in its center (figure 2d).

Natural convection

Most of the previously mentioned and also commonly known examples of turbulence have something particular in common. The flow is driven by a difference in density that wants to be balanced. This can either be caused by a dissimilarity in temperature or concentration. Imagine a pot of water that you place on a stove to heat it up or an electric kettle (figure 3a). If the temperature difference between the water and the hot bottom plate is only marginal, the heat will only slowly diffuse through the system. If the difference in heat is higher than some critical value, convection rolls will develop where the hot, lighter fluid combines to thermal plumes and rises up until it cools down. At that point it will increase its density and sink down until it heats up again. The water in this case will heat up much faster than from pure diffusion since the convection causes mixing through large-scale circulation which drives the flow and therefore distributes the heat much more effectively. On a larger scale, convection cells are responsible for huge weather structures around our planet (figure 3b). Air gets heated up close to the equator, rises and then moves towards the poles while cooling down. This phenomenon spans over multiple distinct circulation cells, called Hadley, Ferrel, and Polar cells. Below the surface in the Earth's mantle, large thermal plumes support the so called mantle convection (figure 3c), carrying heat from the Earth's core towards the crust causing volcanic eruptions and tectonic activity. Not only planets like Earth are driven by convection. Even stars like the Sun have a convection zone where plasma is transported to the surface cooling down from $2,000,000^{\circ}\text{C}$ to about $5,500^{\circ}\text{C}$ (figure 3d).

Figure 3: (a) Picture of water boiling in an electric kettle [15]. (b) Visualization of atmospheric cells [16] and (c) simulations of mantle convection on Earth [18]. (d) Illustration of the convection zones within a Sun-like star [20].

Figure 4: Side view of the thermal structures from a three-dimensional numerical simulation of Rayleigh-Bénard convection, where a large-scale circulation is formed between hot, denser fluid raising up and cool, lighter fluid falling down [27].

Rayleigh-Bénard convection

In this dissertation, I want to further investigate thermal convection. For this a canonical system in flow physics, called Rayleigh-Bénard convection, is used. It is defined as the flow confined between a hot plate on the bottom and a cold plate on top (figure 4). This is a system of unstable stratification, which creates turbulent flow, if the temperature difference between bottom and top plates is large enough. It is based on the work of Henri Bénard (1874–1939) and John William Strutt (1842–1919), whom we better know as Lord Rayleigh. Bénard created the first experimental setup. It is a mathematically well defined system, necessary boundary conditions are numerically easy to implement, and energy balances between global input and output hold, because the system is closed. Using this, turbulent flows can be studied from a very fundamental aspect while achieving realistic flow behavior.

Governing equations

Rayleigh-Bénard flow is governed by two dimensionless control parameters. The Rayleigh number quantifies the strength of the thermal forcing of the system. It is defined as

$$Ra = \beta g H^3 \Delta / (\kappa \nu), \quad (2)$$

where β is the thermal expansion coefficient, g the gravitational acceleration, H the distance between the plates, and $\Delta = T_{bottom} - T_{top}$ the temperature difference between the plates. κ is the thermal diffusivity and ν the kinematic viscosity, also called momentum diffusivity of the fluid. The Prandtl number depends only on the properties of the fluid between the plates:

$$Pr = \nu / \kappa. \quad (3)$$

The box size of a simulation is defined by the aspect ratio:

$$\Gamma = L / H, \quad (4)$$

with L the horizontal length of the plates.

In this work the commonly used Oberbeck-Boussinesq approximations are applied, which assume that the fluid density ρ depends only linearly on the temperature T in the buoyancy term and that material properties of the fluid, such as β , κ , and ν do not depend on the temperature at all. The flow is mathematically defined by the Navier-Stokes equations. They read:

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla P + \left(\frac{Pr}{Ra} \right)^{1/2} \nabla^2 \mathbf{u} + \theta \hat{z}, \quad \nabla \cdot \mathbf{u} = 0, \quad (5)$$

$$\frac{\partial \theta}{\partial t} + \mathbf{u} \cdot \nabla \theta = \frac{1}{(RaPr)^{1/2}} \nabla^2 \theta. \quad (6)$$

Here, $\mathbf{u} = u(x, y, z)$ is the velocity normalized by $\sqrt{g\beta\Delta H}$, t the time normalized by $\sqrt{H/(g\beta\Delta)}$, θ the temperature normalized by Δ and P the kinematic pressure normalized by $g\beta\Delta H$. All quantities are now dimensionless.

The most important output parameter of the flow is the Nusselt number Nu , which is a non-dimensional expression of the heat transfer between the plates:

$$Nu = QH/(\kappa\Delta). \quad (7)$$

$Q = \overline{w'T'} - \kappa\partial T/\partial z$ is the constant vertical heat flux, w' the velocity fluctuations in wall-normal direction, T' the temperature fluctuations.

Boundary layers

For turbulent wall bounded flows such as classical Rayleigh-Bénard convection, the flow can be divided into two different regions: The bulk and the boundary layers. Most of the flow lies in the bulk region where the flow does not directly feel the effect of the wall. Only the flow very close to the plates is part of the boundary layers. Here, it becomes important that a fluid must adhere to the wall and the velocity must be continuous at the interface. For pure Rayleigh-Bénard convection, these are the applied temperature at the plates and a velocity of zero and thus a thermal and a viscous (kinetic) boundary layer emerge. The boundary layers are of special interest for us, since they are responsible for most of the heat transfer between the plates. In proximity of a wall, the heat transfer experiences the most resistance and therefore the boundary layer dynamics strongly impact the Nusselt number. Due to their small thickness, boundary layers are very demanding to resolve. In numerical simulations it needs to be ensured that enough grid points lie within the boundary layer and in experiments measurements boundary layers can easily become as thin as a very small fraction of the cell height H . This can easily be in the order of only millimeters with experimental setups in the order of meters. The boundary layer thickness does not only depend on the previously described flow input parameters, but locally also on the flow structures. For instance a plume impacting at the wall will have a different footprint than an emitting one.

Guide through thesis

In the foregoing sections some very basic terminology was introduced. This is now followed by six scientific chapters, each with its own more detailed introduction. In the first part, the focus will lie on pure large-scale Rayleigh-Bénard convection and the existence of superstructures will be discussed. Most experiments and numerical simulations have been focusing on rather small aspect ratios to be able to resolve very large Rayleigh numbers. In pursuit of achieving turbulent flows with higher and higher thermal forcing, researchers often resort to very limited aspect ratios to keep the flow resolution feasible. Vice versa, since many natural instances of convection are linked to very large aspect ratios, studying very large flow patterns significantly restricts the realizable Rayleigh number. There is not much insight yet into the actual development of large thermal structures at high Ra and until recent years it was not quite clear if the large-scale structures will wash out if the thermal forcing becomes too high or if they will survive as so called superstructures. In chapter 1, simulations of very large aspect ratios at high Rayleigh number are presented and the existence of superstructures with the size of 6–7 times the distance between the plates is discussed. Using the same data, the superstructures were then further analyzed by employing a specific averaging technique, which isolates the large-scale structures in the flow field (chapter 2). This way important flow quantities, such as heat transport and shear stress at the wall, can be studied as well as the behavior of the boundary layers along the large-scale wind.

The second part of this dissertation explores the emergence of large-scale structures in mixed convection. Here, first the similarities between pressure (Poiseuille) and wall driven (Couette) flows with added unstable stratification are discussed in chapter 3. Afterwards the numerical simulations are extended to sheared Rayleigh-Bénard turbulence, where a Couette-type wall shearing is added to the unstably stratified flow. A wide variety of different combinations of thermal and shear forcing is presented in chapter 4. Different flow structures, which can be linked to real life phenomena, appear while the flow undergoes a transition between a regime where the thermal forcing from the temperature difference between the plates is dominant and a regime where the shear forcing induced by the walls is the superior driving of the convection. In chapter 5 the numerical dataset is extended to a variation in the Prandtl number. While the previous data assumed $Pr = 1$, now also different flow properties are considered, which can have a significant impact on the effect of the applied

thermal and shear forcing.

To better understand the behavior of large-scale structures and their interaction with smaller scales closer to the plates, it is vital to have the possibility to also visually observe the different structures that were found in the numerical data. Due to the extremely large resolution required for the simulations that have been performed for this dissertation, three-dimensional visualization of flow structures becomes nontrivial due to the sheer size of the flow fields. It is therefore necessary to perform such visualization remotely on a computing cluster, similar to the simulations themselves. In chapter 6 different visualization techniques are discussed, which also resulted in the cover of this dissertation.

Turbulent thermal superstructures in Rayleigh-Bénard convection*

We report the observation of superstructures, i.e. very large-scale and long living coherent structures in highly turbulent Rayleigh-Bénard convection up to Rayleigh $Ra = 10^9$. We perform direct numerical simulations in horizontally periodic domains with aspect ratios up to $\Gamma = 128$. In the considered Ra number regime the thermal superstructures have a horizontal extend of 6–7 times the height of the domain and their size is independent of Ra . In the last 20 years, laboratory experiments and numerical simulations have focused on small aspect ratio cells in order to achieve the highest possible Ra . However, here we show that also for very high Ra integral quantities such as the Nusselt and volume averaged Reynolds number only converge to the large aspect ratio limit around $\Gamma \approx 4$, while horizontally averaged statistics such as standard deviation and kurtosis converge around $\Gamma \approx 8$, and the integral scale converges around $\Gamma \approx 32$, and the peak position of the temperature variance and turbulent kinetic energy spectra only around $\Gamma \approx 64$.

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1.1 Introduction

Turbulence is characterized by chaotic, vigorous fluctuations. Therefore it is surprising to observe very large-scale coherent structures in turbulent flows such as channel [28, 29], pipe [30], or turbulent boundary layer flows [31–33]. To observe these superstructures (figure 1.1), very large experimental or numerical domains are necessary. So far, superstructures have been observed in pressure and shear driven turbulent flows. However, up to now they have not been reported in highly turbulent thermally driven turbulence, where a preferred flow direction is absent, reflected in the community’s focus on experiments and simulations in small aspect ratio cells. Here we study thermal superstructures, defined as the largest horizontal flow scales that develop, such that their flow characteristics, size, and shape are independent of the system geometry, in highly turbulent thermal convection. So, even though the large-scale circulation (LSC) observed at very high Ra in $\Gamma \sim 0.5$ – 1.0 cells is a fascinating feature of flow organization [26, 34–37], such a LSC in a confined cell is not a thermal superstructure according to our definition since the geometrical and dynamical features depend on the system geometry.

The most popular model of thermal convection is Rayleigh–Bénard (RB) flow [26, 37–40], where the dimensionless control parameters are the Rayleigh (Ra) and Prandtl (Pr) numbers, parameterizing the dimensionless temperature difference and the fluid properties. Major advances have been achieved in the last few decades in theoretically understanding the global transfer properties of the flow. Namely, the unifying theory of thermal convection [41–43] describes the Nusselt Nu (dimensionless heat transport) and Reynolds Re number (dimensionless flow strength) dependence on Ra and Pr well. In addition, experiments and simulations agree excellently up to $Ra \sim 10^{11}$ due to major developments in experimental and numerical techniques [26, 37, 39, 40].

However, the effect of the third dimensionless quantity, the aspect ratio $\Gamma = W/H$, where W is the cell’s width and H its height, is much less understood. According to the classical view, strong turbulence fluctuations at high Ra should ensure that the effect of the geometry is minimal as the entire phase space is explored statistically by the flow [44, 45]. This view would justify the use of small aspect ratio domains, which massively reduces the experimental or numerical cost to reach the high Ra number regime relevant for industrial applications and astrophysical and geophysical phenomena, while maintaining the essential physics. Therefore, in a quest to study RB convection at ever

increasing Ra , most experiments and simulations have focused on relatively small aspect ratio. Many studies have been performed for $\Gamma \lesssim 2$, while very high Ra number cases are even limited to $\Gamma \sim 0.2\text{--}0.5$. This approach allowed the discovery of the ultimate regime of thermal convection [46], already predicted by Kraichnan in 1962 [47] and later by Grossmann and Lohse [48].

Although heat transfer in industrial applications takes place in confined systems, the aspect ratio in many natural instances of convection is extremely large [26, 37, 39, 40]. Very large flow patterns have, for example, been observed in moist convection simulations [49–51], high Ra number non-penetrative convection [52], and in plane Couette [53, 54] at low Re . For RB convection just above onset of convection, experiments [55–61] and simulations in large periodic [62–65] and in very large aspect cylindrical [66–72] domains have revealed beautiful flow patterns [73–75]. Correlations between single point measurements [57, 61] and PIV measurements at high Ra [58] have shown a transition between a single and multi-roll structure when Γ exceeds roughly 4, while simulations at $\Gamma = 6.3$ and $Ra = 9.6 \times 10^7$ [72] observed that large regions of warm rising and cold sinking fluid are still present. Previously, Ref. [62, 64] showed with simulations from onset up to $Ra = 10^7$ and for aspect ratios up to 20 that the size of the largest flow structures increases with increasing Ra . These simulation results agree well with the classical experiments performed by Fitzjarrald [55] in rectangular containers. In addition, Ref. [62, 64] found that at $Ra = 10^5$ and 10^6 the size of thermal superstructures peaks at *intermediate* Pr . Furthermore, Ref. [63] presented the emergence of large-scale flow patterns up to $Ra = 10^7$ and $\Gamma = 2\pi$. Later, Ref. [65] showed in simulations with aspect ratios up to 12π that, after an initial growth period, the size of thermal superstructures becomes constant as function of time.

There is no clear insight into the development of thermal superstructures at higher Ra . However, at larger Ra the development is still unexplored. In this regime the behavior could be quite different as it is only for these large Ra where the flow becomes turbulent and the coherence length scale becomes considerably smaller than $0.1H$. In this previously “unexplored” highly turbulent regime classical theories would predict that turbulent superstructures disappear. In this work we will show (i) that thermal superstructures survive at high Ra , (ii) that the thermal superstructures have pronouncedly different flow characteristics than LSC in smaller domains, and (iii) that the domain size to obtain convergence to the large aspect ratio limit depends on the quantity of interest.

Figure 1.1: Snapshots at different magnifications for the simulation at $Ra = 10^8$ and $\Gamma = 64$. The first and second row show snapshots of the temperature and vertical velocity at mid-height and the third and fourth row show the corresponding snapshots at BL height. The columns from left to right present successive zooms of the area indicated in the black box.

1.2 Numerical method

We performed direct numerical simulations (DNS) of periodic RB convection in very large computational domains and at high Ra using AFiD. The code uses a second order, energy conserving, finite difference method. Here, we use no-slip conditions, constant temperature boundary conditions at the bottom and top plates, and periodic boundary conditions in the horizontal directions. Details can be found in literature [76–78] and at www.AFiD.eu. The control parameters are $Ra = \beta g \Delta H^3 / (\nu \kappa)$ and $Pr = \nu / \kappa$, where β is the thermal expansion coefficient, g the gravitational acceleration, Δ the temperature difference between the top and bottom plates, H the height of the fluid domain, ν the kinematic viscosity, and κ the thermal diffusivity of the fluid. We performed 33 simulations at $Ra = 2 \times 10^7; 10^8; 10^9$ in the aspect ratio range $\Gamma = 1\text{--}128$ and $Pr = 1$. We took great care to perform all simulations consistently and followed the resolution criteria set by Ref. [79] and Ref. [80]. The simulation at $Ra = 10^9$ for $\Gamma = 32$ is performed on a $12288 \times 12288 \times 384$ grid. The statistical convergence of integral flow quantities such as Nu and Re is within a fraction of a percent. The convergence of higher order statistics is, unavoidably, less due to the slow dynamics of the thermal superstructures, whose existence will be revealed.

1.3 Results

We first look at a visualization of the flow at $Ra = 10^8$ in a $\Gamma = 64$ cell in figure 1.1. The first row displays the temperature field at mid-height. The different subfigures in this row present the flow structures more clearly by successive zoom-ins. One can easily discern the significance of a sufficiently large aspect ratio. The second row, which shows the mid-height vertical velocity field, displays a remarkable disparity with the temperature field. We find that in large aspect ratio cells the correlation coefficient between temperature and vertical velocity is only about 0.5 at mid-height, while this correlation is about 0.7 at BL height. The third and fourth row show the temperature and vertical velocity at BL height. It is impressive to see that the large-scale thermal structures at mid-height leave a visible imprint in the BL, i.e. the warm (red) areas at mid-height (top row) correspond to warm areas (brighter

Figure 1.2: The temperature variance $E_\theta(k)$ and TKE $E_u(k)$ spectra at (a,b) mid-height and (c,d) BL height at $Ra = 10^8$ and (e,f) at mid-height at $Ra = 2 \times 10^7$ for different Γ . Here k is the circular wave number $k = (k_x^2 + k_y^2)^{1/2}$. The zoom in panel a shows the peaks of $\Gamma = 16; 32; 64$ with error bars displaying the distance to the next captured wavenumber.

areas) in the BL (third row). This imprint is quantified by the correlation of the temperature field at mid-height and BL height, which is about 0.3, i.e. small but statistically relevant.

To determine the horizontal extent of the thermal superstructures, we calculated the turbulent kinetic energy (TKE) $E_u(k)$ and thermal variance $E_\theta(k)$ spectra at BL height and mid-height. The spectra represent the time average obtained in the statistical stationary state. Figure 1.2 shows that the wavenumber of maximal energy, respectively, thermal variance decreases with increasing aspect ratio until it slowly saturates, but for $Ra = 10^8$ we cannot conclude whether the peak position of the spectra is fully converged. In figure 1.2e,f we can observe that the results for $Ra = 2 \times 10^7$ do reveal a clear convergence of the peak location of the spectra around $\Gamma \approx 64$. The slow convergence of the peak location of the spectra shows that extremely large domains are necessary to accurately capture thermal superstructures, i.e. the domain size must be much larger than the average size of the superstructures. The temperature variance spectra at mid-height and BL height indicate that the spectrum peak is located around $k \approx 1$, which corresponds to a structure size of about 6–7 times the domain height. This is of similar size as obtained in the classical works [62–65] for Ra up to 10^7 . Also the peak of the TKE spectrum at BL height is located around $k \approx 1$. This reflects the large-scale

Figure 1.3: Height profile of (a) the standard deviation and (b) the kurtosis at $Ra = 10^8$.

pattern visible in the horizontal velocity components as the spectrum of the vertical velocity component at BL height peaks around $k \approx 30$ ($\approx 0.21H$), which corresponds to the plume size at BL height presented in figure 1.1, see also the work of Ref. [63]. For $Ra = 10^8$ and $\Gamma = 32$ we verified that the shown spectra are converged up to $k \approx 700$ by performing separate simulations on a $6144 \times 6144 \times 192$ and a $8192 \times 8192 \times 256$ grid. For the TKE spectrum at mid-height the main peak is located close to $k = 2$, which indicates that the velocity structures at mid-height are smaller than the temperature structures. This further emphasizes that the correlation between the vertical velocity and temperature at mid-height is less than naively expected.

As the location of the peak of the spectrum is difficult to converge we look at the so-called integral scale [63]. Here we calculate the integral length scale based on the temperature variance $\Lambda_\theta = 2\pi \int [E_\theta(k)/k]dk / \int E_\theta(k)dk$ and TKE $\Lambda_u = 2\pi \int [E_u(k)/k]dk / \int E_u(k)dk$ spectra. We emphasize that the integral length scales do not correspond to the spectral peaks discussed in the previous section. Figure 1.4a reveals that Λ_θ and Λ_u converge to a large aspect ratio limit around $\Gamma \approx 32$. For $\Gamma \lesssim 8$, when there is only one convection roll in the domain, Λ_θ and Λ_u increase roughly linearly with the domain size. For $\Gamma = 16$ and low Ra Λ_θ is similar to the value found for $\Gamma = 8$, while for higher Ra it is close to the large aspect ratio limit. We speculate that this phenomenon could be due to the existence of multiple turbulent states at $\Gamma = 16$, similarly to what is observed in, for example, Taylor-Couette [81] and 2D RB flow [82, 83].

To investigate how the flow structures influence horizontally averaged higher order statistics, we present the standard deviation and kurtosis of the temperature as function of height in figure 1.3. The curves show a clear separation between the flow characteristics in small and in large aspect ratio cells. In

Figure 1.4: (a) Integral scale at mid-height based on the temperature variance Λ_θ and the TKE spectra Λ_u , (b) Nusselt number, (c) vertical Reynolds number Re_v , and (d) horizontal Reynolds number Re_h as function of Γ normalized with the value at $\Gamma = 1$. (e) Re_v/Re_h as function of Γ .

contrast to the spectra and integral length scales we find that horizontally averaged higher order statistics already converge to the large aspect ratio limit around $\Gamma \approx 8$, while figure 1.4 reveals that integral quantities such as Nu and Re are already converged around $\Gamma \approx 4$. Figure 1.4b shows that Nu as function of Γ reaches a maximum around $\Gamma \approx 0.75$ for all Ra considered here, while it decreases sharply for $\Gamma \lesssim 0.5$. The figure also reveals that in smaller domains the horizontal motion is suppressed, while the vertical motion and heat transfer in the system are much less sensitive to the aspect ratio. Consequently, the vertical velocity is much stronger than the horizontal velocity in small domains, while the horizontal and vertical velocity components are nearly equal in large aspect ratio domains, see figure 1.4e. Thus in large aspect ratio cells the horizontal mixing in the interior domain is stronger than in smaller aspect ratio cells, which results in the lower correlation of the temperature and vertical velocity observed in large aspect ratio cells. We find that the correlation between temperature and vertical velocity converges to the large aspect ratio limit around $\Gamma = 8$.

1.4 Conclusions

In summary, we highlighted the existence of thermal superstructures in highly turbulent RB flow. The observed structure sizes are significantly bigger than the structures found near onset of convection [73] or the structures found in 2D RB [82, 83], but similar in size as obtained in the classical works [62–65], which studied thermal superstructures up to $Ra = 10^7$ in simulation with aspect ratio up to about 40. Surprisingly, while classical theory would predict that these flow structures should be washed out at high Ra when the flow becomes turbulent, we do not find any sign that the superstructures get weaker when Ra is increased. Our simulations show for the first time that the peak location of the temperature variance and TKE spectra converge around $\Gamma \approx 64$, which is a sign that the characteristics of the thermal superstructures become truly independent of the domain size. Here we also show that the horizontal velocity increases rapidly when the domain size is enlarged until it converges to its large aspect ratio limit around $\Gamma \approx 4$. This leads to more vigorous mixing in large domains, which is reflected in the lower correlation between temperature and vertical velocity in large domains when compared to small domains. While vertical velocity and heat transfer are much less sensitive to the domain size, we find that the large-scale motions have a visible effect on the heat transfer.

Thermal superstructures have a profound influence on flow statistics. Interestingly, we find that integral quantities such as Nu and Re reach the large aspect ratio limit already around $\Gamma \approx 4$, while this limit is only reached around $\Gamma \approx 8$ for horizontally averaged higher order statistics, around $\Gamma \approx 32$ for the integral length scales, and around $\Gamma \approx 64$ for the peak location of the temperature variance and TKE spectra. Thus the minimal domain size required to reach the large aspect ratio limit result depends on the quantity of interest. The observation that simple statistics are accurately captured in a smaller domain than necessary to converge spectra is similar to the situation in channel [28, 29], pipe [30] and turbulent boundary layer flow [31–33]. However, we note that the thermal superstructures are very different than large-scale structures discovered in pipe, channel, and boundary layer flow. First of all, the absence of a mean flow direction means that the thermal superstructures have a similar extend in all horizontal directions, whereas in channel, pipe and boundary layer flows the large-scale flow features are very long and elongated [31–33]. In addition, the thermal superstructures have a size that is independent of the distance to the wall, while superstructures appear to be

limited to the logarithmic region in turbulent boundary layer flow [84] or the outer layer for pipe and channel flow [85].

Further research is required to investigate how the Pr number influences the formation of thermal superstructures at high Ra . In addition, the observations that the kurtosis of the temperature distribution convergence to the Gaussian value, and the weak correlation between the temperature and vertical velocity in the bulk are very intriguing phenomena and need further investigation in order to determine how these observations are related to the coherency of the large-scale flow patterns.

Flow organization in laterally unconfined Rayleigh-Bénard turbulence*

We investigate the large-scale circulation (LSC) of turbulent Rayleigh-Bénard convection in a large box of aspect ratio $\Gamma = 32$ for Rayleigh numbers up to $Ra = 10^9$ and at a fixed Prandtl number $Pr = 1$. A conditional averaging technique allows us to extract statistics of the LSC even though the number and the orientation of the structures vary throughout the domain. We find that various properties of the LSC obtained here, such as the wall-shear stress distribution, the boundary layer thicknesses and the wind Reynolds number, do not differ significantly from results in confined domains ($\Gamma \approx 1$). This is remarkable given that the size of the structures (as measured by the width of a single convection roll) more than doubles at the highest Ra as the confinement is removed. An extrapolation towards the critical shear Reynolds number of $Re_s^{\text{crit}} \approx 420$, at which the boundary layer (BL) typically becomes turbulent, predicts that the transition to the ultimate regime is expected at $Ra_{\text{crit}} \approx \mathcal{O}(10^{15})$ in unconfined geometries. This result is in line with the Göttingen experimental observations [36, 46]. Furthermore, we confirm that the local heat transport close to the wall is highest in the plume impacting region, where the thermal BL is thinnest, and lowest in the plume emitting region, where the thermal BL is thickest. This trend, however, weakens with increasing Ra .

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2.1 Introduction

Rayleigh-Bénard (RB) convection [26,37,39,40] is the flow in a box heated from below and cooled from above. Such buoyancy driven flow is the paradigmatic example for natural convection which often occurs in nature, e.g. in the atmosphere. For that case, a large-scale horizontal flow organization is observed in satellite pictures of weather patterns. Other examples include the thermohaline circulation in the oceans [7], the large-scale flow patterns that are formed in the outer core of the Earth [86], where reversals of the large-scale convection roll are of prime importance, convection in gaseous giant planets [87] and in the outer layer of the Sun [88]. Thus, the problem is of interest in a wide range of scientific disciplines, including geophysics, oceanography, climatology, and astrophysics. For a given aspect ratio and given geometry, the dynamics in RB convection are determined by the Rayleigh number $Ra = \beta g \Delta H^3 / (\kappa \nu)$ and the Prandtl number $Pr = \nu / \kappa$. Here, β is the thermal expansion coefficient, g the gravitational acceleration, Δ the temperature difference between the horizontal plates, which are separated by a distance H , and ν and κ are the kinematic viscosity and thermal diffusivity, respectively. The dimensionless heat transfer, i.e. the Nusselt number Nu , along with the Reynolds number Re are the most important response parameters of the system.

For sufficiently high Ra , the flow becomes turbulent, which means that there are vigorous temperature and velocity fluctuations. Nevertheless, a large-scale circulation (LSC) develops in the domain such that, in addition to the thermal boundary layer (BL), a thin kinetic BL is formed to accommodate the no-slip boundary condition near both the bottom and top plates. Properties of the LSC and the nature of the BLs are highly relevant to the theoretical description of the problem. In particular, the unifying theory of thermal convection [41–43,48] states that the transition from the classical to the ultimate regime takes place when the kinetic BLs become turbulent. This transition is shear based and driven by the large-scale wind, underlying the importance of the LSC to the overall flow behavior.

So far, the LSC and BL properties have mainly been studied in small aspect ratio cells, typically for $\Gamma = 1/2$ and $\Gamma = 1$. Various studies have shown that the BLs indeed follow the laminar Prandtl-Blasius (PB) type predictions in the classical regime [26,89–95]. Previous studies by, for example Ref. [96] and Ref. [97], have used results from direct numerical simulations (DNS) in aspect ratio $\Gamma = 1$ cells to study the properties of the BLs in detail. Ref. [96] showed

that an extrapolation of their data gives that for $Pr = 0.786$ the critical shear Reynolds number of 420 is reached at $Ra \approx 1.2 \times 10^{14}$, while Ref. [97] predict a value of $Ra \approx 3 \times 10^{13}$.

Despite the wealth of studies in low aspect-ratio domains, many natural instances of thermal convection take place in very large aspect ratio systems, as mentioned above. Previous research has demonstrated that several flow properties are significantly different in such unconfined geometries. Ref. [62] and Ref. [65] performed DNS at $Ra = \mathcal{O}(10^7)$ and $\Gamma = 20$. They observed large-scale structures by investigating the advective heat transport and found the most energetic wavelength of the LSC at $4H-7H$. Recently, DNS by Ref. [98] for $\Gamma = 128$ and $Ra = \mathcal{O}(10^7-10^9)$ also reported ‘superstructures’ with wavelengths of 6–7 times the distance between the plates. Similar findings were made by Ref. [99] over a wide range of Prandtl numbers $0.005 \leq Pr \leq 70$ and Ra up to 10^7 . It was shown that the signatures of the LSC can be observed close to the wall, which Ref. [63] described as clustering of thermal plumes originating in the BL and assembling the LSC. Ref. [100] showed that the presence of the LSC leads to a pronounced peak in the coherence spectrum of temperature and wall-normal velocity. Based on DNS at $\Gamma = 32$ and $Ra = \mathcal{O}(10^5-10^9)$, they determined that the wavelength of this peak shifts from $\hat{l}/H \approx 4$ to $\hat{l}/H \approx 7$ as Ra is increased.

Ref. [98] have shown that in periodic domains, the heat transport is maximum for $\Gamma = 1$ and reduces with increasing aspect ratio up to $\Gamma \approx 4$ when the large-scale value is obtained. They also found that fluctuation-based Reynolds numbers depend on the aspect ratio of the cell. However, other than the structure size, it is mostly unclear how the large-scale flow organization and BL properties are affected by different geometries. Not only is the size of the LSC more than 2 times larger without confinement (note that $\hat{l}$ measures the size of two counter-rotating rolls combined), but also other effects, such as corner vortices, are absent in periodic domains. Therefore one would expect differences in wind properties and BL dynamics. It is the goal of this chapter to investigate these differences. Doing so comes with significant practical difficulty due to the random orientation of a multitude of structures that are present in a large box. To overcome this, we adopt the conditional averaging technique that was devised in Ref. [101] to reliably extract LSC features even under these circumstances. Details on this procedure are provided in section §2.3 after a description of the dataset in §2.2. Finally, in §2.4 and §2.5 we present results on how superstructures affect the flow properties in comparison to the flow formed in a cylindrical $\Gamma = 1$ domain [96] and summarize our findings in §2.6.

Ra	$N_x \times N_y \times N_z$	Nu	$\hat{l}/H$	v_{RMS}/V_{ff}	λ_θ^*/H	tV_{ff}/H
1×10^5	$2048 \times 2048 \times 64$	4.35	4.4	0.2172	0.115	1500
4×10^5	$2048 \times 2048 \times 64$	6.48	4.5	0.2214	0.077	1500
1×10^6	$3072 \times 3072 \times 96$	8.34	4.9	0.2198	0.060	1500
4×10^6	$3072 \times 3072 \times 96$	12.27	5.4	0.2152	0.041	1500
1×10^7	$4096 \times 4096 \times 128$	15.85	5.9	0.2107	0.032	1000
1×10^8	$6144 \times 6144 \times 192$	30.94	6.3	0.1968	0.016	500
1×10^9	$12288 \times 12288 \times 384$	61.83	6.6	0.1805	0.008	75

Table 2.1: Data from [98] and [100] for the global Nusselt number, the grid resolution (N_x, N_y, N_z) in streamwise, spanwise, and wall-normal direction, the location of the coherence spectra peak $\hat{l}$, the root mean square velocity $v_{RMS} = \sqrt{\langle v_x^2 + v_y^2 + w^2 \rangle_V}$ non-dimensionalized with the free-fall velocity $V_{ff} = \sqrt{\beta g H \Delta}$, the estimated thermal BL thickness $\lambda_\theta^*/H = 1/(2Nu)$, and the amount of non-dimensional time units used for our statistical analysis tV_{ff}/H .

2.2 Numerical method

The data used in this chapter have previously been presented by Ref. [98] and Ref. [100]. A summary of the most relevant quantities for this study can be found in table 2.1; note that there and elsewhere we use the free-fall velocity $V_{ff} = \sqrt{\beta g H \Delta}$ as a reference scale. In the following, we briefly report details on the numerical method for completeness. We carried out periodic RB simulations by numerically solving the three-dimensional incompressible Navier-Stokes equations within the Boussinesq approximation. They read:

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla P + \left(\frac{Pr}{Ra} \right)^{1/2} \nabla^2 \mathbf{u} + \theta \hat{z}, \quad (2.1)$$

$$\nabla \cdot \mathbf{u} = 0, \quad (2.2)$$

$$\frac{\partial \theta}{\partial t} + \mathbf{u} \cdot \nabla \theta = \frac{1}{(RaPr)^{1/2}} \nabla^2 \theta. \quad (2.3)$$

Here, $\mathbf{u}$ is the velocity vector, θ the temperature, and the kinematic pressure is denoted by P . The coordinate system is oriented such that the unit vector $\hat{z}$ points up in the wall-normal direction, while the horizontal directions are denoted by x and y . We solve (2.1) - (2.3) using AFiD, the second-order finite

Figure 2.1: (a) Premultiplied temperature power spectra $k\Phi_{\theta\theta}$ for $Ra = 10^5; 10^7; 10^9$. The blue line indicates the cut-off wavenumber $k_{\text{cut}} = 2/H$ used for the low-pass filtering. The dashed black lines indicate alternative cut-offs ($k_{\text{cut}} = 1.8/H$ and $k_{\text{cut}} = 2.5/H$) considered in panel (c). The white plusses are located at $k = 0.57/\lambda_\theta^*$ and $z = 0.85\lambda_\theta^*$ (with $\lambda_\theta^* = H/(2Nu)$) in all cases, which corresponds to the location of the inner peak [100] (b) Coherence spectra of temperature and wall-normal velocity at mid-height, figure adopted from Ref. [100]. The black line illustrates the choice of $k_{\text{cut}} = 2/H$ and the legend of figure 2.4a applies for the Ra -trend. (c) Snapshot of temperature fluctuations for $Ra = 10^7$ at mid-height. The black lines show contours of $\theta'_L = 0$ evaluated for different choices of k_{cut} .

difference code developed by Verzicco and coworkers [76, 77]. We use periodic boundary conditions and a uniform mesh in the horizontal direction and a clipped Chebyshev-type clustering towards the plates in the wall-normal direction. For validations of the code against other experimental and simulation data in the context of RB we refer to Ref. [76, 80, 102–104].

The aspect ratio of our domain is $\Gamma = L/H = 32$, where L is the length of the two horizontal directions of the periodic domain. The used numerical resolution ensures that all important flow scales are properly resolved [79, 80]. We note that the grid resolution at $Ra = 10^9$ still has 11 grid points in the thermal and kinetic boundary layer, while the criteria by Ref. [79] state that 8 grid points are sufficient in this case. In appendix A.1 we give further details on the simulations and show that the average of the horizontal velocity components is almost zero.

In this chapter, we define the decomposition of instantaneous quantities into their mean and fluctuations such that $\psi(x, y, z, t) = \Psi(z) + \psi'(x, y, z, t)$, where $\Psi = \langle \psi(x, y, z, t) \rangle_{x,y,t}$ is the temporal and horizontal average over the whole domain and ψ' the fluctuations with respect to this mean.

2.3 Conditional Averaging

Extracting features of the LSC in large aspect ratio cells poses a significant challenge. The reason is that there are multiple large-scale structures of varying sizes, orientation, and inter-connectivity at any given time. It is therefore not possible to extract properties of the LSC by using methods that rely on tracking a single or a fixed small number of convection cells, which have been proven to be successful in analyzing the flow in small [96, 105] to intermediate [106] aspect-ratio domains. To overcome this issue, we use a conditional averaging technique developed in Ref. [101], where this framework was employed to study the modulation of small-scale turbulence by the large flow scales. This approach is based on the observation of Ref. [100] that the pre-multiplied temperature power spectra $k\Phi_{\theta\theta}$ (shown in figure 2.1a) is dominated by two very distinct contributions. One is due to the ‘superstructures’ whose size (relative to H) increases with increasing Ra and typically corresponds to wavenumbers $kH \approx 1$ –1.5. The other contribution relates to a ‘near-wall peak’ with significantly smaller structures whose size scales with the thickness of the BL [100]. This implies that this peak shifts to larger k (scaled with H) as the BLs get thinner at higher Ra . Hence, there is a clear spectral gap between

superstructures and small-scale turbulence, which widens with increasing Ra , as can readily be seen from figure 2.1a. This figure also demonstrates that a spectral cut-off $k_{\text{cut}} = 2/H$ is a good choice to separate superstructure contributions from the other scales over the full Ra range $10^5 \leq Ra \leq 10^9$ considered here.

The choice for $k_{\text{cut}} = 2/H$ is further supported by considering the spectral coherence

$$\gamma_{\theta w}^2(k) = \frac{|\Phi_{\theta w}(k)|^2}{\Phi_{\theta\theta}(k)\Phi_{ww}(k)}, \quad (2.4)$$

where Φ_{ww} and $\Phi_{\theta w}$ are the velocity power spectrum and the co-spectrum of θ and w , respectively. The coherence γ^2 may be interpreted as a measure of the correlation *per scale*. The results at $z = 0.5H$ in figure 2.1b indicate that there is an almost perfect correlation between θ' and w' at the superstructure scale. At larger wavenumbers, this correlation is seen to drop significantly. For the lower Ra values, the coherence rises again at the very small scales. However, almost no energy resides at the scales corresponding to the high-wavenumber peak in $\gamma_{\theta w}^2$ (see figure 2.1a and for a more detailed discussion Ref. [100]), such that the coherence there is of little practical relevance. The threshold $k_{\text{cut}} = 2/H$ effectively delimits the large-scale peak in $\gamma_{\theta w}^2$ towards larger k for all Ra considered, such that this value indeed appears to be a solid choice to distinguish the large-scale convection rolls from the remaining turbulence. To confirm this, we overlay a snapshot of θ' with zero-crossings of the low-pass filtered signal (with cut-off wavenumber k_{cut}) θ'_L in figure 2.1c. These contours reliably trace the visible structures in the temperature field. Furthermore, it becomes clear that slightly different choices for k_{cut} do not influence the contours significantly. This is consistent with the fact that only limited energy resides at the scales around $k \approx 2/H$, such that θ'_L only changes minimally when k_{cut} is varied within that range. In the following, we adopt $k_{\text{cut}} = 2/H$ to obtain θ'_L except when we study the effect of the choice for k_{cut} .

We use θ'_L evaluated at mid-height to map the horizontal field onto a new horizontal coordinate d . To obtain this coordinate, first the distance d^* to the nearest zero-crossing in θ'_L is determined for each point in the plane. This can be achieved efficiently using a nearest-neighbor search. Then the sign of d is determined by the sign of θ'_L , such that d is given by

$$d = \text{sgn}(\theta'_L)d^*. \quad (2.5)$$

Figure 2.2: Illustration of the conditional averaging method based on simulation data for $Ra = 10^7$. (a) Temperature fluctuation field at mid-height and corresponding distance field (right). The black lines correspond to the zero-crossings $\theta'_L = 0$ relative to which the distance d^* is defined (see blow-up in panel b). Note that by definition isolines $\theta'_L = 0$ correspond to contours of $d = 0$ in the distance field. (b) Illustration of the distance definition; for every point d^* is equal to the radius of the smallest circle around that point which touches a $\theta'_L = 0$ contour. (c) Illustration of the decomposition of the horizontal velocity v , here at boundary layer height, into the parallel v_p and the normal v_n component to the gradient vector d . The color scheme in (b) and (c) indicates the d -field as in (a).

Figure 2.3: Contour plot of the conditionally averaged temperature $\bar{\theta}/\Delta$ for $Ra = 10^7$. The arrows show $\bar{w}/V_{ff}$ and $\bar{v}_p/V_{ff}$ and are plotted every 24 and every 6 data points along d and z , respectively. The white line is the streamline which passes through z^*/H at $d = 0$.

All results presented here are with reference to the lower hot plate. Hence $d < 0$ and $d > 0$ correspond to plume impacting and plume emitting regions, respectively. The averaging procedure is illustrated in figure 2.2a,b. Another important aspect is a suitable decomposition of the horizontal velocity component v . Figure 2.2c shows how we decompose v into one component (v_p) parallel the local gradient ∇d , and another component (v_n) normal to it. This ensures that v_p is oriented normal to the zero-crossings in θ'_L for small $|d|$, where the wind is strongest. However, at larger $|d|$, the orientation may vary from a simple interface normal, which accounts for curvature in the contours. It should be noted that the d -field is determined at mid-height and consequently applied to determine the conditional average at all z -positions. This is justified since Ref. [100] showed that there is a strong *spatial* coherence of the large scales in the vertical direction. Therefore, the resulting zero-contours would almost be congruent if θ'_L was evaluated at other heights. The time-averaged conditional average is obtained by averaging over points of constant d , while we make use of the symmetry around the midplane to increase the statistical convergence. Mathematically, the conditioned averaging results in a triple decomposition according to $\psi(x, y, z, t) = \Psi(z) + \bar{\psi}(z, d) + \psi(x, y, z, t)$, where the overline indicates conditional and temporal averaging. As bin-size of the d -array we have used the horizontal grid spacing $dx = \Gamma/N_x$.

Applying the outlined method to our RB dataset results in a representative large-scale structure like the one depicted in figure 2.3 for $Ra = 10^7$. In general, we find $\bar{\theta} < 0$ with predominantly downward flow for $d < 0$, while lateral flow towards increasing d dominates in the vicinity of $d = 0$. In the plume emitting region $d > 0$ the conditioned temperature $\bar{\theta}$ is positive and the flow upward. In interpreting the results it is important to keep in mind that the averaging is ‘sharpest’ close to the conditioning location ($d = 0$) and ‘smears out’ towards

Figure 2.4: (a) PDF of the normalized distance parameter $d/\hat{l}$ using all available snapshots. (b) Sample velocity profile, locally determined in (x,y) , to illustrate the slope method (λ) and the level method (ℓ) used to determine the instantaneous BL thicknesses.

larger $|d|$ as the size of individual structures varies. We normalize d with $\hat{l}$ to enable a comparison of results across Ra . Based on the location of the peak in γ^2 , Ref. [100] found that the superstructure size is $\hat{l} = 5.9H$ at $Ra = 10^7$. As indicated, the conditionally averaged flow field in figure 2.3 corresponds to approximately half this size.

We present the probability density function (PDF) of the distance parameter d in figure 2.4a. The data collapse to a reasonable degree, indicating that there are no significant differences in how the LSC structures vary in time and space across the considered range of Ra . Visible deviations are at least in part related also to uncertainties in determining $\hat{l}$ via fitting the peak of the γ^2 -curve.

The LSC is carried by v_p , which is also supported by the fact that the velocity component normal to the gradient ∇d averages to zero, i.e. $\bar{v}_n \approx 0$, for all d . The determination of the viscous BL thickness is therefore based on v_p only. We use the ‘slope method’ to determine the viscous (λ_u) and thermal (λ_θ) BL thickness. Both are determined locally in space and time and are based on instantaneous wall-normal profiles of θ and v_p , respectively. As sketched in figure 2.4b, λ is given by the location at which linear extrapolation using the wall-gradient reaches the level of the respective quantity. Here the ‘level’ (e.g. $u_l(x,y) = \max_{z \in I}(v_p(x,y,z))$ for velocity) is defined as the local maximum within a search interval I above the plate. In agreement with Ref. [96] we find that the results for both thermal and viscous BL do not significantly depend on

Figure 2.5: (a) Conditioned temperature $\bar{\theta}/\Delta$ at $d = 0$ and in the plume impacting ($d/\hat{l} = -0.25$) and in the plume emitting region ($d/\hat{l} = 0.25$) for various Ra , see legend in (c). (b) Wind velocity $\bar{v}_p/V_{ff}$ at $d = 0$ versus z/H at the same Ra . The inset shows the sensitivity of the results to different choices of k_{cut} in the range $1.8 \leq k_{cut}H \leq 2.5$ (same range used in figure 2.1) for $Ra = 10^7$. (c) Mean wind velocity at $d = 0$ normalized by its maximum value for various Ra (see legend). The dashed black lines in (c) represent experimental data from Ref. [105] at $\Gamma = 1$ for $Ra = 1.25 \times 10^9$ (short dash) and $Ra = 1.07 \times 10^{10}$ (long dash) and the dotted black line represents the Prandtl-Blasius profile.

the search region when it is larger than $I = 4\lambda_\theta^*$. Therefore, we have adopted this search region in all our analyses.

In figure 2.5a we present the conditionally averaged temperature $\bar{\theta}$ as a function of z/H at three different locations of $d/\hat{l}$. Consistent with the conditioning on zero-crossings in $\theta'_L = 0$, we find that $\bar{\theta} \approx 0$ for all z at $d = 0$. In the plume impacting ($d/\hat{l} = -0.25$) and emitting ($d/\hat{l} = 0.25$) regions, $\bar{\theta}$ is respectively negative and positive throughout. On both sides, $\bar{\theta}$ attains nearly constant values in the bulk, the magnitude of which is decreasing significantly with increasing Ra .

Profiles for the mean wind velocity $\bar{v}_p(z)$ at $d = 0$ are shown in figure 2.5b,c. These figures show that the viscous BL becomes thinner with increasing Ra , while the decay from the velocity maximum to 0 at $z/H = 0.5$ is almost linear for all cases. We note that of all presented results the wind profile is most sensitive to the choice of the threshold k_{cut} . The reason is that the obtained wind profile depends on both the contour location and orientation.

Figure 2.6: (a) Timescale $\mathcal{T}$ versus Ra using different methods. The datasets are: The time needed to circulate the flow along a streamline, which passes through z^*/H at $d = 0$ (red circles), see figure 2.3; the timescale calculated with the EAM method of Ref. [99] (blue squares). We also show the Ref. [99] data itself, which were calculated for the smaller $Pr = 0.7$ (black diamonds). The dashed line shows $\mathcal{T}/T_{ff} = (7.7 \pm 1.5) \times Ra^{0.139 \pm 0.014}$. (b) Average velocity v_{wind} determined along the streamline chosen in (a), normalized with v_{RMS} . (c) Comparison between the length of the streamline and the circumference $\pi(0.25\hat{l} + 0.5H)$ of the ellipse (EAM method), both used to calculate the respective timescale in (a).

To provide a sense for the variations associated with the choice of k_{cut} , we compare the present result at $Ra = 10^7$ to what is obtained using alternative choices ($k_{cut} = 1.8/H$ and $k_{cut} = 2.5/H$) in the inset of figure 2.5b. This plot shows that results within the BL are virtually insensitive to the choice of k_{cut} while the differences in the bulk consistently remain below 5%. In panel (c) of figure 2.5 we re-plot the data from figure 2.5b normalized with the BL thickness $\bar{\lambda}_u(d = 0)$ and the velocity maximum $\bar{v}_p^{\max}$. The figure shows that the velocity profiles for the different Ra collapse reasonably well for $z \lesssim \bar{\lambda}_u$. A comparison to the experimental data by Ref. [105], which were recorded in the center of a slender box with $\Gamma = 1$ and $Pr = 4.3$, reveals that, although the overall shape of the profiles is similar, there are considerable differences in the near-wall region. With their precise origin unknown, these discrepancies could be related to the differences in Pr and Γ .

Another interesting question that we can address based on our results concerns the evolution timescale $\mathcal{T}$ of the LSC. We estimate $\mathcal{T}$ as the time it takes a fluid parcel to complete a full cycle in the convection roll obtained from the conditional average. To do this we compute the streamline that passes through the location z^*/H of the velocity maximum $\bar{v}_p(z^*/H) = \bar{v}_p^{\max}$ at $d = 0$ as shown in figure 2.3. The integrated travel time $\mathcal{T}$ along this averaged streamline as a function of Ra is presented in figure 2.6a. We find $\mathcal{T}/T_{ff} \gg 1$, i.e.,

the typical timescale of the LSC dynamics is much longer than the free-fall time $T_{ff} = \sqrt{H/(\beta g \Delta)}$. Up to $Ra = 10^7$ the timescale $\mathcal{T}$ grows approximately according to $\mathcal{T}/T_{ff} = (7.7 \pm 1.5) \times Ra^{0.139 \pm 0.014}$, but the trend flattens out at Ra beyond that value. For the determination of all uncertainties in this chapter we have used a 95% confidence interval.

To compare our results to other estimates in the literature, we also adopt the method used by Ref. [99] to estimate $\mathcal{T}$. These authors assumed the LSC to be an ellipse, used v_{RMS} as the effective velocity scale and introduced a empirical prefactor of 3 (which is equivalent to assuming a velocity scale $1/3 v_{RMS}$). The results for the ‘elliptical approximation method (EAM)’, using $1/3 v_{RMS}$ as the velocity scale, are compared to the corresponding results by Ref. [99] in figure 2.6a. Results are consistent between the two methods in terms of the order of magnitude. However, the actual values, especially at lower Ra , differ significantly, and also the trends do not fully agree. The streamline approach allows us to determine the average convection velocity along the streamline $v_{wind} \equiv \mathcal{L}/\mathcal{T}$, where $\mathcal{L}$ is the length of the streamline. Figure 2.6b show that v_{wind} is indeed proportional to v_{RMS} with $v_{wind} \approx 0.45 v_{RMS}$ in the considered Ra number regime. In figure 2.6c, we present $\mathcal{L}$ along with the ellipsoidal estimate used in Ref. [99]. From this, it appears that an ellipse does not very well represent the streamline geometry. Further, it becomes clear that it is the difference in the length-scale estimate that leads to the different scaling behaviors for $\mathcal{T}$ in figure 2.6a.

It should additionally be noted that the present approach provides information on the typical turnover timescale of the superstructure in an averaged sense. This is different from Ref. [107] who studied turnover times for individual fluid particles. Particles may linger for long times in either the core of the structures or within the boundary layers, leading to a very wide distribution of timescales in the latter case.

2.4 Wall shear stress and heat transport

The shear stress $\bar{\tau}_w$ at the plate surface is defined through

$$\bar{\tau}_w/\rho = -\nu \langle \partial_z \bar{v}_p \rangle_t. \quad (2.6)$$

Here ∂_z is the spatial derivative in wall-normal direction. In figure 2.7a we show that the normalized shear stress $\bar{\tau}_w/\bar{\tau}_w^{\max}$ as a function of the normalized

Figure 2.7: (a) Normalized shear stress $\bar{\tau}_w$ as a function of $d/\hat{l}$ and (b) mean shear stress $\langle \bar{\tau}_w \rangle_J$ and maximum shear stress $\bar{\tau}_w^{\max}$ versus Ra . The filled symbols show data of the present study ($\Gamma = 32$ periodic domain), where the data for $Ra \geq 4 \times 10^6$ can be fitted as $\bar{\tau}_w^{\max}/(\rho V_{ff}^2) = (0.12 \pm 0.04) \times Ra^{0.242 \pm 0.020}$ and $\langle \bar{\tau}_w \rangle_J/(\rho V_{ff}^2) = (0.10 \pm 0.04) \times Ra^{0.236 \pm 0.016}$. The open symbols represent the data of Ref. [96] for $\Gamma = 1$ with a cylindrical domain. The blue shading in figure 2.7a. We use the average over this interval to evaluate the wind properties and indicate this by $\langle \rangle_J$. In figure 2.7b the data for mean $\langle \bar{\tau}_w \rangle_J$ and for maximum $\bar{\tau}_w^{\max}$ wall shear stress are compiled for the full range of Ra considered. Both quantities are seen to increase significantly as Ra increases. Around $Ra = 1 \times 10^6 - 4 \times 10^6$ we can see a transition point at which the slope steepens. For lower Ra the scaling of $\langle \bar{\tau}_w \rangle_J$ is much flatter. A fit to the data for $Ra \geq 4 \times 10^6$ gives

distance $d/\hat{l}$ is nearly independent of Ra . Similar to findings in smaller cells [96], the curves are asymmetric with the maximum ($d/\hat{l} \approx -0.05$) shifted towards the plume impacting region. The value of $\bar{\tau}_w/\bar{\tau}_w^{\max}$ drops to about 0.25 in both the plume impacting ($d/\hat{l} = -0.25$) and the plume emitting region ($d/\hat{l} = 0.25$).

We use the good collapse of the $\bar{\tau}_w/\bar{\tau}_w^{\max}$ profiles across the full range of Ra considered to separate regions with significant shear from those with little to no lateral mean flow. We define the ‘wind’ region based on the approximate criterion $\bar{\tau}_w/\bar{\tau}_w^{\max} \gtrsim 0.5$, which leads to the interval $J = \{d/\hat{l} \mid d/\hat{l} \in [-0.2 : 0.15]\}$ that is indicated by the blue shading in figure 2.7a. We use the average over this interval to evaluate the wind properties and indicate this by $\langle \rangle_J$. In figure 2.7b the data for mean $\langle \bar{\tau}_w \rangle_J$ and for maximum $\bar{\tau}_w^{\max}$ wall shear stress are compiled for the full range of Ra considered. Both quantities are seen to increase significantly as Ra increases. Around $Ra = 1 \times 10^6 - 4 \times 10^6$ we can see a transition point at which the slope steepens. For lower Ra the scaling of $\langle \bar{\tau}_w \rangle_J$ is much flatter. A fit to the data for $Ra \geq 4 \times 10^6$ gives

$$\frac{\bar{\tau}_w/\rho}{V_{ff}^2} \sim Ra^{0.24}, \quad (2.7)$$

for both $\langle \bar{\tau}_w \rangle_J$ and $\bar{\tau}_w^{\max}$. Overall, we find that the shear stress at the wall due

Figure 2.8: (a) Local heat flux $\overline{Nu}$ at the wall normalized by the global heat flux Nu as function of the normalized spatial variable $d/\hat{l}$. (b) Values in the impacting ($-0.3 \leq d/\hat{l} \leq -0.2$) and emitting ($0.2 \leq d/\hat{l} \leq 0.3$) range as a function of Ra .

to the turbulent thermal superstructures (in the periodic $\Gamma = 32$ domain with $Pr = 1$) compares well with the shear stress in a cylindrical $\Gamma = 1$ domain by Ref. [96] with $Pr = 0.786$. Most importantly, the scaling with Ra is the same for both cases. The actual shear stress seems to be somewhat higher in the cylindrical aspect ratio $\Gamma = 1$ domain than in the periodic domain in which the flow is unconfined. In part this difference may be related to the difference in Pr . Besides that, as we will show in the next section, the shear Reynolds number is slightly lower for the periodic domain than in the confined domain.

Next, we consider the local heat flux at the plate surface, given by

$$\overline{Nu}(d) \equiv -\frac{H}{\Delta} \partial_z \bar{\theta}(d), \quad (2.8)$$

which is plotted in figure 2.8a for the full range of Ra . In all cases $\overline{Nu}/Nu$ is higher than one on the plume impacting side ($d < 0$). This is consistent with the impacting cold plume increasing the temperature gradient in the BL locally. The fluid subsequently heats up while it is advected along the plate towards increasing d by the LSC. As a consequence, the wall gradient is reduced and $\overline{Nu}$ decreases approximately linearly with increasing $d/\hat{l}$, which is consistent with observations by Ref. [106] and Ref. [96]. This leads to the ratio $\overline{Nu}/Nu$ dropping below 1 for $d > 0$. For increasing Ra , the local heat flux becomes progressively more uniform across the full range of d . To quantify this, we plot the mean local heat fluxes in the plume impacting and emitting

Figure 2.9: Large-scale turbulent heat transport term $(\widetilde{\theta w})/(Nu\kappa\Delta/H)$ evaluated in (a) the plume impacting region, (b) for small $|d|$ around zero, and (c) in the plume emitting region.

regions, respectively, in figure 2.8b. The former is decreasing while the latter is increasing with increasing Ra , bringing the two sides closer. Again, and in both cases, a change of slope is visible in the range of $Ra = 1 \times 10^6$ – 4×10^6 . In this context it is interesting to note that in a recent study on two-dimensional RB convection at $\Gamma = 2$ [108] it was found that at significantly higher $Ra \gtrsim 10^{11}$ the heat transport in the plume emitting range dominated, reversing the current situation. If we boldly extrapolate the trend for $Ra \geq 4 \times 10^6$ in our data, we can estimate that a similar reversal may occur at $Ra \approx \mathcal{O}(10^{12}\text{--}10^{13})$, see figure 2.8b.

A possible mechanism that might explain this behavior is increased turbulent (or convective) mixing, which can counteract the diffusive growth of the temperature BLs. To check this hypothesis, we plot the heat transport term $(\widetilde{\theta w}) \equiv \overline{w\theta} - \overline{w}\overline{\theta}$ in figure 2.9. The normalization in the figure is with respect to the total heat flux Nu , the plotted quantity reflects the fraction of Nu carried by $(\widetilde{\theta w})$. It is obvious from these results that the convective transport contributes significantly, even within the BL height $\langle \bar{\lambda}_\theta \rangle_J$. Moreover, this relative contribution is independent of Ra (except for the lowest value considered) in the plume impacting region (see figure 2.9a). However, figure 2.9b shows that already around $d = 0$ the convective transport in the BL increases with increasing Ra . This trend is much more pronounced in the plume emitting region $d > 0.2$, see figure 2.9c. Hence, convective transport in the BL plays an increasingly larger role for $d \geq 0$ with increasing Ra . Its effect is to smooth

Figure 2.10: (a) Thermal BL thickness $\bar{\lambda}_\theta$ normalized by the estimated thermal BL thickness λ_θ^* and (b) viscous BL thickness $\bar{\lambda}_u$ normalized by the mean viscous BL thickness in the interval $d/\hat{l} \in J$ versus normalized distance $d/\hat{l}$. The color indicates the Rayleigh number, see legend.

out the near-wall region, thereby increasing the temperature gradient at the wall. It is conceivable that the increased convective transport in the near-wall region (provided the trend persists) eventually leads to a reversal of the $\overline{Nu}(d)$ trend observed at moderate Ra in figure 2.8a.

2.5 Thermal and viscous boundary layers

Next, we study how the BL thicknesses λ_θ and λ_u vary along the LSC. In figure 2.10a we present $\bar{\lambda}_\theta$, normalized by λ_θ^* . As expected from figure 2.8, $\bar{\lambda}_\theta$ is generally smaller in the plume impacting region and then increases along the LSC. However, unlike $\overline{Nu}$, $\bar{\lambda}_\theta$ is not determined by the gradient alone but also depends on the temperature level (see figure 2.4b for the definition of the level) such that differences arise. Specifically, $\bar{\lambda}_\theta / \lambda_\theta^*$ is rather insensitive for $Ra \geq 4 \times 10^6$ in the plume impacting region ($d/\hat{l} < -0.1$). Furthermore, for $Ra \geq 10^7$, the growth of the thermal BL with $d/\hat{l}$ comes to an almost complete stop beyond $d = 0$, which is entirely consistent with the conclusions drawn in the discussion on $\widetilde{(\theta w)}$ above. Finally, we note that $\bar{\lambda}_\theta$ is generally larger than the estimate λ_θ^* , which agrees with previous observations by Ref. [96].

There is no obvious choice for the normalization of the viscous BL thickness and we therefore present $\bar{\lambda}_u$ normalized with its mean value $\langle \bar{\lambda}_u \rangle_J$ in figure 2.10. Overall these curves for $\bar{\lambda}_u$ exhibit a similar trend as we observed previously for $\bar{\lambda}_\theta$. The values of $\bar{\lambda}_u$ are smaller in the plume impacting region

Figure 2.11: (a) Mean BL thicknesses versus Ra for the present data at $\Gamma = 32$ (filled symbols) and those of Ref. [96] (open symbols, W.S.W.) and Ref. [97] (x, S.S.), both with $\Gamma = 1$. The dashed line shows $\langle \bar{\lambda}_\theta \rangle_J / H = (4.7 \pm 0.9) \times Ra^{-0.298 \pm 0.012}$. (b) Most probable BL ratio $\bar{\Lambda}^{MP}$ versus normalized distance $d/\hat{l}$ for various Ra .

($d < 0$) and the variation with Ra is limited. Also for $\bar{\lambda}_u/\langle \bar{\lambda}_u \rangle_J$ the growth with increasing d is less pronounced the higher Ra and the curves almost collapse for $d > 0$ at $Ra \geq 10^7$.

Figure 2.11a shows $\langle \bar{\lambda}_\theta \rangle_J$ and $\langle \bar{\lambda}_u \rangle_J$ as a function of Ra . For the thermal BL thickness, the scaling appears to be rather constant over the full range and from fitting $4 \times 10^6 \leq Ra \leq 10^9$ we obtain

$$\langle \bar{\lambda}_\theta \rangle_J / H = (4.7 \pm 0.9) \times Ra^{-0.298 \pm 0.012}. \quad (2.9)$$

The reduction of the viscous BL thickness $\langle \bar{\lambda}_u \rangle_J$ with Ra is significantly slower than for the thermal BL thickness $\langle \bar{\lambda}_\theta \rangle_J$. For low Ra , $\langle \bar{\lambda}_u \rangle_J < \langle \bar{\lambda}_\theta \rangle_J$. However, due to the different scaling of the two BL thicknesses, $\langle \bar{\lambda}_u \rangle_J > \langle \bar{\lambda}_\theta \rangle_J$ for $Ra \approx 4 \times 10^6$. Comparing the periodic $\Gamma = 32$ data with the confined $\Gamma = 1$ case reported in Ref. [96] and Ref. [97], we note that the results for $\langle \bar{\lambda}_\theta \rangle$ agree closely between the two geometries. The scaling trends for $\langle \bar{\lambda}_u \rangle$ also appear to be alike in both cases. However, the viscous BL is significantly thinner in the smaller box, with a slight difference between the two datasets of $\Gamma = 1$, which may be due to the difference in Pr . This situation is similar, and obviously also related to, the findings we reported for the comparison of the wall-shear stress in figure 2.7b.

We further computed the most probable instantaneous BL ratio $\bar{\Lambda}^{MP}(d) \equiv \text{mode}(\Lambda(d(x, y), t|d = \text{const.}))$, where *mode* indicates the most common value of the instantaneous BL ratio $\Lambda = \lambda_\theta/\lambda_u$, and present results in figure 2.11b.

Figure 2.12: Comparison of mean BL thicknesses versus Ra using the slope method and the location of the respective temperature and velocity levels (level method). The dashed lines show $\langle \bar{\lambda}_\theta \rangle_J / H = (4.7 \pm 0.9) \times Ra^{-0.298 \pm 0.012}$ and $\langle \bar{\ell}_\theta \rangle_J / H = (8.6 \pm 3.1) \times Ra^{-0.283 \pm 0.023}$.

Since the statistics of Λ were found to be quite susceptible to outliers, we decided to report the most probable value $\bar{\Lambda}^{MP}$ as this provides a more robust measure than the mean. The Prandtl-Blasius BL theory for the flow over a flat plate suggests that $\Lambda = 1$ for $Pr = 1$. The figure shows that $\bar{\Lambda}^{MP}$ is almost constant as function of $d/\hat{l}$. However, unexpectedly, $\bar{\Lambda}^{MP}$ turns out to depend on Ra . For $Ra = 10^5$, $\bar{\Lambda}^{MP} \approx 2$, which is larger than the theoretical prediction, but similar to the ratio of the means reported in figure 2.11a. $\bar{\Lambda}^{MP}$ decreases with Ra and approaches the predicted value of 1 for $Ra = 10^9$. We note that, although this Ra dependence is not expected, it was also observed by e.g. Ref. [96].

When interpreting results for the BL thicknesses, it should be kept in mind that different definitions exist in the literature [61, 70, 89, 90, 93, 109–113]. We note that values may depend on the boundary layer definition that is employed. To get at least a sense for which of the observations transfer to other possible BL definitions, we compare the results for λ (the slope method) to those obtained by the location of the temperature and velocity levels ($\bar{\ell}$) (level method, see figure 2.4b) in figure 2.12. We note that the scalings versus Ra are very similar, albeit not exactly the same, for both definitions of the BL thickness. However, the offset between $\bar{\lambda}$ and $\bar{\ell}$ is not the same for velocity and temperature. As a consequence, there is no crossover between $\bar{\ell}_\theta$ and $\bar{\ell}_u$ within the range of Ra considered.

Figure 2.13: (a) Wind Reynolds number Re_{wind} versus Ra obtained in a periodic $\Gamma = 32$ domain compared to the corresponding values obtained by Ref. [96] and Ref. [97], both for a cylindrical $\Gamma = 1$ domain. We also show the predictions from the unifying theory [41, 42] using the updated prefactors [43]. The blue dashed line shows $Re_{\text{wind}} = (0.22 \pm 0.05) \times Ra^{0.468 \pm 0.012}$. (b) Re_s versus Ra with estimations for Ra_{crit} . In both panels, we have fitted our own data points only from $Ra = 4 \times 10^6$ onwards to achieve consistent comparisons with the data by Ref. [96], where only data from $Ra = 3 \times 10^6$ on is available. The blue dashed line shows $Re_s = (0.09 \pm 0.04) \times Ra^{0.243 \pm 0.025}$.

In figure 2.13 we compare the wind Reynolds number, which we determined as follows,

$$Re_{\text{wind}} = \langle \bar{u}_l \rangle_J H / \nu, \quad (2.10)$$

with the results of Ref. [96] and Ref. [97]. The figure shows that our Re_{wind} obtained in a periodic $\Gamma = 32$ domain with $Pr = 1$ agree surprisingly well with the results from Ref. [96] obtained in a cylindrical $\Gamma = 1$ sample with $Pr = 0.786$ and with the data of Ref. [97] for $Pr = 0.7$. The Re values obtained by Ref. [96] and Ref. [97] are slightly higher than our values. We note that the lower Pr results in slightly higher Re_{wind} . This means that the main finding in this context is that Re_{wind} in the turbulent superstructures is almost the same, perhaps slightly lower, than in a confined $\Gamma = 1$ sample. We note that the predictions for the wind Reynolds number obtained from the unifying theory for thermal convection [41, 42] are in good agreement with the data. The unifying theory, using the updated constants (see appendix A.2) found by Ref. [43], namely predicts that for $Pr = 1$ the wind Reynolds number scales as $Re_{GL} = 0.40 \times Ra^{0.44}$, while the data for $Ra \geq 4 \times 10^6$ are well approximated by $Re_{\text{wind}} = (0.22 \pm 0.05) \times Ra^{0.468 \pm 0.012}$.

To estimate when the BLs become turbulent we calculate the shear Reynolds number

$$Re_s = \frac{[\bar{u}_l \times \lambda_u^{MP}]^{\max}}{2\nu}. \quad (2.11)$$

We expect the BL to become turbulent and the ultimate regime to set in [41, 48] at $Re_s^{\text{crit}} \approx 420$ [114]. A fit to our data gives

$$Re_s = (0.09 \pm 0.04) \times Ra^{0.243 \pm 0.025}, \quad (2.12)$$

from which we can extrapolate that $Re_s^{\text{crit}} = 420$ is reached at $Ra_{\text{crit}} \approx 1.3 \times 10^{15}$. Of course, this estimate comes with a significant error bar as our data for $\Gamma = 32$ is still far away from the expected critical Ra number. Nevertheless, it agrees well with the result from Ref. [96], who find $Ra_{\text{crit}} \approx 1.2 \times 10^{14}$, and Ref. [97], who determined $Ra_{\text{crit}} = (3 \pm 2) \times 10^{13}$, both for a cylindrical $\Gamma = 1$ cell, and the results from Ref. [105] who find from experiments that $Ra_{\text{crit}} \approx 2 \times 10^{13}$. We emphasize that all these estimates are consistent with the observation of the onset of the ultimate regime at $Ra_* \approx 2 \times 10^{13}$ in the Göttingen experiments [36, 46]. As is explained by Ref. [115] also measurements of the shear Reynolds number in low Pr number simulations by Ref. [94] support the observation of the ultimate regime in the Göttingen experiments.

2.6 Conclusions

We have used a conditional averaging technique to investigate the properties of the LSC and the boundary layers in $\Gamma = 32$ RB convection for unit Prandtl number and Rayleigh numbers up to $Ra = 10^9$. The resulting quasi-two-dimensional representation of the LSC allowed us to analyze the wind properties as well as wall shear and local heat transfer. We found the distribution of the wall shear stress $\bar{\tau}_w$ to be asymmetric. The maximum of $\bar{\tau}_w$ is located closer to the plume impacting side and its value increases as $\bar{\tau}_w^{\max}/(\rho\beta gH\Delta) \sim Ra^{0.24}$ with increasing Ra . The local heat transfer at the wall, represented by the conditioned Nusselt number $\bar{Nu}$, has its highest values in the plume impacting zone at all Ra considered here. Going from the plume impacting towards the plume emitting region, $\bar{Nu}$ is seen to decrease consistently as is expected from the fluid near the hot wall heating up. However, as Ra is increased, the differences in $\bar{Nu}$ even out more and more. For the plume emitting side in particular, we were able to connect this trend to increased advective transport in the wall-normal direction at higher Ra . When extrapolating the trends for $\bar{Nu}$ to Ra higher than those available here, our results appear consistent with Ref. [108]. These authors observed a reversal of the $\bar{Nu}$ -distribution in 2D RB turbulence above $Ra \gtrsim 10^{11}$ with higher values of the heat transport in the emitting region.

Further, we examined the thermal and the viscous BLs. At low Ra , both increase along d in an approximately linear fashion, whereas flat plate boundary layer theory would suggest a growth proportional $\sqrt{d}$ [114]. As Ra increases, and especially for $d > 0$, the growth becomes successively weaker and stops entirely beyond $Ra \gtrsim 10^8$. Again, this is likely a consequence of the increased convective mixing in this region. For increasing Ra , both $\bar{\lambda}_\theta$ and $\bar{\lambda}_u$ become thinner, with $\bar{\lambda}_\theta$ showing an effective scaling of $\langle \bar{\lambda}_\theta \rangle_J/H \sim Ra^{-0.3}$. At $Ra \gtrsim 4 \times 10^6$ we observed a crossover point where the thermal BL becomes smaller than the viscous BL. It should be noted that the crossover appears specific to the definition of $\bar{\lambda}$ since a similar behavior was not observed when an alternative definition ($\bar{\ell}$, based on the location of the level) was employed. Nevertheless, the scaling behavior of $\bar{\lambda}$ and $\bar{\ell}$ was seen to be very similar. When calculating instantaneous BL ratios, a convergence to $\bar{\Lambda}^{MP} \rightarrow 1$ for high enough Ra can be observed as predicted by the PB theory for laminar BLs. As pointed out in Ref. [116], the PB limit only strictly applies to wall parallel flow and the ratio is expected to be higher if the flow approaches the

plate at an angle. This incidence angle is higher at smaller Γ which can explain why at comparable Ra the BL ratios reported in Ref. [96] are slightly higher than what is found here.

We expected to find significant differences in the LSC statistics obtained in a confined $\Gamma = 1$ system and a large $\Gamma = 32$ system. However, surprisingly, we find that the thermal BL thickness $\langle \bar{\lambda}_\theta \rangle_J$ obtained for both cases agrees very well. It turns out that the viscous BL thickness $\langle \bar{\lambda}_u \rangle_J$ is significantly larger ($\approx 55\%$ – 65%) for the periodic $\Gamma = 32$ case than in a $\Gamma = 1$ cylinder. However, the wall shear and its scaling with Ra are similar in both cases. Here we find that in a periodic $\Gamma = 32$ domain, the shear Reynolds number scales as $Re_s \sim Ra^{0.243}$. This is a bit lower than the corresponding result for $\Gamma = 1$, although one needs to keep in mind the slight difference in Pr ($Pr = 0.786$ at $\Gamma = 1$ vs. $Pr = 1$ for $\Gamma = 32$) is responsible for part of the observed difference. An extrapolation towards the critical shear Reynolds number of $Re_s^{\text{crit}} \approx 420$ when the laminar-type BL becomes turbulent predicts that the transition to the ultimate regime is expected at $Ra_{\text{crit}} \approx \mathcal{O}(10^{15})$. This is slightly higher than the corresponding result for a $\Gamma = 1$ cylinder, i.e. $Ra_{\text{crit}} \approx \mathcal{O}(10^{14})$, by [96]. However, it should be noted that considering inherent uncertainties and differences in Pr , the results for $\Gamma = 32$ agree with the observed transition to the ultimate regime in the Göttingen experiments [36, 46], as well as with previous measurements of the shear Reynolds number [96, 97]. So surprisingly, we find that in essentially unconfined very large aspect ratio systems, in which the resulting structure size is significantly larger, the differences in terms of Re_{wind} or Re_s with respect to the $\Gamma = 1$ cylindrical case are marginal.

3

Shear/buoyancy interaction in wall bounded turbulent flows*

In this chapter we describe and compare two unstably stratified turbulent flows in a channel forced by pressure gradient and wall shear, respectively, with the aim of evidencing similarities and differences in the heat transfer and flow dynamics. In both cases we find that the combination of the mean flow with the thermal forcing produces an increase of the friction coefficient and a non-monotonic dependence of the heat transfer on the mean flow strength. This behavior might be relevant for the prediction of the light-wind conditions in weather forecast or, more in general, for mixed convection applications.

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3.1 Introduction

Nature and technology have plenty of examples in which heat transport is mediated by the motion of a fluid. When the latter is the result only of the thermal induced buoyancy, we refer to as natural convection. On the other hand, if the flow features are essentially independent of the heat transfer the phenomenon is called forced convection. Most of the relevant cases occurring in reality, however, fall in between the two categories since the mean flow is forced externally but the heat transfer affects its features: these phenomena are referred to as *mixed convection*. The dynamics of atmosphere and oceans but also building ventilation or industrial cooling is most of the times in the regime of mixed convection [117] which is the most difficult to characterize.

In this context, the current practice in engineering is to rely on heat transfer and skin friction predictions for natural and forced convection and to ‘blend’ them through the Richardson number (later defined) that weights the relative importance of buoyancy and friction [118, 119]. Unfortunately, owing to the strong nonlinear nature of the equations, the interaction of the two effects can generate dynamics and structures that are found in none of the two regimes. This is certainly the case of elongated streets of clouds [120], patterns in sand dunes [121] and rows of unburned trees in forest fires [122]. Understanding in detail the heat transfer and flow dynamics in mixed convection would therefore be important either to assess the reliability of the empirical correlations and to give insights for more accurate wall models on which the simulations of real systems rely.

An additional motivation for performing this study is the transition to the ‘ultimate’ regime in natural convection, predicted by Ref. [47]. It occurs when the boundary layers become turbulent and the heat transfer increases more steeply with the thermal forcing. Unfortunately, temperature is relatively inefficient to enhance momentum and boundary layers transition to turbulence only for very high values of the forcing that has been achieved only in few experiments [46] and recently in two-dimensional numerical simulations [108]. On the other hand, despite the considerable effort and the progress of nowadays computers, this ultimate regime is still out of reach of three-dimensional numerical simulation [123] and reliable computations will not be presumably possible before one decade. However, since the boundary layer turbulence is induced by the strong wall shear, it might be possible that when the latter is introduced by a forcing exerted directly on the flow (either by a pressure

Figure 3.1: Sketch of the problem with the main flow parameters.

gradient or by a wall motion), the transition to the ultimate regime could be obtained for smaller values of the thermal forcing, affordable to the three dimensional direct numerical simulation by the present computers.

With the two motivations described above in mind, in this chapter we illustrate and discuss the results of some three-dimensional numerical simulations of the unstably stratified turbulence in a channel where the flow is forced either by an imposed pressure gradient or by an imposed wall velocity.

3.2 Problems and numerical methods

We consider the flow in a plane channel whose walls, at a distance H , are horizontal and the lower is at a temperature T_h hotter than the upper T_c ; the gravity vector is perpendicular to them and directed towards the hotter plate so that the flow is unstably stratified (figure 3.1). The flow is unbounded and periodic in the horizontal directions while the plates are no-slip and they can slide with an imposed opposite velocity u_w in the streamwise (x) direction to generate a plane Couette flow. Alternatively, the flow can be forced by a streamwise pressure gradient Π with fixed no-slip plates to enforce a plane Poiseuille flow. Following the restrictions on the size of the computational box

for the Poiseuille flow [124] we have used a domain of $\Gamma_x \times \Gamma_y = 8H \times 4H$ when the flow was forced by a pressure gradient. On the other hand, for the Couette flow, according to Ref. [125], the computational domain was increased to $\Gamma_x \times \Gamma_y = 9\pi H \times 4\pi H$ in order to accommodate the elongated flow structures. The problem is solved by integrating numerically the unsteady, incompressible, three-dimensional Navier-Stokes equations with the Boussinesq approximation for a viscous Newtonian fluid that, in non-dimensional form, read:

$$\begin{aligned} \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} &= -\nabla P - \Pi \hat{x} + \theta \hat{z} + \left(\frac{Pr}{Ra}\right)^{1/2} \nabla^2 \mathbf{u} & \nabla \cdot \mathbf{u} &= 0, \\ \frac{\partial \theta}{\partial t} + \mathbf{u} \cdot \nabla \theta &= \frac{1}{(RaPr)^{1/2}} \nabla^2 \theta. \end{aligned} \quad (3.1)$$

Here $\mathbf{u}$ is the velocity vector, P the pressure and θ the temperature fields. $\hat{x}$ and $\hat{z}$ are unit vectors pointing, respectively, in the streamwise and wall-normal directions, Π is an externally imposed pressure gradient. The length and temperature scales are H and $\Delta T = T_h - T_c$ while the velocity scale is u_w for the Couette flow and u_b , the channel bulk velocity, for the Poiseuille flow. The Rayleigh and Prandtl numbers are then defined as $Ra = g\beta\Delta TH^3/(\nu\kappa)$ and $Pr = \nu/\kappa$ being, g the gravity acceleration, β the isobaric thermal expansion coefficient, ν the kinematic viscosity and κ the thermal diffusivity of the fluid. It is useful to introduce also τ_w as the time- and surface-averaged wall viscous stress to define the friction velocity $u_\tau = \sqrt{\tau_w/\rho}$ with ρ the fluid density. If the external pressure gradient is defined as $\Pi = 2u_\tau^2/H$ the flow maintains a constant mass flow rate in time. Owing to the imposed temperature difference and the resulting wall viscous stress a heat flux $Q = \lambda \langle \partial T / \partial z \rangle_w$ will be produced being λ the thermal conductivity of the fluid and $\langle \dots \rangle_w$ the surface and time averaged value of the derivative evaluated at one of the walls. If Q is made non-dimensional by the analogous quantity obtained only for molecular conduction, the Nusselt number is obtained as $Nu = QH/(\lambda\Delta T)$. Finally, the relative importance of thermal buoyancy and wall shear on the flow dynamics can be quantified by the Richardson number $Ri = Ra/(Re^2Pr)$, with the Reynolds number $Re = uH/\nu$ and $u = u_w$ or $u = u_b$ depending if the flow is Couette or Poiseuille, respectively.

The equations are integrated numerically discretizing the variables on a staggered Cartesian mesh by central second-order accurate finite-difference schemes that, in the limit of vanishing viscous and diffusive terms and time integration error, preserve the energy of the flow. The equations are advanced

Figure 3.2: Comparison of the results obtained from the AFiD code [78] and the code by Bernardini et al. (2014) [124]. Panels (a,b) are for the Couette flow at $Re = 3000$: (a) mean streamwise velocity profile as a function of $\eta = (z - H/2)/(H/2)$; (b) mean streamwise velocity profile in wall units. (c) Friction coefficient for the Couette flow versus Reynolds number. The dashed line shows the Prandtl turbulent friction law [126]. (d) Nu as a function of Ra for pure Rayleigh-Bénard flow.

in time by a fractional-step method using low storage third-order Runge-Kutta scheme; all the terms are computed explicitly in time except for the viscous and diffusive terms with derivatives in the wall-normal direction that instead are computed implicitly. For every simulation, the spatial resolution requirements have been satisfied according to the standard of Ref. [79].

Both the numerical code for the Poiseuille- and that for the Couette-flow adopt a numerical scheme very similar to that described in Ref. [127] and they are described more in detail in Ref. [124] and Ref. [78], respectively, the latter being implemented also for GPU architectures. As a consistency check and for a cross-validation of the two codes, both of them have been used to simulate a plane Couette flow without thermal stratification ($Ra = 0$); for a Reynolds number $Re = 3000$, the mean streamwise velocity profile, both, in external and wall units is reported in figures 3.2a,b and a perfect agreement between the codes can be observed. Another important quantity for the Couette flow is the friction coefficient $C_f = 2\tau_w/(\rho u_w^2)$ that relates the imposed wall velocity with the generated wall shear stress. The results for different Reynolds numbers are reported in figure 3.2c showing that not only the two codes are in excellent

agreement but they also agree with the Prandtl turbulent friction law [126]

$$\sqrt{\frac{2}{C_f}} = \frac{1}{K} \log \left(Re \sqrt{\frac{C_f}{2}} \right) + C, \quad (3.2)$$

with the classical parameters $K = 0.41$ and $C = 5$. Further results for this flow can be found in Ref. [125]. Finally, the natural convection flow ($Re = 0$) has been computed in the range $10^6 \leq Ra \leq 10^9$ and the Nusselt number computed with the two codes, again obtaining the same results (figure 3.2d).

In the next section we will discuss some results for the flow with mechanical forcing and unstable thermal stratification. In all simulations the Rayleigh number is fixed to $Ra = 10^6$ and the Prandtl number to $Pr = 1$; the Reynolds number is instead varied in the range $0 \leq Re \leq 10^4$ to reach the buoyancy-dominated, the mixed and the shear-dominated regimes.

3.3 Results

When the flow is simultaneously driven by a mechanical forcing in the x -direction and a thermal counterpart in the z -direction there are competing effects that result in very different flow organization and global parameters. Instantaneous plane sections of the temperature field, in midplane and for the Couette-like flow, are reported in figure 3.3 for the same Rayleigh number ($Ra = 10^6$) and three different Reynolds numbers $Re = 0, 2000$ and 4000 . The parameters have been selected to show the buoyancy dominated, the intermediate and the shear-dominated regimes. It can be observed that as the Reynolds number increases the flow changes the organization from patchy with irregular x - y orientation to a more regular arrangement with a preferred streamwise direction. For different Re , either the spacing and the waviness of the elongated structures changes and the same features have been observed also in the Poiseuille flow with unstable stratification described in Ref. [129] also for a wider range of Rayleigh and Reynolds numbers.

The three dimensional structure of the elongated hot ‘streaks’ can be seen from figure 3.4 where the Couette-like flow at $Ra = 10^6$ and $Re = 3000$ is shown. It is worth mentioning that despite the turbulent nature of the flow and the intense unpredictable fluctuations, the structures are quite pinned in space and this feature does not depend on the finite size of the computational box, as recently confirmed by Ref. [130].

Figure 3.3: Instantaneous snapshots of the temperature field sampled at the plane halfway between the plates ($z = H/2$). Flow with wall shear at $Ra = 10^6$ and $Pr = 1$: a) $Re = 0$; b) $Re = 2000$; c) $Re = 4000$. (Adapted from Ref. [128]).

Figure 3.4: Perspective view of the instantaneous three-dimensional temperature field for the flow with wall shear at $Ra = 10^6$, $Re = 3000$ and $Pr = 1$. Only a hot temperature isosurface is shown and the lower plate is sliding in the positive x -direction.

Interesting results of these simulations are the evolution of the Nusselt number and friction coefficient as function of the Reynolds number reported in figure 3.5. It is quite intuitive to imagine that the thermal plumes detaching vertically in the wall-normal direction mix low- and high-momentum fluid particles thus increasing the friction with respect to the unperturbed flow: this is evident from figure 3.5b both, for the Couette- and Poiseuille-like flows, and it had been already observed by Ref. [131] as well as in the applied engineering context [119]. However, the same enhanced mixing, responsible for the increase of friction, should promote also the convective heat transfer and this is reflected in the widely used empirical correlations in the form $Nu \simeq A \times Re^b$ with A and b problem dependent parameters that are always positive [119]. In contrast with the expectations, figure 3.5a shows an initial decrease of the Nusselt number before the expected increase and this is true either for the Couette- and the Poiseuille-like flows. If the Richardson number is computed for all the simulations it appears that the minimum in the heat transfer is achieved for $Ri \simeq 1$ where buoyancy and shear effects are of the same order of magnitude. In other words it appears that when the flow is buoyancy dominated ($Ri \rightarrow \infty$) the heat is transferred by the large-scale recirculations driven only by temperature differences as in pure Rayleigh-Bénard convection. On the other hand, for the shear dominated flow ($Ri \rightarrow 0$) it is the mechanical forcing that produces the elongated flow structures responsible for the forced convective heat transfer. In the regime in between ($Ri \simeq 1$) non of the two mechanisms is effective and as a results the heat transfer is weakened.

Figure 3.5: (a) Nusselt number normalized by the value for pure thermal convection as a function of Re at $Ra = 10^6$ and $Pr = 1$. (b) Friction coefficient as a function of Re for the same flow as in panel (a).

The same behavior has been observed also for higher Rayleigh numbers in the Poiseuille-like flow [129, 132] and in the Couette-like flow [128].

3.4 Conclusions

In this chapter we have show and discussed direct numerical simulations of Poiseuille and Couette turbulent flows with unstable temperature induced stratification. The main result is that both flows show an increase of the friction coefficient that is produced by the enhanced momentum mixing due to the detachment of the thermal plumes from the walls. For the heat transfer coefficient, however, an initial decrease is observed for increasing Reynolds number until the Richardson number attains values of the order of unity. Beyond this threshold the heat transfer start increasing with Re . This study thus confirms that the regime of mixed convection ($Ri \approx 1$), where neither the buoyancy nor the shear effects dominate the flow, is the most difficult to parameterize and its behavior can not be described by ‘blending’ the asymptotic results obtained for $Ri \rightarrow \infty$ and $Ri \rightarrow 0$.

Flow organization and heat transfer in turbulent wall sheared thermal convection*

We perform direct numerical simulations of wall sheared Rayleigh-Bénard (RB) convection for Rayleigh numbers up to $Ra = 10^8$, Prandtl number unity, and wall shear Reynolds numbers up to $Re_w = 10000$. Using the Monin-Obukhov length L_{MO} we observe the presence of three different flow states, a buoyancy dominated regime ($L_{MO} \lesssim \lambda_\theta$; with λ_θ the thermal boundary layer thickness), a transitional regime ($0.5H \gtrsim L_{MO} \gtrsim \lambda_\theta$; with H the height of the domain), and a shear dominated regime ($L_{MO} \gtrsim 0.5H$). In the buoyancy dominated regime, the flow dynamics is similar to that of turbulent thermal convection. The transitional regime is characterized by rolls that are increasingly elongated with increasing shear. The flow in the shear dominated regime consists of very large-scale meandering rolls, similar to the ones found in conventional Couette flow. As a consequence of these different flow regimes, for fixed Ra and with increasing shear, the heat transfer first decreases, due to the breakup of the thermal rolls, and then increases at the beginning of the shear dominated regime. In the shear dominated regime the Nusselt number Nu effectively scales as $Nu \sim Ra^\alpha$ with $\alpha \ll 1/3$, while we find $\alpha \simeq 0.30$ in the buoyancy dominated regime. In the transitional regime, the effective scaling exponent is $\alpha > 1/3$, but the temperature and velocity profiles in this regime are not logarithmic yet, thus indicating transient dynamics and not the ultimate regime of thermal convection.

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4.1 Introduction

Rayleigh-Bénard (RB) convection, i.e. the flow in a box heated from below and cooled from above, is one of the paradigmatic fluid dynamical systems [26, 37, 39, 40]. The dynamics of RB convection driven by an imposed temperature difference is controlled by the Rayleigh number

$$Ra = \beta g H^3 \Delta / (\kappa \nu), \quad (4.1)$$

which is the non-dimensional temperature difference between the horizontal plates, and the Prandtl number

$$Pr = \nu / \kappa, \quad (4.2)$$

which is the ratio between kinematic viscosity and thermal diffusivity. In equations (4.1) and (4.2), H is the distance between the plates, β the thermal expansion coefficient of the fluid, g the gravitational acceleration, Δ the temperature difference between the top and bottom plate, and κ and ν the thermal diffusivity and kinematic viscosity, respectively. Length scales are normalized by H unless specified otherwise. While for purely thermally driven flows Ra and Pr are enough to characterize the flow, when an external shear is introduced an additional control parameter is needed. In this work, we analyze the effect of the wall shear Reynolds number

$$Re_w = H u_w / \nu, \quad (4.3)$$

where u_w is the velocity of the wall. The ratio between buoyancy and shear driving can be expressed using the bulk Richardson number

$$Ri = Ra / (Re_w^2 Pr), \quad (4.4)$$

which can be seen as alternative control parameter for either Ra or Re_w .

Important responses of the system are the Nusselt number

$$Nu = QH / (\kappa \Delta), \quad (4.5)$$

which is the dimensionless vertical heat flux, the friction Reynolds number

$$Re_\tau = H u_\tau / \nu, \quad (4.6)$$

and the skin friction coefficient

$$C_f = 2\tau_w/(\rho u_w^2). \quad (4.7)$$

Here $Q = \overline{w'T'} - \kappa\partial T/\partial z$ is the constant vertical heat flux, with w' and T' the fluctuations for wall-normal velocity and temperature, respectively, and $u_\tau = \sqrt{\tau_w/\rho}$ the friction velocity, with τ_w the mean wall shear stress and ρ the density of the fluid.

For pure RB convection ($Re_w = 0$) and strong enough thermal driving, i.e. high enough Ra , the flow in the bulk region becomes fully turbulent. For even stronger thermal driving, beyond some critical Ra number Ra_c , the boundary layers also become turbulent, and the system reaches the regime of so-called ultimate convection [41,42,47,48]. This ultimate regime sets in when the shear Reynolds number at the boundary layers is sufficiently high so that the boundary layer becomes turbulent, leading to a strong increase in the heat transport, quantified by the Nusselt number. Ref. [35] found that the transition to the ultimate regime sets in around $Ra_c \sim \mathcal{O}(10^{14})$. While in the classical regime one generally finds $Nu \sim Ra^{0.31}$, in the experimentally accessible ultimate regime an effective scaling of $Nu \sim Ra^{0.38}$ is observed, in agreement with theoretical predictions [48].

The transition to the ultimate regime has also been observed in direct numerical simulations (DNS) of two-dimensional RB convection [108]. In Taylor-Couette flow, which is an analogous system, experiments and DNS have observed the ultimate regime as well [133]. However, so far, the ultimate regime has not yet been achieved in DNS of three-dimensional RB flows [80,134] as the required computational time to achieve this is still out of reach. Here, in an attempt to trigger the transition to the ultimate regime, we add a Couette type shearing to the RB system to increase the shear Reynolds number in the boundary layers.

In Couette flow the top and bottom walls move in opposite directions [53, 135, 136] with constant u_w and just as in other examples of wall-bounded turbulence [32,137,138] the flow is dominated by elongated streaks, which have been observed in experiments [139] and DNS [140,141], even at relatively low shear Reynolds numbers [142]. Ref. [125,143] and Ref. [144] showed that these streaks in Couette flow have much longer characteristic length scales than in Poiseuille flow, where the flow is forced by a uniform pressure gradient rather than by wall shear. Ref. [145] showed that these large-scale flow structures even survive when the small-scale structures are artificially suppressed. Recently, Ref. [130] found that the streak length increases with increasing shear Reynolds

number and that some correlation in the streamwise direction remains visible up to a length of almost 160 times the distance between the plates.

Investigating the interaction between buoyancy and shear effects is also very important to better understand oceanic and atmospheric flows [146–148]. For example, early experiments on sheared thermal convection by Ref. [149] and Ref. [150] showed the appearance of large-scale structures. Ref. [151] showed that in channel flow unstable stratification increases the longitudinal velocity fluctuations close to the wall, while in the bulk region, the temperature fluctuations are drastically lowered. Furthermore, recent experiments by Ref. [152] investigated the plume spacing in sheared convection and found a scaling law that connects the mean spacing of the plumes with Re_w , Ra , and Pr .

Early simulations of sheared convection were performed by Ref. [153] and Ref. [154] for $Ra \lesssim \mathcal{O}(10^5)$. Ref. [154] found that in Couette-RB flow the addition of shear at low Ra initially increases the heat transport. However, for $Ra \gtrsim 150,000$ the heat transport decreases as the added shear breaks up the large-scale structures. More recently, Ref. [131, 155] showed that also in Poiseuille-RB the heat transfer first decreases when the applied pressure gradient is increased. The reason is that for intermediate forcing the longitudinal wind disturbs the thermal plumes, which therefore lose their coherence. Only with a strong enough pressure gradient, a heat transfer enhancement is found.

The Richardson number quantifies the ratio between the buoyancy and shear forces in Couette-RB and Poiseuille-RB based on the applied temperature difference and wall shear Reynolds number. Another way to quantify the ratio between buoyancy and shear forces is to determine the Monin-Obukhov length [156, 157]

$$L_{MO}/H = u_\tau^3 / (\overline{w'\theta'} \beta g H), \quad (4.8)$$

which indicates up to which distance from the wall the flow is dominated by shear. Note that L_{MO}/H is a response parameter, in contrast to Ri , which is a control parameter. Ref. [129] found that the Monin-Obukhov length scales as $L_{MO}/H \approx 0.15/Ri^{0.85}$ for channel flow with unstable stratification. In appendix B.1 we show that here for Couette-RB $L_{MO}/H \approx 0.16/Ri^{0.91}$.

In this study, we investigate the effect of an additional Couette type shearing on the heat transfer in RB convection in an attempt to trigger the boundary layers to become fully turbulent and hence observe the transition to the ultimate regime. Figure 4.1 shows a flow visualization of the temperature field obtained from one of our simulations, which reveals large-scale meandering streaks that are formed near the hot plate. We performed simulations over a

Figure 4.1: Volume rendering of the thermal structures rising from the heated plate in a simulation with $Ra = 4.6 \times 10^6$ and $Re_w = 8000$. The plate dimensions are $9\pi H \times 4\pi H$, in streamwise and spanwise direction, respectively, where H is the distance between the plates. The red colors show hot thermal structures emerging from the hot plate, while the blue structures show vorticity formations in the flow. For further details of the flow visualization, see Ref. [158].

Figure 4.2: (a) Streamwise (n_x) resolution used in the simulations as function of Ra and Re_w , see table 4.2 for details. (b) Re_τ versus Re_w obtained from the simulations. In agreement with Ref. [125] and Ref. [159] we find that $Re_\tau \sim Re_w^{0.87}$ for large Re_w .

wide parameter range, spanning $10^6 \leq Ra \leq 10^8$ and $0 \leq Re_w \leq 10^4$, while $Pr = 1$ has been used in all cases, see figure 4.2a. Despite the very strong forcing for the largest Ra and Re_w , we did not yet achieve ultimate turbulence. We were limited by our requirement of using large domain sizes as recommended by Ref. [129] to ensure convergence of the main flow properties.

The remainder of this chapter is organized as follows. In §4.2 we present the simulation method. We discuss the heat transfer and skin friction measurements in §4.3.1 and §4.3.2, respectively. A discussion of the identified flow regimes is given in §4.4. The concluding remarks follow in §4.5.

4.2 Simulation details

We numerically solve the three-dimensional incompressible Navier-Stokes equations within the Boussinesq approximation, which in non-dimensional form read:

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla P + \left(\frac{Pr}{Ra}\right)^{1/2} \nabla^2 \mathbf{u} + \theta \hat{\mathbf{z}}, \quad \nabla \cdot \mathbf{u} = 0, \quad (4.9)$$

N_x	N_y	N_z	Re_τ	L_{MO}/H	Nu	$C_f/10^{-3}$
1024	512	384	708.0	0.138	25.66	10.03
1296	648	384	703.6	0.137	25.37	9.902
1536	768	384	700.6	0.137	25.19	9.818
1728	864	384	700.0	0.136	25.15	9.805

Table 4.1: Grid convergence study for $Ra = 1.0 \times 10^8$, $Pr = 1$, and $Re_w = 10000$ in a $2\pi H \times \pi H \times H$ domain. N_x , N_y , N_z indicate the resolution in the streamwise (x), spanwise (y), and wall-normal (z) direction, respectively. The other columns show the friction Reynolds number Re_τ , the Monin-Obukhov length L_{MO}/H , the Nusselt number Nu , and the friction coefficient C_f . Additional information on the grid convergence study is provided in figure 4.3.

$$\frac{\partial \theta}{\partial t} + \mathbf{u} \cdot \nabla \theta = \frac{1}{(RaPr)^{1/2}} \nabla^2 \theta, \quad (4.10)$$

with $\mathbf{u}$ the velocity non-dimensionalized by the free-fall velocity $\sqrt{g\beta H\Delta}$, t the time non-dimensionalized by $\sqrt{H/(g\beta\Delta)}$, θ the temperature non-dimensionalized by the temperature difference between the plates Δ , and P the kinematic pressure non-dimensionalized by $g\beta\Delta H$. All our length scales are non-dimensionalized by H , implying that we set the plate distance to unity in this work.

To solve equations (4.9) - (4.10) we employ the second-order finite difference code AFiD [77], which has been validated many times against other numerical and experimental results [76, 80, 102–104, 134, 160]. The code uses periodic boundary conditions with uniform mesh spacing in the horizontal directions and supports a non-uniform grid distribution in the wall-normal direction. For this study, we used the GPU version of the code [78] to allow efficient execution of many large-scale simulations. The Couette flow forcing is realized by moving both walls in opposite directions with a velocity of u_w , and the results for the classic Couette flow case match excellently with the results by Ref. [125]. For example, figure 4.2b shows that for Couette flow $Re_\tau \sim Re_w^{0.87}$, which agrees very well with the Couette data of Ref. [125] and Ref. [159].

All simulations in this study were performed in a large $9\pi H \times 4\pi H \times H$ box, in streamwise, spanwise and wall-normal direction [125, 141], which is required to capture the large-scale structures formed in Couette flow [125, 130, 159]. We adopted the grid distribution used by Ref. [125, 129], which is based on the resolution requirements for pure buoyant flow [79] and pure channel flow [124], which is very similar to our flow configuration. The average

Figure 4.3: (a) Nu and (b) the streamwise velocity fluctuations for simulations at $Ra = 10^8$ and $Re_w = 10000$ performed using different grid resolutions. The simulations are performed in a box of $2\pi H \times \pi H \times H$ in streamwise, spanwise, and vertical direction, respectively. The displayed resolutions indicate the extrapolated streamwise resolutions that correspond to the full $9\pi H \times 4\pi H \times H$ box, see table 4.1 for details. Note that the simulation results are converged for the grid resolution used in this study.

horizontal grid spacing in the mixed convection simulations is $\Delta_{x,y}^+ \lesssim 4$. In the wall-normal direction the boundary layer are resolved up to 1.6 Kolmogorov lengths. For the case at $Ra = 10^8$ and $Re_w = 10000$, i.e. the most challenging simulation of this study, we used a horizontal grid spacing of less than three wall units in both horizontal directions. There are 54 grid points in each boundary layer to ensure that the boundary layers are resolved up to 1.3 Kolmogorov lengths. We present a grid refinement check, which was performed in a smaller $2\pi H \times \pi H \times H$ domain to keep the test manageable, for this case in table 4.1. Figure 4.3 confirms that the simulations are fully resolved for the chosen resolution. As further validation, we show in §4.3.2 that our data excellently agree with the Couette data from Ref. [125]. We make sure that all simulations have reached the statistically stationary state before collecting data. Table 4.2 shows the simulation parameters for the main cases presented in this study.

Ra	Pr	Re_w	N_x	N_y	N_z	Re_τ	Ri	L_{MO}/H	Nu	$C_f/10^{-3}$
0	1	2000	1280	1024	256	131.9	0	0	0	8.695
0	1	3000	1280	1024	256	185.8	0	0	0	7.673
0	1	4000	1280	1024	256	238.1	0	0	0	7.089
0	1	6000	1280	1024	256	340.6	0	0	0	6.446
0	1	8000	2048	1280	256	439.7	0	0	0	6.041
0	1	10000	3072	1536	256	540.9	0	0	0	5.852
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1.0×10^6	1	0	1280	1024	256	—	∞	0	8.343	∞
1.0×10^6	1	2000	1280	1024	256	161.7	0.250	0.645	6.557	13.07
1.0×10^6	1	3000	1280	1024	256	203.0	0.111	1.218	6.869	9.158
1.0×10^6	1	4000	1280	1024	256	251.7	0.063	2.022	7.891	7.922
1.0×10^6	1	6000	2048	1280	256	355.2	0.028	4.259	10.52	7.008
1.0×10^6	1	8000	3072	1536	256	452.2	0.016	7.212	12.82	6.390
1.0×10^6	1	10000	4608	2304	320	554.3	0.010	11.00	15.49	6.145
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2.2×10^6	1	0	1280	1024	256	—	∞	0	10.40	∞
2.2×10^6	1	2000	1280	1024	256	176.3	0.550	0.316	7.866	15.53
2.2×10^6	1	3000	1280	1024	256	215.3	0.244	0.583	7.788	10.30
2.2×10^6	1	4000	1280	1024	256	261.9	0.138	0.953	8.568	8.576
2.2×10^6	1	6000	2048	1280	256	363.0	0.061	1.983	10.96	7.319
2.2×10^6	1	8000	4096	2048	256	462.8	0.034	3.351	13.44	6.692
2.2×10^6	1	10000	4608	2304	320	566.4	0.022	5.123	16.12	6.416
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4.6×10^6	1	0	1280	1024	256	—	∞	0	12.83	∞
4.6×10^6	1	2000	1280	1024	256	190.2	1.150	0.156	9.353	18.09
4.6×10^6	1	3000	1280	1024	256	237.3	0.511	0.306	9.502	12.51
4.6×10^6	1	4000	1280	1024	256	276.1	0.288	0.475	9.626	9.526
4.6×10^6	1	6000	2048	1280	256	377.2	0.128	0.982	11.88	7.903
4.6×10^6	1	8000	4096	2048	256	474.0	0.072	1.645	14.08	7.021
4.6×10^6	1	10000	4608	2304	320	578.7	0.046	2.513	16.76	6.697

Table 4.2: Main simulations considered in this work.

Ra	Pr	Re_w	N_x	N_y	N_z	Re_τ	Ri	L_{MO}/H	Nu	$C_f/10^{-3}$
1.0×10^7	1	0	1280	1024	256	—	∞	0	16.18	∞
1.0×10^7	1	2000	1280	1024	256	213.2	2.500	0.078	12.41	22.73
1.0×10^7	1	3000	1280	1024	256	265.8	1.111	0.156	12.02	15.69
1.0×10^7	1	4000	1280	1024	256	306.0	0.625	0.243	11.78	11.70
1.0×10^7	1	6000	2048	1280	256	391.2	0.278	0.466	12.85	8.502
1.0×10^7	1	8000	4096	2048	256	493.4	0.156	0.785	15.30	7.607
1.0×10^7	1	10000	6144	3072	320	595.0	0.100	1.180	17.85	7.080
2.2×10^7	1	0	3072	1536	256	—	∞	0	19.86	∞
2.2×10^7	1	2000	3072	1536	256	236.4	5.500	0.036	16.62	27.94
2.2×10^7	1	3000	3072	1536	256	296.5	2.445	0.075	15.77	19.53
2.2×10^7	1	4000	3072	1536	256	341.4	1.375	0.119	15.24	14.57
2.2×10^7	1	6000	3072	1536	256	429.1	0.611	0.233	15.43	10.23
2.2×10^7	1	8000	4096	2048	256	514.0	0.344	0.374	16.52	8.255
2.2×10^7	1	10000	6144	3072	320	607.6	0.220	0.552	18.01	7.383
1.0×10^8	1	0	4096	2048	256	—	∞	0	31.14	∞
1.0×10^8	1	2000	4096	2048	256	283.9	25.00	0.007	29.34	40.31
1.0×10^8	1	3000	4096	2048	256	360.1	11.11	0.017	27.85	28.82
1.0×10^8	1	4000	4096	2048	256	425.7	6.250	0.029	26.83	22.66
1.0×10^8	1	6000	4608	2304	320	534.7	2.778	0.059	25.81	15.88
1.0×10^8	1	8000	6144	3072	320	628.5	1.563	0.097	25.72	12.35
1.0×10^8	1	10000	6912	3456	384	713.3	1.000	0.139	26.03	10.18

Table continued from previous page.

Figure 4.4: Nu as a function of Ra and Re_w in Couette-RB flow.

4.3 Global flow characteristics

4.3.1 Effective scaling of the Nusselt number

Figure 4.4 shows that the heat transfer increases with increasing Ra and Re_w and that for a given Ra number a minimum heat transfer is obtained at some intermediate Re_w . Ref. [155] showed that the minimum is caused by the thermal plumes being swept away by the shear. Figure 4.5a shows cross-sections for constant Ra which reveal that the location of the minimum heat transfer at constant Ra shifts towards higher Re_w with increasing Ra . For high enough Re_w , the behavior of Nu converges towards $Nu \sim 0.0013Re_w$. Figure 4.5b, where Nu is normalized by the RB value for the respective Ra , shows that the drop in Nu becomes less pronounced and is observed at higher Re_w when Ra is increased. This is a good indication that the thermal plumes become stronger and therefore harder to disturb by the applied shear. For $Ra = 10^8$ the decrease in Nu at $Re_w = 2000$ is only $\sim 5\%$ while the data for other Ra show percentages up to the high twenties. A more detailed analysis would need more data points for low Re_w , which are difficult to obtain due to

Figure 4.5: (a) Nu and (b) Nu normalized by the RB value $Nu_{Re_w=0}$ as a function of Re_w .

the computational time that is required for each simulation.

The results indicate that the heat transfer is influenced by the ratio of the buoyancy and shear forces. Therefore the bulk Richardson number Ri or the above-defined Monin-Obukhov length, which take the ratio of these forces into account, are natural control and response parameters to identify the different flow regimes. Although the Monin-Obukhov theory itself is only valid for shear dominated flow, which does not necessarily exist in all our simulations, we use the Monin-Obukhov length as an objective criterion to distinguish between buoyancy and shear driven flow. This choice builds on a long and rich tradition to use the Monin-Obukhov length to characterize mixed convective flows, namely on the seminal works by Ref. [161] and Ref. [156]. Its use has significantly advanced the understanding of mixed convective flows. The Monin-Obukhov length is relevant as it characterizes the effects of both friction and buoyancy, the main physical effects in this system, by a single length scale. Also, in this case, we show that the Monin-Obukhov length is a relevant parameter that gives insight into the behavior of the flow. From the data in table 4.2, we find $L_{MO}/H \approx 0.16/Ri^{0.91}$ (see appendix B.1). In figure 4.6a the Monin-Obukhov length is compared to the thermal boundary layer thickness λ_θ , which is determined from $\lambda_\theta = H/(2Nu)$. Since L_{MO}/H is the fraction of the domain in which the shear forcing is dominant $L_{MO} \geq 0.5H$ indicates when the flow is completely shear dominated. This allows us to define three different flow regimes, namely a buoyancy dominated regime ($L_{MO} \lesssim \lambda_\theta$), a transitional regime ($0.5H \gtrsim L_{MO} \gtrsim \lambda_\theta$), and a shear dominated regime ($L_{MO} \gtrsim 0.5H$). At the moment we cannot more accurately

Figure 4.6: (a) The Monin-Obukhov length as function of Ra for different Re_w . The Monin-Obukhov length (solid lines) is compared to the thermal boundary layer thickness (dashed lines) and to 0.5 to define the flow regime (buoyancy dominated, transitional, shear dominated) of each simulation, see details in the text. Open symbols indicate $L_{MO} < 0.5H$. See appendix B.2 for more information. (b) Nu as function of Ra . The numbers indicate the scaling exponent α in $Nu \sim Ra^\alpha$. The $\alpha = 0.37$ effective scaling line is plotted for visual reference only.

determine the Monin-Obukhov length at which the transition takes place, but the presented ranges provide a good indication of the required thermal and shear forcing to achieve the different regimes. A similar behavior has also been observed in convective boundary layers, where Ref. [162] find a cell dominated regime for $-z_i/L_{MO} \gtrsim 20$, where z_i is the convective boundary layer thickness, a cell and roll dominated regime as transitional state, and a roll dominated regime for $-z_i/L_{MO} \lesssim 5$.

Figure 4.6b shows that the heat transfer in the buoyancy dominated regime scales as $Nu \simeq Ra^{0.30}$, which is in agreement with results for classical RB convection ($Re_w = 0$, Ref. [26]). For the shear dominated regime we find that the effective scaling exponent α in $Nu \sim Ra^\alpha$ is $\alpha \ll 1/3$ and in the transitional regime we find $\alpha > 1/3$. An effective scaling exponent larger than $1/3$ is one of the characteristics of the ultimate regime. It should occur when the boundary layers have transitioned to the turbulent state, which is indicated by their logarithmic profiles. Our analysis in §4.4.2 shows that this is not yet the case in this transitional regime. Instead, for intermediate shear, the heat transfer is decreased with respect to the RB case. The locally larger effective scaling exponent simply is a consequence of the fact that with increasing Ra the heat transfer, which was decreased at intermediate shear, must again converge to the RB case.

Figure 4.7: (a) Skin friction coefficient C_f as a function of Re_w . (b) Zoom-in of the gray area shown in panel (a), now on a logarithmic scale, showing the data for pure Couette flow ($Ra = 0$, stars) and $Ra = 10^6$. Note that $C_f(Ra = 0)$ follows the expected laminar result (---) until $Re_w = 650$ – 700 and then jumps to the turbulent curve ($\cdots$). For Couette-RB, i.e. the up-pointing triangle, no jump is observed.

4.3.2 Skin Friction

In figure 4.7 we compare the measured skin friction coefficient for different Re_w and Ra with Prandtl’s turbulent friction law [163]:

$$\sqrt{\frac{2}{C_f}} = \frac{1}{\mathcal{K}} \log \left(Re_w \sqrt{\frac{C_f}{2}} \right) + C. \quad (4.11)$$

Following Ref. [125] we use a von Kármán constant $\mathcal{K} = 0.41$ and $C = 5$. The figure shows that the skin friction increases with Ra and decreases with Re_w . At fixed Ra the relative strength of the thermal forcing decreases for high Re_w , and therefore the obtained friction coefficient converges to the Prandtl law. This agrees very well with the findings of Ref. [131] and Ref. [129] for Poiseuille-RB flow. In figure 4.7b we focus on the data for small Re_w . The skin friction in pure Couette flow follows the expected laminar result $C_f = 4/Re_w$ [4] until a transition to the turbulent state occurs around $Re_w = 650$ – 700 . Ref. [164] discuss that in pipe flow this jump is caused by the formation of puffs and slugs. Ref. [165] attribute this discontinuous jump in C_f to the lack of restoring forces in plane Couette flow (similar to pipe, channel, and boundary layer flows). For the Couette-RB case we do not observe such a discontinuous jump.

Figure 4.8: Instantaneous snapshots of temperature fields at mid-height for a subdomain of the parameter space, see figure 4.2a and table 4.1, focusing on $Ra = 1.0 \times 10^6$ – 2.2×10^7 and $Re_w = 0$ –4000. The panels have colored borders depending on the flow regime they display: buoyancy dominated (white), transitional (blue), and shear dominated (orange) regime. An overview of temperature fields over the whole domain can be found in appendix B.3. The color range for the snapshots in this figure and in figures 4.9, 4.10, 4.11, and B.3 is adjusted such that the most important thermal structures are clearly visible.

Instead, this sheared RB case is another example, next to the application of Coriolis, buoyancy, and Lorentz forces discussed by Ref. [165], which shows that restoring forces can prevent a discontinuous jump in $C_f(Re_w)$. Ref. [142], on the other hand, claim that all transitions to turbulence should be continuous if the used box size is large enough. From this figure we can also judge whether the boundary layer is turbulent or not. When the slope of C_f approaches the one of pure Couette flow the boundary layers are turbulent. We consider the boundary layer as non-turbulent when this slope starts to strongly deviate from the Prandtl law.

4.4 Local flow characteristics

4.4.1 Organization of turbulent structures

To further investigate the dynamics of the different regimes we show visualizations of the temperature field for all simulations in figure 4.8 and appendix B.3. We decided to show the flow at mid-height because there the flow is least affected by the walls. In the buoyancy dominated regime the primary flow structure resembles the large-scale flow found in RB convection [98]. In the transitional regime ($L_{MO} \lesssim 0.5H$), the thermal forcing dominates part of the bulk where large elongated thermal plumes transform into thin straight elongated streaks when L_{MO} approaches $0.5H$. In figure 4.8 and in the appendix this manifests itself as a very visual line diagonally through the diagram, splitting the more thermal and the more shear dominated cases. In the shear dominated regime ($L_{MO} \gtrsim 0.5H$) we find large-scale meandering structures, similar to the ones found in pressure-driven channel flow with unstable stratification [129]. This significant change in flow structure can be linked to the minimum in Nu in figure 4.5. The reason for the minimum is that at intermediate shear the thermal convection rolls are broken up, while the shear is not yet strong enough to increase the heat transfer directly. This observation is in agreement with earlier works described above [129, 131, 154, 155].

In figure 4.9 we present a clear overview of the behavior of the flow structures versus the flow control parameters combined in the bulk Richardson number. On the left side, we compare the different values of Ri with the visually observed flow structures. We find a range of Ri in which the flow

Figure 4.9: Left: Ri versus Re_w for different Ra . Open symbols indicate the presence of thin straight elongated streaks (see third snapshot from top). The dashed line indicates $L_{MO} = 0.5H$. In the middle: instantaneous snapshots of temperature fields at mid-height. Right: Nu as a function of Ri for different Re_w . An indication of the effective scaling exponent γ in $Nu \sim Ri^\gamma$ in the different regimes is also given. For a more detailed quantification of the different flow regimes in the presented snapshots, we refer to the Monin-Obukhov lengths documented in table 4.2.

undergoes a change from the transitional to the shear dominated regime. This happens in a range of $0.2 \lesssim Ri \lesssim 0.7$. In the right panel, we can also detect this trend, where the effective scaling exponent γ in $Nu \sim Ri^\gamma$ changes from $\gamma = 0.05 \pm 0.01$ to $\gamma = 0.37 \pm 0.02$. We note that more data points would be necessary to define the transition point more accurately.

Figure 4.9 combines these findings with the above observation that in the shear dominated regime the effective scaling exponent α in $Nu \sim Ra^\alpha$ is much smaller than $1/3$, in the transitional regime $\alpha > 1/3$, and in the buoyancy dominated regime $\alpha \simeq 0.30$. When we compare the regime transitions with the results in figure 4.5 it becomes clear that the lowest heat transfer for a given Ra occurs at the end of the transitional regime before the emergence of the thin straight elongated streaks. Due to the large computational time that is required for each simulation the number of considered cases is limited, which makes it difficult to pinpoint exactly when the heat transfer is minimal and what the flow structure looks like in that case. However, we note that the onset of the shear dominant regime corresponds to the point where the heat transfer starts to increase as the additional shear can then more effectively enhance the overall heat transport.

To get more insight into the boundary layer dynamics in the different regimes, we show the temperature and streamwise velocity at the boundary layer height for $Ra = 4.6 \times 10^6$ in figure 4.10. At this Rayleigh the flow is

Figure 4.10: Instantaneous near-wall snapshots at $z^+ \approx 0.5$ of the temperature (left) and streamwise velocity (right) for $Ra = 4.6 \times 10^6$. Re_w increases from top to bottom. For a more detailed quantification of the different flow fields in the presented snapshots, we refer to the values for the Monin-Obukhov length in table 4.2. The color range for the snapshots in this figure is adjusted such that the most important thermal structures are clearly visible.

in the transitional regime for $Re_w = 2000$ and $Re_w = 3000$, and in the shear dominant regime for $Re_w \geq 4000$. For all cases we observe a clear imprint of the large-scale structures observed at mid-height, see figure 4.8 and appendix B.3. This indicates that the large-scale dynamics have a pronounced influence on the flow structures in the boundary layers [98]. The figure also reveals that in the transitional and shear dominated regime the lowest temperatures at boundary layer height are observed in the high-speed streak regions, which indicates that the regions with the highest shear contribute most to the overall heat flux.

4.4.2 Flow statistics

We now present the streamwise temperature variance spectra $E_\theta(k)$ in figure 4.11 to analyze the size of the large-scale structures as function of the Monin-Obukhov length. The position of the peak in the temperature spectrum indicates the wavelength of the most prominent thermal structure [98]. In panel (b) and (c) we plot the evolution of these wavelengths versus the absolute size of the flow domain. Therefore we define $k_{x_{peak}}$ and $k_{y_{peak}}$ as the wavenumbers of the peak in the respective energy spectrum and $\ell_x = 2\pi/k_{x_{peak}}$ and $\ell_y = 2\pi/k_{y_{peak}}$ as the respective wavelengths. If the spectrum does not show a clear peak but keeps growing for small k , the structure size is limited by the box size, which is $\Gamma_x = 9\pi$ in streamwise (figure 4.11b) and $\Gamma_y = 4\pi$ in spanwise direction (figure 4.11c).

For $L_{MO} \rightarrow \infty$, $\ell_x \approx \Gamma_x H$, which is expected since for pure Couette flow, structures much larger than 9π are expected [130]. $\ell_y \approx 0.8\pi H = 0.2\Gamma_y H$ for the highest shear case, but here more data points are needed for a clearer determination of its behavior. In the other limit of $L_{MO} \rightarrow 0$, i.e. in the transitional regime as the RB case (buoyancy dominated regime) is not shown due to the logarithmic axis, the large-scale structures are elongated over the whole streamwise length, which is consistent with figure 4.8 and appendix B.3. For pure RB convection, where $L_{MO} = 0$, ℓ_x decreases to $\ell_x \approx 2\pi H$, which is in agreement with Ref. [98]. In the spanwise direction, the flow converges already much earlier to the RB case where $\ell_y \approx 2\pi H = 0.5\Gamma_y H$. In the shear dominated regime, where the flow meanders, the structure size in streamwise direction drops to about half the box length. In the spanwise direction, this flow regime is present as a local peak in panel (c). Due to the minimal number of data points, it is not possible to fully assess the behavior of ℓ_x and ℓ_y versus

Figure 4.11: (a) Overview of streamwise temperature variance spectra at mid-height at $Ra = 4.6 \times 10^6$ for the different flow regimes. (b,c) Shows the evolution of peaks in streamwise and spanwise temperature variance spectra, respectively, versus the Monin-Obukhov length. The spectra were evaluated on three-dimensional snapshots and are subsequently time-averaged.

Figure 4.12: (a) Mean streamwise velocity and (b) temperature profiles, where $u^+ = u/u_\tau$ and, following Ref. [129], $T^+ = T/T_\tau$ with the friction temperature $T_\tau = Q/u_\tau$ for $Ra = 4.6 \times 10^6$.

L_{MO} for all Ra and Re_w . Nevertheless, the minimum in ℓ_x and peak in ℓ_y in the shear dominated regime are very distinct.

To further quantify the cases shown in figure 4.10, in figure 4.12 we show the streamwise velocity and temperature profiles for fixed $Ra = 4.6 \times 10^6$ and increasing Re_w from 2000 to 10000. As can be seen, for the wall Reynolds number in the transitional range up to $Re_w \approx 4000$ (see corresponding curve in figure 4.9a) neither the temperature nor the streamwise velocity profiles are logarithmic. This indicates that the boundary layers are not yet turbulent in this state. Hence, the higher Nu scaling in this transitional regime is not caused by a triggered transition to the ultimate regime. Note that spatio-temporally chaotic flow with thermal plume detachment from the walls must not be confused with turbulent flow. The temporal fluctuations in this regime can in fact be considerable, but given the small shear Reynolds numbers, the flow is still not turbulent. Here we use the definition of turbulence as absence of large-scale coherence in space and time.

In contrast, in the shear dominated regime (beyond $Re_w \approx 4000$ for this $Ra = 4.6 \times 10^6$) the streamwise velocity and temperature profiles do start to converge to a logarithmic profile with further increasing Re_w , reflecting the onset of the ultimate regime. This observation is in agreement with previous findings for Couette-RB [166–169] and Poiseuille-RB [129, 131].

In figure 4.13 we show the same statistical quantities as in figure 4.12, but now for fixed $Re_w = 6000$. For $Ra \gtrsim 10^7$ the flow is in the transitional regime and for $Ra \lesssim 10^7$ the flow undergoes a transition into the shear dominated regime. Just as in figure 4.12 we observe that the temperature and streamwise velocity profiles are not logarithmic in the transitional regime. As the Richardson number decreases with decreasing Ra , we see that the profiles converge towards a logarithmic behavior. From a comparison with table 4.2 we find that

Figure 4.13: (a) Mean streamwise velocity and (b) temperature profiles, where $u^+ = u/u_\tau$ and $T^+ = T/T_\tau$ with $T_\tau = Q/u_\tau$ for $Re_w = 6000$. $T_{Ra=0}^+$ was determined through a passive-scalar temperature field.

$Ri \lesssim 0.2$ seems to be required to achieve logarithmic temperature and velocity profiles. A comparison with the results shown in figure 4.9 confirms that $Ri \approx 0.2$ is indeed the threshold where the flow undergoes its transition to the shear dominated regime. This is also consistent with the work of Ref. [129], who report a regime with the increased importance of friction at $Ri \approx 0.1$. For the parameter regime under investigation, the effective scaling exponent α in the shear dominated regime is well below $1/3$. In both figures we can detect a non-monotonic behavior of both u^+ and T^+ for low Re_w and high Ra . The non-monotonic temperature profile indicates the formation of different flow layers, i.e. heat that is carried by hot plumes originating from the bottom plate gets entrapped somewhere in the middle of the domain. Similarly, some of the cold plumes originating from the top plate also get trapped. Several further statistical quantities are presented in appendix B.4.

4.5 Conclusions

We performed direct numerical simulations of turbulent thermal convection with Couette type flow shearing. We presented cases in a range $10^6 \leq Ra \leq 10^8$ and $0 \leq Re_w \leq 10^4$, achieving up to $Re_\tau \approx 710$. For fixed Rayleigh number we obtain a non-monotonic progression of Nu similarly to what was previously observed in unstable stratification with a pressure gradient [155]. The addition of imposed shear to thermal convection first leads to a reduction of the heat transport by disrupting the turbulent system before the shear becomes strong enough to create meandering streaks that efficiently transport the heat away

from the wall. As the impact of the thermal plumes on the flow decreases with increasing shear, the skin friction coefficient at constant Ra drops with increasing Re_w .

Using the Monin-Obukhov length L_{MO} and the thermal boundary layer thickness λ_θ , we identify three flow regimes. In the buoyancy dominated regime ($L_{MO} \lesssim \lambda_\theta$) large thermal plumes dominate the flow. With decreasing Richardson number we first find a transitional regime ($0.5H \gtrsim L_{MO} \gtrsim \lambda_\theta$), before the shear dominated flow regime with large-scale meandering streaks is obtained. For given Ra the minimum heat transport is found before the onset of this shear dominated regime when thin straight elongated streaks dominate the flow. We find that in the transitional regime the effective scaling exponent α in $Nu \sim Ra^\alpha$ is larger than $1/3$. An analysis of the flow characteristics shows that the temperature and streamwise velocity profiles are not logarithmic in this transitional regime, which one would expect when this high scaling exponent would indicate the onset of the ultimate regime. We want to investigate in future studies whether it is possible to further increase the thermal and sheared forcing far enough to trigger the occurrence of a logarithmic velocity profile in the boundary layer and thus the ultimate convection in Couette-RB, but considerably more CPU-time is required for that.

5

The effect of the Prandtl number on turbulent sheared thermal convection*

In turbulent wall sheared thermal convection, there are three different flow regimes, depending on the relative relevance of thermal forcing and wall shear. In this paper we report the results of direct numerical simulations of such sheared Rayleigh-Bénard convection, at fixed Rayleigh number $Ra = 10^6$, varying the wall Reynolds number in the range $0 \leq Re_w \leq 4000$ and Prandtl number $0.22 \leq Pr \leq 4.6$, extending our prior work by [128], where Pr was kept constant at unity and the thermal forcing (Ra) varied. We cover a wide span of bulk Richardson numbers $0.014 \leq Ri \leq 100$ and show that the Prandtl number strongly influences the morphology and dynamics of the flow structures. In particular, at fixed Ra and Re_w , a high Prandtl number causes stronger momentum transport from the walls and therefore yields a greater impact of the wall shear on the flow structures, resulting in an increased effect of Re_w on the Nusselt number. Furthermore, we analyze the thermal and kinetic boundary layer thicknesses and relate their behavior to the resulting flow regimes. For the largest shear rates and Pr numbers, we observe the emergence of a Prandtl- von Karman log-layer, signaling the onset of turbulent dynamics in the boundary layer.

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5.1 Introduction

Buoyancy and shear are crucial processes in fluid dynamics and key for many flow related phenomena in nature and technology. A paradigmatic example of buoyancy driven flow is Rayleigh-Bénard (RB) convection, a system where the fluid is heated from below and cooled from above [26, 37, 39, 40]. The flow is controlled by the Rayleigh number $Ra = \beta g H^3 \Delta / (\kappa \nu)$, which quantifies the non-dimensional thermal driving strength between the two horizontal plates. Here, H is their distance, β the thermal expansion coefficient of the fluid, g the gravitational acceleration, Δ the temperature difference across the fluid layer, κ and ν the thermal diffusivity and kinematic viscosity, respectively. Furthermore, the Prandtl number is defined as $Pr = \nu / \kappa$, which is the ratio between momentum and thermal diffusivities. An important output of the flow is the heat transport between the plates, which can be non-dimensionally quantified by the Nusselt number $Nu = QH / (\kappa \Delta)$, with $Q = \langle wT \rangle_{A,t} - \kappa \langle \partial_z T \rangle_{A,t}$ the mean vertical heat flux, where $\langle \dots \rangle_{A,t}$ indicates the mean over time and a horizontal plane.

On the other hand, for flows driven by wall shear stress, a commonly used model problem is the Couette flow [53, 135, 136]. We adopt a geometry in which the bottom and top walls slide in opposite directions with a wall-tangential velocity u_w and the forcing can be expressed non-dimensionally by the wall Reynolds number $Re_w = H u_w / \nu$. The relevant flow output is now the wall friction, quantified by the friction coefficient $C_f = 2\tau_w / (\rho u_w^2)$, with ρ the fluid density and τ_w the surface- and time-averaged wall shear stress. Turbulent Couette flow is dominated by large-scale streaks [125, 139–144]. These remain correlated in the streamwise direction for a length up to about 160 times the distance between the plates [130].

Combining both, buoyancy and wall shear forcings, yields a complex system that is relevant in many applications, especially for atmospheric and oceanic flows [146–148]. Also in sheared thermal convection large-scale structures emerge, as experiments have shown [149, 150]. Investigations on channel flows with unstable stratification [151] revealed that temperature fluctuations in the bulk decrease while velocity fluctuations close to the wall increase for stronger unstable stratification.

Numerical simulations of wall sheared convection [153, 154] have revealed that adding shear to buoyancy increases the heat transport for low Ra , but causes also the large-scale structures to weaken thus decreasing the heat trans-

Figure 5.1: Phase diagram of simulation runs. We show two panels to better illustrate our choice of simulation input parameters, which were determined based on Re_w (left panel) and Ri (right panel). $Re_w = 2000; 3000; 4000$ were chosen to be consistent with Ref. [128] and to cover the shear dominated regime. The squared symbols show the data points for $Re_w = 0$ for completeness and independently of the y-axis, since they cannot be directly included in the logarithmic scale. To have a sufficient amount of data in the thermal buoyancy dominated regime, we picked $Ri = 100$ as most thermal dominated case and then logarithmically spaced three more data points.

port for $Ra \gtrsim 150,000$. Similar phenomena have been observed in Poiseuille-RB, where the wall parallel mean flow is driven by a pressure gradient rather than the wall shear: in this case the Nu decrease was attributed to the disturbance of the longitudinal wind on the thermal plumes [129, 131, 155]. This plume-sweeping mechanism, causing a Nusselt number drop, was also observed in [128], who report very long, thin streaks, similar to those of the atmospheric boundary layer where these convection rolls are called cloud streets [170–172].

In both flows, Couette-RB and Poiseuille-RB, the ratio between buoyancy and mechanical forcings can be best quantified by the bulk Richardson number

$$Ri = \frac{Ra}{Re_w^2 Pr}, \quad (5.1)$$

which is a combination of the flow governing parameters Ra , Re_w and Pr . In the Couette-RB flow of [128], Ri was used to distinguish between three different flow regimes, namely thermal buoyancy dominated, transitional, and shear dominated, similarly to the case of stably stratified wall turbulence, where [173] distinguish between the buoyancy dominated, buoyancy affected and turbulence dominated regimes.

Indeed, sheared stably or unstably stratified flows are present in many different situations involving both liquids and gases. Therefore the fluid properties, as reflected in the Prandtl number, play a major role [174]. In the atmosphere it results $Pr = \mathcal{O}(1)$ while in ocean dynamics $Pr = \mathcal{O}(10)$. However, a much larger Pr variation is found in industrial applications. E.g. $Pr \approx \mathcal{O}(10^{-3})$ for liquid metals [175], which are for example in use for cooling applications in nuclear reactors [176] or $Pr \approx \mathcal{O}(10^3)$ for molten salts or silicone oils [177] for high-performance heat exchangers.

Despite this staggering range of Prandtl numbers encountered in real applications, the vast majority of studies on sheared, thermally stratified flows have been performed only at $Pr = \mathcal{O}(1)$. To overcome this limitation, in this paper we extend the work of [128] for $Pr = 1$ by analyzing the parameter space $0 \leq Re_w \leq 4000$ and $0.22 \leq Pr \leq 4.6$ while keeping the Rayleigh number constant at $Ra = 10^6$ (see figure 5.1 for the complete set of simulations).

The present study can be considered similar and complementary to that of [178] who carried out numerical simulations with a large Pr variation for a *stably* stratified Couette flow.

The chapter is divided in the following manner. Section 5.2 briefly reports the numerical method. Section 5.3 focuses on the global transport properties and section 5.4 on the boundary layers. The paper ends with conclusions (section 5.5).

5.2 Numerical method

The three-dimensional incompressible Navier-Stokes equations with the Boussinesq approximation are integrated numerically. Once non-dimensionalized, the equations read:

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla P + \left(\frac{Pr}{Ra}\right)^{1/2} \nabla^2 \mathbf{u} + \theta \hat{z}, \quad \nabla \cdot \mathbf{u} = 0, \quad (5.2)$$

$$\frac{\partial \theta}{\partial t} + \mathbf{u} \cdot \nabla \theta = \frac{1}{(PrRa)^{1/2}} \nabla^2 \theta, \quad (5.3)$$

with $\mathbf{u}$ the velocity, normalized by $\sqrt{g\beta\Delta H}$, and θ the temperature, normalized by Δ . t is the time normalized by $\sqrt{H/(g\beta\Delta)}$ and P the pressure in multiples

Ra	Pr	Re_w	Ri	N_x	N_y	N_z	Re_τ	L_{MO}/H	Nu	$C_f/10^{-3}$
1.0×10^6	0.22	0	∞	2592	2048	256	–	0	7.37	∞
1.0×10^6	0.22	213	100.0	2592	2048	256	57.90	0.006	7.33	147.5
1.0×10^6	0.22	357	35.86	2592	2048	256	74.80	0.013	7.24	88.28
1.0×10^6	0.22	597	12.76	2592	2048	256	99.81	0.031	6.98	55.90
1.0×10^6	0.22	1000	4.546	2592	2048	256	133.0	0.080	6.44	35.37
1.0×10^6	0.22	2000	1.137	2592	2048	256	197.0	0.286	5.89	19.41
1.0×10^6	0.22	3000	0.505	2592	2048	256	246.7	0.538	6.14	13.53
1.0×10^6	0.22	4000	0.284	2592	2048	256	291.5	0.884	6.17	10.62
1.0×10^6	0.46	0	∞	1728	1458	192	–	0	7.92	∞
1.0×10^6	0.46	147	100.0	1728	1458	192	43.75	0.005	7.82	176.1
1.0×10^6	0.46	279	27.99	1728	1458	192	60.63	0.014	7.58	94.69
1.0×10^6	0.46	528	7.803	1728	1458	192	85.08	0.041	6.98	51.97
1.0×10^6	0.46	1000	2.175	1728	1458	192	120.2	0.128	6.26	28.91
1.0×10^6	0.46	2000	0.544	1728	1458	192	175.0	0.414	5.96	15.33
1.0×10^6	0.46	3000	0.241	1728	1458	192	217.8	0.787	6.04	10.54
1.0×10^6	0.46	4000	0.136	1728	1458	192	260.7	1.287	6.33	8.493

Table 5.1: Main simulations considered in this work. The columns from left to right indicate the input and output parameters and the resolution in streamwise, spanwise, and wall-normal direction (N_x, N_y, N_z). The simulations for $0 \leq Re_w \leq 1000$ were chosen to allow the first nonzero Re_w at $Ri = 100$. The other two $Re_w < 1000$ simulations for each Pr respectively were logarithmically evenly spaced in Re_w . Data of Ref. [128] have been used for $Pr = 1$; $Re = 0$; 2000; 3000; 4000. The data of the Monin-Obukhov length was added for consistency with Ref. [128], although not specifically discussed in this chapter.

Ra	Pr	Re_w	N_x	N_y	N_z	Re_τ	Ri	L_{MO}/H	Nu	$C_f/10^{-3}$
1.0×10^6	1	0	∞	1280	1024	256	—	0	8.34	∞
1.0×10^6	1	100	100.0	1280	1024	128	31.85	0.004	8.20	202.9
1.0×10^6	1	215	21.63	1280	1024	128	47.31	0.014	7.82	96.86
1.0×10^6	1	464	4.645	1280	1024	128	72.95	0.056	6.95	49.44
1.0×10^6	1	1000	1.000	1280	1024	128	113.5	0.223	6.56	25.75
1.0×10^6	1	2000	0.250	1280	1024	256	161.7	0.645	6.56	13.07
1.0×10^6	1	3000	0.111	1280	1024	256	203.0	1.218	6.87	9.158
1.0×10^6	1	4000	0.063	1280	1024	256	251.7	2.022	7.89	7.922
1.0×10^6	2.2	0	∞	1536	1296	162	—	0	8.50	∞
1.0×10^6	2.2	67	100.0	1536	1296	162	22.88	0.003	8.38	230.3
1.0×10^6	2.2	166	16.52	1536	1296	162	37.02	0.015	7.68	99.65
1.0×10^6	2.2	407	2.741	1536	1296	162	63.08	0.081	6.82	47.99
1.0×10^6	2.2	1000	0.455	1536	1296	162	100.4	0.336	6.62	20.18
1.0×10^6	2.2	2000	0.114	1536	1296	162	144.2	0.936	7.04	10.39
1.0×10^6	2.2	3000	0.050	1536	1296	162	194.1	1.845	8.72	8.373
1.0×10^6	2.2	4000	0.028	1536	1296	162	246.1	3.052	10.75	7.573
1.0×10^6	4.6	0	∞	2048	1536	192	—	0	8.51	∞
1.0×10^6	4.6	47	100.0	2048	1536	192	16.68	0.003	8.31	255.9
1.0×10^6	4.6	130	12.85	2048	1536	192	29.59	0.016	7.51	103.5
1.0×10^6	4.6	360	1.678	2048	1536	192	53.01	0.101	6.77	43.38
1.0×10^6	4.6	1000	0.217	2048	1536	192	87.65	0.459	6.75	15.36
1.0×10^6	4.6	2000	0.054	2048	1536	192	137.1	1.382	8.58	9.397
1.0×10^6	4.6	3000	0.024	2048	1536	192	189.0	2.685	11.56	7.936
1.0×10^6	4.6	4000	0.014	2048	1536	192	240.4	4.441	14.39	7.225

Table continued from previous page.

of $g\beta\Delta H$.

Equations (5.2) and (5.3) are solved using the AFiD GPU package [78] which bases on a second-order finite-difference scheme [77]. The code has been validated and verified several times [76, 80, 102–104, 134, 160]. We use a uniform discretization in horizontal, periodic directions and a non-uniform mesh, with an error function-like node distribution in the wall-normal direction. To implement the sheared Couette-type forcing we move the top and bottom walls in opposite directions with velocities $\pm u_w$, i.e., relative velocity $2u_w$ between the two plates.

Following [128], we performed our simulations in a $9\pi H \times 4\pi H \times H$ domain, which are the streamwise, spanwise and wall-normal directions, respectively. The grid resolutions are also based on [128] and then further modified to account for the Prandtl number variation in this study.

5.3 Flow organization & transport properties

5.3.1 Organization of turbulent structures

Using as guideline the description of [128] we observe that also in the present case the flow can be classified in buoyancy dominated, transitional and shear dominated regimes (see figure 5.2 and table 5.1 for a full overview). As shown in [128], for $Pr = 1$ and increasing Re_w , we observe the thermal buoyancy dominated regime at $Re_w = 0$ while already at $Re_w = 1000, 2000$ the compact thermal structures elongate into streaks and evidence the transitional regime. Further increasing the wall shear causes the streaks to meander in the spanwise direction which indicates the shear dominated regime ($Re_w = 3000, 4000$).

As $Pr = \nu/\kappa$ exceeds unity, kinematic viscosity overtakes thermal diffusivity and the wall shear affects the flow structures in the bulk easier. In fact, it can be observed that already for $Re_w = 1000$ the flow shows the meandering behavior of the shear dominated regime. For $Pr = 4.6$ and $Re_w = 4000$ the shear is strong enough to make the effect of the thermal forcing negligible, as confirmed by the flow structures similar to the plane Couette flow.

Conversely, for Prandtl numbers smaller than unity, the shear is less effective for a given Re_w and the bulk flow is more dominated by the thermal structures. In the case of $Pr = 0.22$, a wall shear of $Re_w = 1000$ is not strong

Figure 5.2: Snapshots of the temperature field at mid-height ($z/H = 0.5$) for a subdomain of the parameter space. The applied wall shear is in x -direction, while y is the spanwise coordinate.

Figure 5.3: (a) Nu versus Re_w for varying Pr . The curves show a more or less pronounced minimum $Nu^{\min}$ at a certain shear Reynolds number $Re_w(Nu^{\min})$. (b) shows $Nu(Re_w = 0)$ versus Pr . (c) shows $Re_w(Nu^{\min})$ versus Pr . Note that the error bars for these values are considerable, given our limited resolution in Re_w . Nonetheless, we include a power law fit into the figure.

enough to fully disturb the plumes and only the next data point at $Re_w = 2000$ shows signs of elongated streaks.

From the panels of figure 5.2 it is evident how Pr changes the relative strength of momentum and thermal diffusivities: A higher Prandtl number, corresponding to a larger kinematic viscosity, increases the momentum transfer from the boundaries to the bulk and the transition to the shear dominated regime occurs at a lower Re_w than for a corresponding low Pr flow. Vice versa, for small Prandtl numbers, the thermal dominated regime is more persistent and the shear dominated flow features appear only at high Re_w . These findings are consistent with those of Ref. [128] that the Richardson number Ri , which is constant for constant $Re_w^2 Pr$ (see equation (5.1)), determines the flow regime.

5.3.2 Heat transfer

The Nusselt number Nu is plotted in figure 5.3 as function of Re_w , showing a non-monotonic behavior. The common feature is that for increasing wall shear, Nu first decreases and then increases as already observed in [128] for $Pr = 1$. In the present case, however, the specific values are strongly dependent on Pr , as seen in figure 5.3c. The effect of Pr is strongly dependent on the

Figure 5.4: Mean wall-normal temperature profiles (left) and side view snapshots of temperature fields (right), i.e. streamwise cross-sections, for (a) $Pr = 0.22; Re_w = 0$, (b) $Pr = 0.22; Re_w = 4000$, and (c) $Pr = 1; Re_w = 4000$. For all right panels only $x/H = 0-4\pi$ is shown for better visibility and $y/H = 2\pi$ was chosen for the spanwise location, in which periodic boundary conditions are employed.

amount of shear added to the system. For pure Rayleigh-Bénard convection ($Re_w = 0$), Nu increases with Pr for $Pr < 1$ and saturates to a constant value for $1 < Pr < 4.6$, see figure 5.3b, in agreement with the findings of [179] and [43]. For increasing Re_w , the effect of the wall shear on the heat transfer is more pronounced for increasing Pr , because of the higher momentum transfer from the boundaries to the bulk. This is confirmed both by the initial Nu decrease up to 20% of the RB value at $Pr = 4.6$ and the subsequent strong increase by more than 50% for the highest Re_w . In both cases the effects of the momentum transfer are enhanced by the high Prandtl number. We mention that the non-monotonic behavior of the Nusselt number observed here is a frequently occurring feature of flows in which more than one parameter concur to determine the value of the heat transfer; other known cases have been reported by [155] and [129] for Poiseuille-RB flow, [180] and [181] for thermal convection with rotation or [182] for severe lateral confinement, though the exact interplay between the forces in these cases are different.

5.3.3 Flow layering

The initial Nu decrease can be understood upon considering that the added wall shear perturbs the thermal RB structures and produces a horizontal flow layering that weakens the vertical heat flux. Once the wall shear is strong enough, however, the flow undergoes a transition to a shear dominated regime

and the vertical cross-stream motion generated by the elongated streaks makes up for the suppressed RB structures, thus starting the Nusselt number monotonic increase [128]. To better understand the effect of the horizontal flow layering, we discuss the results of figure 5.4. In these ‘side views’ (i.e., stream-wise cross-sections) of the temperature field snapshots and the corresponding top views of figure 5.2, we can observe how the flow changes from thermal plumes to straight thin streaks and then to meandering structures. As expected, the increase in wall shear causes the flow to become more turbulent. But the change in the large-scale structures is also very recognizable. Here, the transitional regime displays a more unexpected behavior. In contrast to what is seen in panels 5.4(a,c), where the flow structures appear clearly divided into hot and cold columns, in panel 5.4b the structures are more complex. Due to the wall shear and the thereby imposed horizontal flow, the vertical structures are disturbed, the flow is not able to reach the opposite hot/cold wall, but is instead trapped in a warm/cool state in the bulk of the flow. The fluctuations in the flow are not strong enough to mix the bulk and therefore the heat gets insulated in a stably stratified layer in the middle of the flow. This layering causes the total heat transfer to decrease and is the reason for the drop in Nu for low Re_w in figure 5.3. Because of the heat entrapment in the bulk layer, relatively cold fluid comes very close to relatively warm fluid and the temperature gradients in wall-normal direction increase significantly. In the atmosphere, this phenomenon can be observed as cloud streets, which, similar to the here observed high-shear end of the transitional regime, manifests as long streaks of convection rolls [170–172].

5.4 Boundary layers

5.4.1 Boundary layer thicknesses

A complementary way to better understand the Pr -dependence of the flow dynamics and the transport properties is to study the viscous and thermal boundary layer thicknesses λ_u and λ_θ , respectively. Here, we define both λ_θ and λ_u by extrapolating the linear slopes of the mean temperature and mean streamwise velocity close to the walls, similarly to [79]. The dependence of λ_u and λ_θ on Ri and Pr is shown in figure 5.5. Here we use as abscissa the Richard-

son number. Given that $Ra = 10^6$ is constant, we have $Ri \propto (Pr Re_w^2)^{-1}$. At every Pr , for increasing Ri – and therefore decreasing shear – λ_θ initially grows, then reaches a plateau around $Ri \approx 1$ and eventually decreases slowly to converge to the pure RB value (figure 5.5a). For comparison, we also plot $Nu(Ri)$ in figure 5.5c. Given that $\lambda_\theta \propto (Nu)^{-1}$ to a good approximation, the behavior of the thermal boundary layer thickness is consistent with the Nusselt number of figures 5.3 and 5.5c. The different flow regimes can be identified either from the different slopes of λ_θ versus Ri or from those of $Nu(Ri)$. The slope is positive in the shear dominated region (small Ri), approximately zero in the transitional regime and then negative in the thermal buoyancy dominated regime.

As the Richardson number indicates the relative strength of buoyancy and shear, the non-monotonic behavior of the thermal boundary layer can be expected. For $Ri \gtrsim 1$, the flow is not dominated by shear, and therefore an increase of Ri , which is consistent with a decrease of Re_w for constant Ra and Pr , strengthens the thermal plumes and therefore the heat transfer, which results in a smaller thermal boundary layer. The reason for the λ_θ increase for $Ri \lesssim 1$ is that in this region the thermal forcing is weak and the flow is mainly driven by the shear. In this case the thermal boundary layer is slaved to the viscous boundary layer which, according to the expectations, monotonically thickens as the wall shear weakens. From figure 5.5b we can see that indeed λ_u monotonously increases with increasing Ri .

Note that the viscous boundary layer thickness has a stronger dependence on Pr than the thermal boundary layer thickness. Qualitatively, larger Pr reflects stronger momentum diffusivity and therefore a thicker viscous boundary layer. Note that part of this strong increase of λ_u with Pr simply reflects that Ri is kept constant, because, to achieve this, Re_w has to decrease as $\propto Pr^{-1/2}$ to keep Ri fixed, see equation (5.1). However, in the shear dominated regime (high Pr or low Ri), λ_u grows faster than in the other regimes and this is especially true for the flows with higher Pr . In fact, in these cases the thermal boundary layer is nested within the viscous one and the dynamics of the latter is not sensitive to the former. This is not the case for small $Pr < 1$ because then λ_u evolves inside λ_θ whose thinning with increasing Ri counteracts the thickening of the viscous boundary layer.

To further stress the importance of the relative thicknesses of the thermal and the viscous boundary layer, we show their ratio versus Ri in figure 5.5d. We can see that λ_θ/λ_u increases for decreasing Pr at fixed Ri since the kinetic boundary layer thickness is driven by the momentum diffusivity. At fixed Pr

Figure 5.5: (a) Thermal boundary layer thickness λ_θ and (b) kinetic boundary layer thickness λ_u as function of the Ri -number for various Pr -numbers and fixed $Ra = 10^6$. Note that the scale is the same in both (a) & (b). (c) $Nu(Ri)$ compared to $H/(2\lambda_\theta(Ri))$. (d) Ratio of thermal and kinetic boundary layer thickness vs Ri .

Figure 5.6: Velocity and temperature wall profiles for $Pr = 0.22$ (left), $Pr = 1$ (middle) and $Pr = 4.6$ (right) for various Re_w . (a-c) Mean streamwise velocity and (d-f) mean temperature profiles. Here $u^+ = u/u_\tau$ and $T^+ = T/T_\tau$, with the friction temperature $T_\tau = Q/u_\tau$. The dashed lines in (a-c) show the linear profile for $z^+ \ll 10$ and the Prandtl- von Kármán log-law of the wall $u^+(z^+) = \kappa^{-1} \log z^+ + B$, with $\kappa = 0.41$ and $B = 5$.

the behavior of the boundary layer ratio is more complex: it always shows a decreasing trend in the high end of Ri which is due to the thinning of the thermal boundary layer. On the other hand, at the low end of Ri one can observe an increase only for $Pr > 1$, which is due to the steep growth of λ_θ with Ri observed in figure 5.5a.

Due to the limited amount of datapoints, we cannot show a more detailed behavior in the extreme case of pure shear forcing. In contrast, in the limit of pure Rayleigh-Bénard convection we do observe the asymptotic trend for λ_θ/λ_u ; there the effect of the shear becomes very small (no imposed shear, all shear due to natural convection roll) and the ratio depends on Pr only. This saturation occurs earlier for smaller Pr , because the thermal forcing dominates over the shear forcing at smaller Ra .

5.4.2 Velocity and temperature wall profiles

For strong enough shear the boundary layers, which are first of laminar type, will eventually become turbulent, considerably enhancing the heat transport. However, for most of the values of the control parameters (Re_w and Pr) of this paper this is hardly the case. This can best be judged from the velocity profiles, which we show in figures 5.6(a-c) for three different values of Pr and various Re_w . Only in the high- Pr range, towards the limit of plane Couette flow, we can see that u^+ evolves towards the well-known Prandtl- von Karman logarithmic behavior $u^+(z^+) = \kappa^{-1} \log z^+ + B$ for high Re_w . Since the shear strongly affects the flow, the boundary layers can transition to turbulence earlier than without shear. But also the large Pr enhance the shear. In fact, at $Pr = 4.6$ already the flow at $Re_w = 3000$ shows the onset of a log-law behavior. The more Pr is decreased, the harder it becomes for the wall shear to disturb the thermal plumes and, as a result, at $Re_w \leq 4000$ and $Pr \leq 2.2$, the log-scaling cannot be attained in our simulations.

Panels 5.6(d-f) show a similar behavior for the mean temperature profiles. One can observe that the temperature profiles converge earlier towards some type of logarithmic behavior. For $Pr = 1$, we can see such behavior for $Re_w = 4000$, whereas at larger $Pr = 4.6$, it already shows up even at $Re_w = 2000$. From the shown temperature profiles, we can also identify the flow layering that was previously discussed in section 5.3.3. When the flow layering occurs, heat gets entrapped in the bulk flow. Since now an additional layer of warm and cool fluid exists in between of the cold and hot regions, T^+ shows a non-monotonic behavior with a drop after the initial peak. This can most prominently be seen in figure 5.6d ($Pr = 0.22$) for the strongest shear $Re_w = 4000$.

5.5 Conclusions

In this chapter we performed DNS of wall sheared thermal convection with $0 \leq Re_w \leq 4000$ and $0.22 \leq Pr \leq 4.6$ at constant Rayleigh number $Ra = 10^6$. Similarly to [128], who analyzed the Ra -dependence of wall sheared thermal convection, we found three flow regimes and quantified them by using the bulk Richardson number and a visual analysis of two-dimensional cross-sectional snapshots. The flow undergoes a transition from the thermal buoyancy domi-

nated to the transitional state when $Ri \lesssim 10$. We found that the meandering streaks of the shear dominated regime start to emerge at $Ri \lesssim 0.1$. Also the behavior of the Nusselt number strongly depends on Pr . For high Prandtl number, the momentum transfer from the walls to the flow is increased and therefore the flow can easier reach the shear dominated regime where the heat transfer is again increased. We analyzed both the thermal and the kinetic boundary layer thicknesses to better understand the transitions of the flow between its different regimes. We found that the thermal boundary layer thickness λ_θ shows a peak in the transitional regime and decreases for both lower and higher Ri . The kinetic boundary layer thickness λ_u increases with increasing Ri and increasing Pr . For very strong Re_w and in particular large Pr we notice the appearance of logarithmic boundary layer profiles, signaling the onset of turbulent boundary layer dynamics, leading to an enhanced heat transport.

Together with the results of [128], we now have analyzed two orthogonal cross-sections of the three-dimensional parameter space (Ra, Pr, Re_w) . More specifically, we have determined $Nu(Ra, Pr, Re_w)$ for the two cross-sections $Nu(Ra, Pr = 1, Re_w)$ in [128] and $Nu(Ra = 10^6, Pr, Re_w)$ here. From standard RB without shear we of course know $Nu(Ra, Pr, Re_w = 0)$, which is perfectly described by the unifying theory of thermal convection by [41, 42] and [43]. The knowledge of the two new cross-sections in parameter space may enable us to extend this unifying theory to sheared convection.

6

A comparative evaluation of three volume rendering libraries for the visualization of sheared thermal convection*

Oceans play a big role in the nature of our planet, about 70% of our earth is covered by water [183]. Strong currents are transporting warm water around the world making life possible, and allowing us to harvest its power producing energy. Yet, oceans also carry a much more deadly side. Floods and tsunamis can easily annihilate whole cities and destroy life in seconds. The earth's climate system is also very much linked to the currents in the ocean due to its large coverage of the earth's surface, thus, gaining scientific insights into the mechanisms and effects through simulations is of high importance. Deep ocean currents can be simulated by means of wall-bounded turbulent flow simulations. To support these very large-scale numerical simulations and enable the scientists to interpret their output, we deploy an interactive visualization framework to study sheared thermal convection. The visualizations are based on volume rendering of the temperature field. To address the needs of supercomputer users with different hardware and software resources, we evaluate different volume rendering implementations supported in the ParaView [184] environment: two GPU-based solutions with Kitware's native volume mapper or NVIDIA's IndeX library, and a CPU-only Intel OSPRay-based implementation.

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Figure 6.1: Snapshot of the three-dimensional temperature field of sheared thermal convection at $Ra = 4.6 \times 10^6$ and $Re_w = 6000$ [128].

6.1 Introduction

Thermohaline ocean circulation [7] is vital for the heat budget of our earth. Manabe and Stouffer [185] observed that it can contribute to a heat increase of up to $\sim 10^\circ\text{C}$ on the yearly averaged mean surface temperatures in the North Atlantic region. Marshall and Schott [6] investigated a vast variety of scales in ocean dynamics and stated that deep convection can be related to mixing layers everywhere in the ocean. Since there are many complex three-dimensional events happening in large-scale fluid bodies such as oceans, it is vital to visualize the three-dimensional and temporal features of such flow simulations.

We study these large-scale bodies of fluids which are sheared by winds or currents and influenced by temperature differences in the flow. A fundamental setup of this natural mechanism is sheared thermal convection (figure 6.1). Many processes in nature are based on heat and momentum transfer and therefore interaction between buoyancy [26, 39] and shear [32, 54].

Rayleigh-Bénard convection, the flow in a box heated from below and cooled from above is a paradigmatic system for thermal convection. We present the use of three different rendering libraries available in ParaView [184] to build a time-dependent volume rendering of thermal convection. The deployment and evaluation of the hardware and software requirements of these libraries was motivated by a showcase submission at the 2018 International Conference for High Performance Computing, Networking, Storage and Analysis. In the accompanying video [186] we are able to display the previously two-dimensionally presented flow structures in a three-dimensional motion. The reader is led through a presentation of one specific flow case with sheared thermal convection and can experience the dynamics of the thermal structures while being informed about different flow parameters.

6.2 Numerical simulations

The direct numerical simulations (DNS) were performed with the second-order finite-difference code AFiD [77], in which the three-dimensional non-dimensional Navier-Stokes equations with the Boussinesq approximation are solved on a staggered grid. We use $\mathbf{u} = u(\mathbf{x}, t)$ as the velocity vector with streamwise, spanwise and wall-normal components. θ is the non-dimensional temperature ranging from $0 \leq \theta \leq 1$. The simulations are performed in a computational box with periodic boundary conditions in streamwise and spanwise directions and confined by a heated plate below and a cooled plate on top. The shearing of the flow is implemented by a Couette flow setting where both top and bottom plates of the flow are moved in opposite directions with the speed u_w keeping the average bulk velocity at zero and therefore minimizing dissipation errors. The domain size is $9\pi h \times 4\pi h \times h$ using a grid of $n_x \times n_y \times n_z = 6912 \times 3456 \times 384$ which is homogeneously distributed in the streamwise and spanwise directions and clustered towards the walls.

The open source finite-difference Navier-Stokes solver AFiD [77] was written in Fortran 90 to study large-scale wall bounded turbulent flow simulations. In collaboration with NVIDIA, USA, the code was ported in its newest version to a GPU setting using an MPI and CUDA Fortran hybrid implementation optimized to run and solve large flow fields [78].

We used data from Blass et al. [128], see chapter 4, for our evaluation of volume rendering implementations, where a parameter study over different input parameters was conducted to study their influence on the flow field.

Figure 6.2: Zoomed snapshots of temperature fields of a sheared and thermally forced transitioning through all flow regimes for $Ra = 2.2 \times 10^6$ and (a) $Re_w = 0$, (b) $Re_w = 2000$, (c) $Re_w = 3000$, (d) $Re_w = 6000$, ranging from θ_{min} (blue) to θ_{max} (red).

Control parameters were the temperature difference between the top and bottom plates as the strength of the thermal forcing, non-dimensionalized as the Rayleigh number Ra , and the wall velocity as the strength of the shear forcing, non-dimensionalized as the wall shear Reynolds number Re_w .

In figure 6.2 we present snapshots of temperature fields at mid-height in different flow regimes. It can be observed that the flow passes from a thermally dominated regime with large thermal convection rolls driving the flow (figure 6.2a) into a regime where the mechanical forcing is dominant. Here, large-scale meandering structures can be observed which are driven by the shearing of the top and bottom plates (figure 6.2d). To undergo a transition between the regimes, the flow has to pass through an intermediate stage, in which the thermal plumes get stretched into large streaks (figure 6.2b). If the shearing is

further increased, these streaks become unstable and start meandering in the final flow state (figure 6.2c,d).

The reason for this streaky flow behavior is the addition of a third dimension to originally quasi-two-dimensional flow structures in pure thermal convection. Such thermal convection rolls are driven solely by the thermal difference between the plates. Once the wall shearing is added, the flow starts to strongly move in streamwise direction, which causes the development of streaks.

In turbulent flows it is very important to research how certain characteristic parameters are influenced by the flow. In thermal convection, the heat transfer, non-dimensionally defined through the Nusselt number Nu is a good indicator if changing flow structures have a supporting effect or may disrupt a previously transport-favorable flow situation.

While two-dimensional visualizations are very helpful in understanding the behavior of the large-scale structures, they don't show the complete scientific picture. They give a good indication of the flow behavior, but to understand thermal turbulence, it is vital to see the whole flow field and the dynamic interaction of turbulent structures with each other. The opportunity to observe the flow evolving and transitioning through different regimes is a great chance to not only statically observe different flow states at fixed locations in space, but to also actually follow the flow on its path to develop thermal plumes, streaks and meandering structures.

It has been previously shown in thermal convection that the large thermal plumes can be traced until very close to the heated and cooled plates [98]. So it is very important to also observe the emergence of structures close to the boundary layer. In the shear dominated regime, which we visualize in the accompanying video [186], we can observe extremely large-scale structures which are caused by a combination of thermal and shear forcing. The detailed visualizations we presented allow us to not only follow the large-scale structures, but also the interaction of small-scale structures much closer to the plates (figure 6.3).

6.3 Volume rendering libraries and setup

We use ParaView v5.6.0, a world-class, open source, multi-platform data analysis and visualization application installed on Piz Daint. Piz Daint, a hybrid Cray XC40/XC50 system, is the flagship supercomputer of the Swiss National

Figure 6.3: Zoom of an snapshot of the temperature field (top) and the vorticity structures (bottom) at $Ra = 2.2 \times 10^6$ and $Re_w = 6000$.

HPC service. We have deployed and tested several solutions within ParaView where parallelism is expressed at different degrees: data-parallel visualization pipelines with GPU-based renderings or multi-threaded parallelism for CPU-based renderings.

The computational domain used for our simulations is made of $6912 \times 3456 \times 384$ grid points. The temperature scalar field stored as *float32* takes 36 GB of memory, an overwhelming size to handle on a normal desktop. Using different parallel programming paradigms has enabled us to provide an engaging environment to promote interactive tuning of visualization options and high productivity for movie generation.

Visualization of three-dimensional scalar fields is a very mature field. Many techniques are available to make some sense of the three-dimensional nature of the data, and its variations throughout the volume. Surface-based renderings with isosurface thresholds or slicing planes have a great appeal in that they are easy to use, and provide unambiguous representations based on clearly defined numerical values. Volume renderings, early applied to medical applications, are also a great fit for scalar visualizations, especially in the realm of time-dependent outputs. They are, however, much more difficult to use. Volume rendering is based on the principle of converting a three-dimensional scalar field onto an RGB (color) volume and an Opacity volume. Transfer functions, often defined in an ad-hoc manner, convert scalar values to colors, and classify the data into regions of different opacities. A volume can then appear as clouds with varying density and color. Their interpretation remains subjective to the user's taste and practice. We refer readers to other sources [187] to dive more deeply into the principles of Volume Rendering.

Volume Rendering can be implemented in different manners. ParaView was chosen because it offers a test-bed for several state-of-the-art implementations which can be selected based on rendering parameters and available hardware.

The largest partition of the Piz Daint supercomputer has nodes equipped with one Intel Xeon E5-2690 (12 cores, 64 GB RAM) and one NVIDIA Tesla P100 GPU (16 GB RAM, OpenGL driver 396.44). Thus our priority is to evaluate the GPU-based implementations. ParaView's default installation enables also a software ray caster for rendering volumes but we have found its performance far below the other options. The lack of advanced parameter settings in the Graphical User Interface (GUI) of ParaView also led us to abandon its evaluation. We tested ParaView's native GPU ray casting implementation against IndeX an NVIDIA library, as well as OSPRay, a software-based library developed by Intel. Doing so, provides a valid option to users of super-

computers not equipped with GPUs. Our performance evaluation is based on ParaView’s benchmarking Python source code[†].

We have in all cases ignored disk-based I/O costs. There is often quite a bit of variability when running on a large distributed file system shared by hundreds of users. Our motivations are rendering-centered, and two-fold: evaluate the memory cost and resources (CPU, GPU) required to get a first image on the screen, and see if color/opacity transfer function editing, as well as other image tuning, can be done interactively, using any of the three methods proposed. In the evaluation of performance costs, ParaView’s benchmark code enables fully automated testing with a careful management of double buffering, turning off all rendering optimizations designed to accelerate interactive viewing, and forcing full-feature rendering before saving images to disk.

In the two GPU-based methods evaluated, we use an EGL-based rendering layer [188] to overcome the need to have a server-side X-Windows server running on the compute node. This enables headless, offscreen rendering with GPU acceleration. We note, however, that although the GPUs provide phenomenal rendering power, they are limited by the available memory (16 GB on our NVIDIA’s Pascal GPUs). For the full size of our simulations outputs, we are actually forced to use data-parallel pipelines on multiple nodes to use the aggregate memory of the different GPUs.

Our third option, uses Intel OSPRay and CPU rendering. HPC compute nodes usually have more memory than their GPU counterparts. We use Piz Daint’s high memory nodes with 128 GB of RAM, where our grid of over 9 billion voxels can be fit easily on a single node.

6.3.1 ParaView’s GPU ray casting

When GPU hardware is present, ParaView’s most efficient mapper is a volume mapper that performs ray casting on the GPU using vertex and fragment programs [189]. The core ray-tracing algorithms are coded in GLSL and require a graphics driver supporting at least OpenGL version 3.2 [190]. The data is stored into a `vtkVolumeTexture` which manages the OpenGL volume texture, its type and internal format. Although this class supports streaming data into separate blocks to make it fit the GPU memory, we have not used this option which imposes a performance trade-off, artificially going over the fixed GPU memory limit. Block streaming, sometimes called data bricking, may also suffer

[†]source code found in `./Wrapping/Python/paraview/benchmark/`

Figure 6.4: Comparison between volume renderings of temperature with ParaView’s OpenGL GPU RayCastMapper (left), and with NVIDIA IndeX (right).

from artifacts at the block boundaries where gradient computations are done to support shading. ParaView’s OpenGL VolumeRayCastMapper binds the 32-bit float scalar field array to a three-dimensional texture image with a call to `glTexImage3D()`. An explicit texture object is created, transferring data from host memory to GPU memory. The maximum achievable performance will be proportional to the total amount of GPU memory, and to the transfer bandwidth over our high speed PCIe3 serial bus connecting the host to the GPU device.

6.3.2 NVIDIA IndeX

NVIDIA IndeX [191] is a three-dimensional visualization SDK developed to enable volume rendering of massive data sets. NVIDIA has worked in tandem with Kitware to bring an implementation of IndeX to ParaView, and we have enjoyed the benefits of a close partnership between the Swiss National Supercomputing Center (CSCS) and NVIDIA, to be able to use IndeX in a multi-GPU setting. We use the ParaView plugin v2.2 with the core library NVIDIA IndeX 2.0.1. The NVIDIA IndeX Accelerated Compute (XAC) interface integrates the core surface and volume sampling programs written in CUDA [192]. For this case, we have used the generic programs provided by IndeX, without custom programming. In figure 6.4 we show side-by-side renderings done with

the two GPU-based libraries, to demonstrate that they produce equivalent images. The ParaView Graphical User Interface ensures that both implementations use identical color and opacity transfer functions and sampling rates. ParaView’s GPU Ray Casting image (left) is used as reference. Differences of illumination are barely noticeable to the human eye.

6.3.3 Intel OSPRay

OSPRay [193] is a ray tracing framework for CPU-based rendering. It supports advanced shading effects, large models and non-polygonal primitives. OSPRay can distribute “bricks” of data as well as “tiles” of the framebuffer, although in our case, we use brick subdivisions only. The Texas Advanced Computing Center has developed a ParaView plugin that enables us to test the possibility of using a ray-tracing based rendering engine for volumetric rendering. This is the best solution for clusters where no GPU hardware is available.

OSPRay can use its own internal Message Passing Interface (MPI) layer to replicate data across MPI processes and composite the image. This would result in linear performance scaling and supports secondary rays used in ParaView’s *pathtracer* mode, but would be prohibitive in terms of communication costs. In this study, we rely on a different parallel computing paradigm. The emphasis is no more on data parallelism, but rather on multi-threaded execution. A complete *software-only* ParaView installation was deployed with an LLVM-based OpenGL Mesa layer. We used Mesa v17.2.8, compiled with LLVM v5.0.0, and the OSPRay v1.7.2 library to provide a very efficient multi-threaded execution path taking advantage of Piz Daint’s second partition of compute nodes. These nodes are built with two Intel Broadwell CPUs (2×18 cores and 64/128 GB RAM). Our cluster management and job scheduling system SLURM provides the specific scheduling options “`--cpus-per-task=72 --ntasks-per-core=2`” to effectively take full advantage of the multi-threading exposed by the LLVM and OSPRay libraries.

6.3.4 Parallel image compositing

ParaView’s default mode of parallel computing is to use data-parallel distribution, whereby sub-pieces of a data grid are processed through identical visualization pipelines. To combine the individual framebuffers of each computing

Figure 6.5: Example of a color and opacity transfer functions to highlight hot and cold plumes.

nodes, ParaView uses Sandia National Laboratory’s IceT [194] compositing library. We use it in its default mode of operation doing sort-last compositing for desktop image delivery. We note here that NVIDIA’s IndeX uses a proprietary compositing library, so for the IndeX tests only, we disable ParaView’s default image compositor.

6.4 Volume rendering of the thermal convection

In visualizing the temperature field, we seek to highlight the turbulence which is best shown by clearly differentiating between cold and hot regions to see how they interact with each other, as seen in figure 6.5. Our movie animation shows an initial phase where region of blue tint is superposed on top of the hotter region. Plumes emerging from the bottom and mixing into the cold regions highlight this phenomenon.

Figure 6.6: Volume rendering with shading based on gradient estimation (left), and with OSPRay-enabled shadows (right).

6.4.1 Visual effects

When presented with multiple visualizations including different illumination and shading, we preferred the renderings which emphasize the amorphous nature of the field data. As can be seen in figure 6.6, shading based on gradient estimation offers little improvement because our data does not have strong gradients, and the use of shadows which at first might seem more appealing, produces images with a strong *surface-like* look, which we discarded upon further analysis.

6.4.2 GPU-based rendering on a single node

Volumetric rendering of high resolution grids has a non-significant cost which we briefly document here. Creating the first frame after data has been read in memory, i.e., the startup cost has a great impact in having users adopt a particular implementation. In a *post-hoc* visualization, data would be read from disk; in an *in-situ* scenario, data might have to be converted to VTK data structures. Thus, we measure performance after the time ParaView has collected all the data and created a bounding-box representation. This startup cost for the first image is also of paramount importance in a movie-making

Rendering library	Startup	ParaView task
OSPRay	1.34 s	18.4 GB
ParaView GPU Mapper	6.17 s	27.2 GB
NVIDIA IndeX	11.84 s	39.2 GB

Table 6.1: Initialization and memory costs for a quarter-size domain on one node.

scenario, where data are read from disk, a single image is computed, and the whole visualization pipeline and hardware resources are flushed to visualize the next timestep.

Unlike ParaView’s native GPU ray caster implementation which does not enable block streaming, the NVIDIA IndeX library processes data by chunks. However, it does so by bringing volume sub-extents *incrementally* into the GPU memory. Early volume chunks are rendered properly as long as the GPU memory is not exhausted. When memory runs out, late chunks actually corrupt the final image. Our attempts to render a 4 billion voxels dataset on a single node did not succeed with NVIDIA IndeX. We observe failures to allocate 64^3 voxel cubes and the final images are corrupted.

We summarize in table 6.1 the time from when volumetric rendering options are enabled, triggering the building of internal structures until the first frame appears. In order to measure the memory cost of all three libraries under evaluation on a single node, we restricted our test sample to a quarter-size domain of the original grid, i.e., 2.28G voxels ($1730 \times 3456 \times 384$), to fit the available GPU RAM. The GPU memory usage[†] settles at 9.1 GB for ParaView native raycaster, and 12.3 GB for NVIDIA IndeX.

We note both a much higher memory consumption on the application side of ParaView and on the GPU memory side for the NVIDIA IndeX implementation. The high initial setup cost incurred by the NVIDIA IndeX library is due to higher volume transfer between CPU and GPU, a cost that increases further when in parallel, as the current implementation of IndeX triggers re-execution of the data I/O due to larger than usual ghost layer requirements. Work is in progress[§] to minimize this impact in a future version of the plugin.

[†]GPU memory usage is measured with the `nvidia-smi` diagnostic tool

[§]personal communication with NVIDIA Dev. team

6.4.3 CPU-based rendering on a single node

If memory costs are substantial, more nodes, and/or more GPUs will be required, increasing the run-time cost of the visualization. Our data domain is quite large, and we are not able to load a half-size domain on a single GPU node. Indeed, both the 64 GB RAM on the node and the 16 GB RAM on the GPU are hard limitations. The OSPRay-based CPU rendering is one way to alleviate this problem. We can load the full size domain on a single node of the multi-core partition of Piz Daint with dual-Xeon chips and 128 GB of RAM. We measured again the startup cost for the first image at full HD resolution (1920x1080 pixels), using 72 execution threads and found them to increase linearly with grid dimensions. We tested the quarter-size, half-size and the full domain and report the delivery of the first image in 1.07, 1.50, and 2.33 s, respectively. The associated cost in RAM is also linear, at 18.4 GB, 36.5 GB and 73 GB, respectively. Of great interest is OSPRay's management of memory. OSPRay volumes can be stored in two different manners. The first variant named *shared structured volume* matches ParaView's data layout. Version 5.6 of ParaView is the first version where this zero-copy access pattern is used and it provides both a faster startup time and a much lower memory footprint, as compared to previous work. Indeed, we reported earlier on the use of OSPRay's alternate implementation called *block bricked volume* whereby data locality in memory is increased by arranging voxel data in smaller chunks. This came however at a higher cost, doubling the memory footprint on the CPU [195].

After the first frame has been built, our experience is that smooth interaction is possible with all three libraries tested. In fact, ParaView supports acceleration shortcuts for lower precision renderings during interactive navigation, enabling a comfortable user experience for mouse-driven interaction, with little degradation of quality. Color and opacity transfer functions editing is also interactive and very intuitive.

Movie quality renderings on the other hand are done with all level-of-details optimizations turned off and we tested the rendering speed of that particular mode in a batch production test. We created an OSPRay-based benchmark test to mimic a navigation fly-through in a full resolution domain, starting from an overall view of the full grid, zooming in, rotating the view-point, and finally zooming in to immerse the viewer in the volume. Our initial view-point has some regions of screen-space empty, where rendering costs at each pixel

Pixel Resolution vs. # of threads	36 threads	72 threads
WXGA (1280×800 pixels)	2.85 s	1.69 s
FHD (1920×1080 pixels)	3.37 s	1.90 s
4K UHD (3840×2160 pixels)	4.81 s	2.73 s

Table 6.2: Average rendering for the full size domain at different pixel resolution

are negligible. We then move quickly into the scene such that the viewport is completely covered by active pixels, that is, all pixel rays hit the volume. We rendered our benchmark test at three different pixel resolution, WXGA (1280×800 pixels), Full HD (1920×1080 pixels) and 4K Ultra HD (3840×2160 pixels), to evaluate the impact of pixel resolution on rendering costs. We also evaluated the use of hyper-threading to further boost performance. Table 6.2 summarizes our average rendering time per frame for 300 frames of navigation.

Our compute nodes are featuring two sockets with eighteen cores each. We note the clear benefit of using hyper-threading to spawn up to seventy-two threads for an increased throughput. We also note that increasing frame buffer resolution to very large sizes is not a showstopper.

6.4.4 Rendering the full domain in parallel

In a post-processing scenario, we have seen that the two GPU-based rendering solutions are limited by the available GPU memory, since our 9-billion voxels data set will not fit on a single GPU. Likewise, in an *in-situ* scenario, the visualization would most likely use a parallel set of nodes. Loading our full-size data, we rounded up our evaluation of all three rendering options, by measuring the initial cost for the first image (after all I/O has been done), and also the average rendering time in a scripted animation loop. Figure 6.7 summarizes our results, with the dataset distributed among 4, 8 and 12 compute nodes.

As expected, startup times decrease almost linearly with the number of compute nodes. For the GPU-based methods, less data is transferred from CPU memory to GPU memory. Our animation benchmark loads a single timestep of data, thus, once the data has migrated to the GPU, there is hardly any CPU to GPU communication apart from a single frame buffer image. For the CPU-based implementation, the build-up of the ray-tracing acceleration

Figure 6.7: Overview of initial cost and average rendering time per frame.

structures takes just over one second so there is less difference across the few tests executed. We see rendering times reduced somewhat linearly since there is less workload. In a movie production setting where all timestep outputs are read once, rendered once and then discarded, the startup cost of any rendering library needs to be weighted against the I/O costs. Although our data I/O statistics show quite a bit of variation because of the high load of our multi user system with over 5000 compute nodes, our simulation data are read, *in average*, in about 32 s (resp. 25, and 16 s) on 4 nodes (resp. 8 and 12 nodes). We see that the initialization of the rendering sub-system has a greater impact than expected, and that in an *in-situ* scenario, it would be the single most important barrier to performance. The initialization of the NVIDIA IndeX is the most significant bottleneck. Discussions with NVIDIA are on-going and our hope is that this will be improved in future versions of the SDK since the library is still in early development. We comment here that the parallel execution of the OSPRay-based volume rendering was made possible by using yet another ParaView mode, letting the OSPRay library take full control of the overall scene and parallel frame compositing. Finally, we highlight the fact that the OSPRay average rendering times per frame in our animation are all

under one second, while it takes a minimum of 8 compute nodes using the NVIDIA IndeX solution. This level of interactivity can be satisfactory during the prototyping phase of a visualization.

6.5 Conclusions

We have discussed three implementations of volume rendering for a thermal convection simulation output of substantial size. Our time-dependent output is stored as a *float32* array of 36GB per timestep. This is a non-trivial size for the most common GPUs. This leaves the scientist with two options: 1) use a data-parallel visualization application with GPU-assisted rendering, or 2) use a *CPU-only* visualization environment which can fit on compute nodes where large memory banks are usually found. Our choice was to deploy a single application, the open-source ParaView, due to its support for different parallel execution paradigms, and for its ability to work with different off-screen and on-screen rendering backends. Having a single application, driven by fully automatized python scripts and a benchmarking suite of tools available in ParaView itself, enabled us to confront all possible implementations with reduced variability.

We tested two GPU-based rendering options. We first used ParaView's native volume rendering which has proved to offer the best compromise between startup time, and interactive performance; We also tested an alternative solution based on a new library in development by NVIDIA. In our current setup, the IndeX library offers superior interactive rendering, however at non-negligible initialization costs.

We evaluated an implementation of volume rendering provided by the Intel OSPRay library, a software-based framework which can take remarkable advantage of a multi-threaded execution layer. This also fits well on a subset of our available hardware, a dual-Xeon based compute node without GPU. Our experiences are of interest for several computer platforms around the world where graphics hardware is not available.

Our emphasis on creating the scientific visualization shown in the accompanying video [186] was two-fold. First, having an interactive environment enabling us to prototype the visualization with large-scale data. The editing of color and opacity transfer functions is the most demanding step in deriving the proper visualization, and we were able to provide an interactive setup using either GPU-, or CPU-based volume rendering. Dealing with long time-

dependent simulation outputs was the second requirement, and the path to achieve high productivity was to use parallel and scalable I/O routines. We used VTK's native XML partitioned file format convention for cartesian image data. This was pivotal for a quick turn-around time. The OSPRay-based implementation had the best performance in both initialization and average rendering time, but suffered from some parallel image compositing artifacts at inter-process boundaries. Given the very high spatial resolution of our grid, these artifacts are only visible at extreme zooming in the vicinity of ghost-cells between MPI-distributed data. To conclude and ensure the best visual quality, the compromise for movie production was to use small subsets of GPU nodes with ParaView's native volume renderer.

The volume rendering benchmarking platform deployed to analyze our large grid simulations provides a unique chance to observe sheared thermal convection in a very simple system with far reaching consequences. Furthermore, the visualizations allow us to have a very good first insight into the interplay between thermal convection and flow shearing by different kinds of wind and flow currents. We are now able to better understand the emergence and behavior of flow structures transporting heat through the system and affecting the flow dynamics.

Conclusions and Outlook

In this dissertation we studied various aspects of large-scale turbulent thermal convection. Firstly, we discussed the existence of thermal superstructures in pure Rayleigh-Bénard (RB) convection which are sized about 6–7 times the height of the domain. In chapter 1 we observed structures that are significantly larger than those at the onset of convection and are not washed out by the large thermal forcing applied in our simulations. They have a similar extent in both horizontal directions due to the lack of mean flow, contrary for example to the later discussed Couette-RB flow. We analyzed the energy signatures of the large-scale structures through temperature variance and TKE spectra and found a saturation in the growth of the structures towards a domain size of $\Gamma \approx 64$, at which the structures become independent of Γ . Other integral quantities show convergence at a much smaller value of Γ . Both Nu and Re already reach their large-scale values at $\Gamma \approx 4$ and calculated integral length scales converge for $\Gamma \approx 32$. Using this information, we then studied RB convection for different Rayleigh numbers at $\Gamma = 32$. To isolate the large-scale contribution of the flow, we employed a novel averaging method, described in chapter 2, which conditionally averages flow quantities along a distance parameter d , combining the data into a quasi-two-dimensional large-scale circulation. We found higher than average Nu in the plume impacting region and lower than average Nu in the plume ejecting region, with a high shear zone in between. We evaluated instantaneous thermal and viscous boundary layer thicknesses along the large-scale circulation and also their most probable ratio, which converges towards unity as predicted by the Prandtl-Blasius approximation for a flat plate laminar boundary layer. Calculations of the wind Reynolds number agree well with the scaling law predicted by the Grossmann-Lohse theory and a scaling of the shear Reynolds number allows us to predict the critical Rayleigh number required for the onset towards the ultimate regime of RB convection at $Ra = \mathcal{O}(10^{14} - 10^{15})$.

Up to chapter 2, we have studied pure RB flow, which can be classified as natural convection. In chapters 3-6 we added a Couette-type wall shear to the unstably stratified flow to create mixed convection. In chapter 3 we compared our flow setup of Couette-RB (thermal forcing with applied wall shear) with

data of Poiseuille-RB (thermal forcing with applied pressure gradient). This chapter is an introduction for the subsequent chapters in which we studied wall sheared thermal convection and also served as a benchmark for our code against available results from literature due to the known similarities between Poiseuille and Couette flow.

In chapter 4 we employed DNS of Couette-RB for a wide variety of thermal and shear forcings. Performing simulations up to $Ra = 10^8$ and $Re_w = 10000$ while keeping the Prandtl number at unity, we found three different flow states. In the thermal buoyancy dominated regime, large convection rolls dominate the flow. With increasing wall shear, the flow starts to undergo a transition towards the shear dominated regime, where large meandering structures drive the flow and increase the heat transport. During this transition, we observed a significant drop in Nu , which we attributed to a flow layering effect in the bulk during the disruption of the thermal convection rolls by the applied wall shear. Depending on the strength of the thermal forcing, this disruption requires a different amount of flow shearing and only for strong enough shear can the flow reach the shear dominated regime where Nu monotonically increases. The minimum Nusselt number can be found just before the onset of the shear dominated regime. Here, we find that the effective scaling exponent in $Nu \sim Ra^\alpha$ is larger than $\alpha = 1/3$, which could be a possible sign of the onset of turbulent boundary layer dynamics. However, this was not confirmed in an analysis of the flow characteristics, which do not show any logarithmic behavior in the transitional regime.

The study of sheared thermal convection was continued in chapter 5, where we added a variation of the Prandtl number in the range of $0.22 \leq Pr \leq 4.6$ to our database. We found that the behavior of the heat transport also strongly depends on Pr , because a high Pr means that the momentum transfer from the walls to the flow is increased and therefore the shear dominated regime is reached more easily. To further analyze the transition between the different flow regimes, we determined both the thermal and the kinetic boundary layer thicknesses. For large Pr and Re_w , we found a logarithmic behavior, indicating an onset of a turbulent boundary layer in the flow statistics, which causes the enhanced heat transport.

In chapter 6 we compared different rendering techniques for CPU and GPU usage. Since our simulations require extremely large resolutions, the visualization of flow structures also becomes non-trivial. To allow for efficient rendering of three-dimensional flow fields, we evaluated multiple visualization techniques and created highly optimized parallel-processing routines for remote rendering

on high performance computing clusters, which were not only very helpful for the present work on sheared Rayleigh-Bénard turbulence, but will also be a great asset for future research.

Although this dissertation made a big scientific step forward in the study of sheared thermal convection, many unanswered questions still remain. We have focused on large-scale structures, which do have a large impact on the flow behavior. We have discussed the topic of necessary domain sizes to allow for the desired flow statistics to fully converge. But also small-scale behavior is very important to study. Due to the limited computational capabilities available and the very large resolutions required, numerical research is very far away from certain real life applications. Therefore it will always also be necessary to further drive the research on very constrained flow, to allow for the investigation of certain flow parameters in small, controlled flow environments, such as the different variations of Rayleigh-Bénard convection. We have added wall shear to thermal convection and achieved a completely new kind of flow behavior. Due to the emergence of large-scale meandering structures, we had to allow the flow to spread in a large, rectangular box. However, this meant that we were again quite limited in the matter of flow resolution. So it has to be determined in the future: How can the computational domain be reduced to allow for an increased thermal and shear forcing? Can compromises be made to learn more about the dynamics of sheared thermal convection at a more turbulent state? What can be learned from simulations in smaller domain sizes that constrain the flow on purpose and make a larger parameter space viable? In chapters 4 and 5 we have determined flow parameters such as the Nusselt number for the two parameter ranges $Nu(Ra, Pr = 1, Re_w)$ and $Nu(Ra = 10^6, Pr, Re_w)$. Furthermore, the unifying theory of thermal convection by Grossmann and Lohse can already quantify $Nu(Ra, Pr, Re_w = 0)$ for pure thermal convection. With our data, we might now be able to extend the Grossmann-Lohse theory to sheared convection.

Appendix A

A.1 Contribution of the horizontal mean velocity

Figure A.1: Maximum contribution of the horizontal mean velocity on the horizontal RMS velocity in percentage points.

In figure A.1 we show that at mid-height the contribution of the horizontal mean velocity $v_{h_{\text{mean}}} = \langle (v_x + v_y)/2 \rangle_A$ on the horizontal RMS velocity $v_{h_{\text{RMS}}} = \sqrt{\langle v_x^2 + v_y^2 \rangle_A}$ is approximately one percentage point. This is in agreement with [62], who find that the energy contained in the mean flow is less than 0.8% of the total kinetic energy.

A.2 Equations of the Grossmann-Lohse Theory

To achieve Re_{GL} in chapter 2, we numerically solve equations (A.1) - (A.4) at every available Ra :

$$\mathcal{F}(x) = (1 + x^4)^{-1/4} \quad (\text{A.1})$$

$$\mathcal{G}(x) = x(1 + x^4)^{-1/4} \quad (\text{A.2})$$

$$(Nu_{GL} - 1)RaPr^{-2} = c_1 \frac{Re_{GL}^2}{\mathcal{G}(\sqrt{Re_L/Re_{GL}})} + c_2 Re_{GL}^3, \quad (\text{A.3})$$

$$Nu_{GL} - 1 = c_3 Re_{GL}^{1/2} Pr^{1/2} \left\{ \mathcal{F} \left[\frac{2a Nu_{GL}}{\sqrt{Re_L}} \mathcal{G} \left(\sqrt{\frac{Re_L}{Re_{GL}}} \right) \right] \right\}^{1/2} \quad (\text{A.4})$$

$$c_4 Pr Re_{GL} \mathcal{F} \left[\frac{2a Nu_{GL}}{\sqrt{Re_L}} \mathcal{G} \left(\sqrt{\frac{Re_L}{Re_{GL}}} \right) \right],$$

As prefactors we used $c_1 = 8.05$, $c_2 = 1.38$, $c_3 = 0.487$, $c_4 = 0.0252$, $a = 0.922$, and $Re_L = (2a)^2$ [43].

B.1 Scaling of L_{MO} vs. Ri

Figure B.1: L_{MO}/H versus Ri and the corresponding fit $L_{MO}/H = 0.16/Ri^{0.91}$ to the data.

In figure B.1 we present the Monin-Obukhov length L_{MO} versus the Richardson number Ri for all simulations. We find that the Monin-Obukhov length scales as $L_{MO}/H = 0.16/Ri^{0.91}$, similar to $L_{MO}/H = 0.15/Ri^{0.85}$ as found by [129] for channel flow with unstable stratification.

B.2 Comparison of L_{MO} and λ_θ

Figure B.2: L_{MO} normalized by the thermal boundary layer thickness λ_θ versus Re_w . For $L_{MO}/\lambda_\theta \lesssim 1$ the flow is in the buoyancy dominated regime.

In figure B.2 we show the ratio between the Monin-Obukhov length L_{MO} and the thermal boundary layer thickness λ_θ , which is determined from $\lambda_\theta = H/(2Nu)$. For $L_{MO}/\lambda_\theta < 1$ the flow is in the buoyancy dominated regime. For higher L_{MO}/λ_θ , the flow first reaches the transitional regime before the shear dominated regime is reached, where $L_{MO}/\lambda_\theta \sim Re_w^{5/2}$.

B.3 Flow field overview

As an addition to figure 4.8 we present in figure B.3 the full overview of temperature snapshots at mid-height, ranging from $Ra = 1.0 \times 10^6$ – 1.0×10^8 and $Re_w = 0$ –10000. All three regimes, i.e. the buoyancy dominated regime, the transitional regime, and the shear dominated regime, can be observed here.

Figure B.3: Instantaneous snapshots of all simulated temperature fields at mid-height, see the caption of figure 4.8 for further details.

B.4 Further Flow Statistics

In addition to the data presented in figures 4.12 and 4.13 we present further flow statistics here. Figure B.4 shows the velocity and temperature fluctuations as function of height for $Ra = 4.6 \times 10^6$ for various wall shear Reynolds numbers. It can be observed that the velocity fluctuations increase with Re_w . The temperature fluctuations show a non-monotonic behavior. The peak temperature fluctuations first increase with increasing Re_w before the peak of the temperature fluctuations decreases with increasing wall shear. Figure B.5 shows the velocity and temperature fluctuations for $Re_w = 6000$ and increasing Ra . u_{peak} and v_{peak} first increase and then monotonically decrease with increasing Ra when thermal forcing is added to Couette flow. Both the wall-normal velocity and the temperature fluctuations decrease completely monotonic for increasing thermal forcing.

Figure B.4: Fluctuations of (a) streamwise, (b) spanwise, and (c) wall-normal velocity, and (d) temperature for $Ra = 4.6 \times 10^6$.

Figure B.5: Fluctuations of (a) streamwise, (b) spanwise, and (c) wall-normal velocity, and (d) temperature for $Re_w = 6000$. $T'^2_{Ra=0}$ was determined through a passive-scalar temperature field.

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Summary

Turbulent thermal convection in all its variations is a very common phenomenon in our daily life. Not only for small applications but also on a large scale, thermal convection is our daily companion. About 70 percent of our Earth is covered by water, thus oceans play a big role in the nature of our planet and the Earth's climate system is heavily linked to it. In this dissertation, the behavior of large-scale structures in such a turbulent flow was studied by means of direct numerical simulations.

In chapter 1 we presented the emergence of superstructures in very turbulent Rayleigh-Bénard (RB) convection in domains reaching horizontal lengths as large as $\Gamma = 128$ times the distance between top and bottom plate. In recent decades, most experiments and simulations have focused on relatively small aspect ratios to achieve very high Rayleigh numbers. However, the structure sizes in many natural instances of convection are very large. In this chapter we also showed that for very high Rayleigh numbers certain domain sizes are necessary to allow statistics to fully converge. We reported that integral quantities such as the heat transfer require an aspect ratio of at least $\Gamma = 4$, while the integral length scale ($\Gamma = 32$) and the signatures of temperature and turbulent kinetic energy ($\Gamma = 64$) need even larger domain sizes to converge.

In chapter 2 we further analyzed the large-scale structures in turbulent RB convection. Here we isolated the large-scale circulation (LSC) using a conditional averaging technique, which allowed us to evaluate statistics independent of the number of LSCs and their orientation. We reported that statistics such as the boundary layer thicknesses and wind Reynolds number do not diverge strongly from results in confined domains at $\Gamma = 1$, although the convection rolls converge to a significantly larger size in our periodic $\Gamma = 32$ domain. The conditional averaging technique also allowed us to investigate local behavior of the statistics in the plume impacting and the plume ejecting region. We showed that the heat transport at the plates is very high when the LSC impacts and very low when it gets emitted back into the bulk flow. Calculating the shear Reynolds number and interpolating towards the critical value of $Re_s^{crit} \approx 420$, we predicted that the transition to the ultimate regime is to be expected at $Ra_{crit} \approx \mathcal{O}(10^{15})$ for unconfined geometries, which is in agreement

with previous experimental observations.

In the further course of this dissertation we have added an additional driving force to the flow. In chapter 3, we discussed flow driven by a pressure gradient (Poiseuille flow) and by wall shear (Couette flow). Here, our code for Couette-RB flow was compared to an external code for Poiseuille-RB flow.

When wall shear is added to pure turbulent thermal convection, the previously nearly two-dimensionally orientated thermal plumes get forced into a three-dimensional state. Depending on the relative amount of wall shear in relation to the thermal forcing, different flow regimes can be extracted. We have presented a wide parameter space of different thermal forcing and wall shear in chapter 4, where we performed simulations of Couette-RB flow in a large and very long rectangular domain, and were able to find three different flow regimes. In the buoyancy dominated regime, the wall shear is nearly negligible and the flow dynamics is very similar to pure thermal convection. Once the shear is increased, the flow enters a transitional regime, where the large-scale structures experience the previously mentioned shift towards a three-dimensional state, which results in thin convection rolls that extend over the full length of the domain in the direction of the wall shear. Once the shear is strong enough to dominate the whole flow field, the shear dominated regime is reached where the elongated convection rolls start to meander. We found that starting from pure thermal convection and adding wall shear, the heat transfer first decreases due to the disruption and breakup of present thermal plumes, and only increases once the shear dominated regime is reached.

In chapter 5 we have added a variation of the fluid properties through an alteration of the Prandtl number to our parameter space. Both liquids and gases are very common to use for applications of sheared thermal convection and their fluid properties play a very important role. We showed that indeed the Prandtl number has a strong influence to the flow dynamics of our system. For high-performance heat exchangers, which usually use molten salts or silicone oils, or in ocean dynamics, the Prandtl number is high and therefore the momentum transport between the walls is strong, leading to a greater effect of the wall shear on the flow structures, while this is much less pronounced at low Prandtl numbers, for example in liquid metals used for cooling in nuclear reactors.

Chapter 6 approaches the topic of sheared thermal convection from the point of different visualization techniques. In this chapter we have used an interactive visualization framework to study the data created by the numerical simulations that we performed for the previous chapters. To use volume

rendering on such large-scale data, certain techniques, such as a parallel computing approach using a supercomputing cluster, are necessary to make these visualizations viable. The results of our volume rendering can be found in several figures of this dissertation, including the front and back cover.

This dissertation is a significant step towards the better understanding of thermal convection on a large scale. Through the study of superstructures, we gained a better idea of necessary domain sizes for future numerical simulations of thermal convection. Our study on sheared RB convection laid the foundation for an extension of the Grossmann-Lohse theory for heat transport to the case of sheared thermal convection, which could universally describe the behavior of the heat transport in form of the Nusselt number $Nu(Ra, Pr, Re_w)$ as a function of thermal forcing, wall shear, and fluid properties. With the work on different visualization techniques, we created the resources necessary for future research to have access to state-of-the-art tools to visualize even very large data sets and therefore allow for a completely new perspective to study turbulent fluid dynamics.

Zusammenfassung

Turbulente thermische Konvektion in all ihren Variationen ist ein sehr bekanntes Phänomen in unserem täglichen Leben. Nicht nur für Anwendungen in kleinskaligem Format, sondern auch in großem Maßstab ist die thermische Konvektion unser täglicher Begleiter. Etwa 70 Prozent unserer Erde sind von Wasser bedeckt. Daher spielen Ozeane eine große Rolle in der Natur unseres Planeten und das Klimasystem der Erde ist eng damit verbunden. In dieser Dissertation wurde das Verhalten großskaliger Strukturen in vergleichbar turbulenten Strömungen mit Hilfe von direkten numerischen Simulationen untersucht.

In Kapitel 1 haben wir die Entstehung von Superstrukturen bei sehr turbulenter Rayleigh-Bénard (RB) Konvektion in Simulationscontainern mit quadratischer Grundfläche vorgestellt, die horizontale Ausmaße von bis zu $\Gamma = 128$ Mal der Höhe des Simulationskörpers erreichen. In den letzten Jahrzehnten haben sich die meisten Experimente und Simulationen auf relativ kleine Aspektverhältnisse konzentriert, um sehr hohe Rayleigh-Zahlen zu erreichen. Allerdings sind die Strömungselemente in vielen natürlichen Fällen von Konvektion sehr groß. In diesem Kapitel haben wir gezeigt, dass auch für sehr hohe Rayleigh-Zahlen bestimmte Mindestgrößen der Simulationscontainer erforderlich sind, damit die Statistiken vollständig konvergieren können. Die Ergebnisse unserer Untersuchungen haben gezeigt, dass integrale Größen wie die Wärmeübertragung ein Seitenverhältnis von mindestens $\Gamma = 4$ erfordern, während die integralen Längenskalen ($\Gamma = 32$) und die Maxima der Signaturen von Temperatur und turbulent kinetischer Energie ($\Gamma = 64$) noch größere Simulationscontainer benötigen, um konvergieren zu können.

In Kapitel 2 haben wir die Superstrukturen in turbulenter RB-Konvektion weiter analysiert. Hier isolierten wir die Großflächenzirkulation (GFZ) mit Hilfe einer konditionierten Mittelungstechnik, die es uns ermöglichte, Statistiken unabhängig von ihrer Anzahl und Ausrichtung auszuwerten. Statistiken wie die Grenzschichtdicken und die Wind-Reynolds-Zahl weichen nicht stark von den Ergebnissen in beschränkten Containern bei $\Gamma = 1$ ab, obwohl die Konvektionsrollen in unseren periodischen, horizontal unbeschränkten Containern von $\Gamma = 32$ zu einem signifikant größeren Endzustand konvergieren. Das Verfahren

der bedingten Mittelwertbildung ermöglichte es uns auch, das Verhalten der thermischen Wolken an den Platten in der Region des Aufpralls und des Abstoßens zu untersuchen. Dabei hat sich gezeigt, dass der Wärmetransport an den Platten sehr hoch ist, wenn die GFZ aufprallt, und sehr niedrig, wenn sie wieder in den Volumenstrom abgegeben wird. Durch Berechnung der Scher-Reynolds-Zahl und Interpolation auf den kritischen Wert von $Re_s^{crit} \approx 420$ lässt sich prognostizieren, dass der Übergang zum ultimativen Regime für horizontal unbeschränkte Simulationscontainer bei $Ra_{crit} \approx \mathcal{O}(10^{15})$ zu erwarten ist, was mit früheren experimentellen Beobachtungen übereinstimmt.

Im weiteren Verlauf dieser Dissertation wurde der Strömung eine zusätzliche treibende Kraft hinzugefügt. In Kapitel 3 haben wir die durch einen Druckgradienten (Poiseuille-Strömung) und durch Wandscherung (Couette-Strömung) angetriebene Strömung erörtert. Hier wurde unser Simulationsprogramm für Couette-RB-Strömung mit einem externen Programm für Poiseuille-RB-Strömung verglichen.

Wenn Wandschub zu reiner turbulenter thermischer Konvektion hinzukommt, werden die vorher fast zweidimensional orientierten thermischen Wolken in einen dreidimensionalen Zustand gezwungen. Abhängig vom relativen Ausmaß der Wandscherung im Verhältnis zum thermischen Antrieb, können verschiedene Strömungsregime extrahiert werden. Wir haben in Kapitel 4 einen breiten Parameterraum mit unterschiedlichen thermischen Antrieben und Wandschubwirkungen vorgestellt, indem wir Simulationen der Couette-RB-Strömung in einem großen und sehr langen rechteckigen Simulationscontainer durchgeführt haben und so drei verschiedene Strömungsregime finden konnten. In dem vom thermischen Auftrieb dominierten Regime ist die Wandscherung nahezu vernachlässigbar und die Strömungsdynamik ist der reinen thermischen Konvektion sehr ähnlich. Sobald die Scherung erhöht wird, tritt die Strömung in ein Übergangsregime ein, in dem die großskaligen Strukturen die bereits erwähnte Verschiebung in einen dreidimensionalen Zustand erfahren, was zu dünnen Konvektionsrollen führt, die sich über die gesamte Länge des Simulationscontainers in Richtung der Wandscherung erstrecken. Sobald die Scherung stark genug ist, um das gesamte Strömungsfeld zu dominieren, beginnen die langgestreckten Konvektionsrollen zu mäandern. Wir konnten zeigen, dass ausgehend von reiner thermischer Konvektion und unter Hinzufügung von Wandscherung der Wärmeübergang zunächst aufgrund des Aufbrechens vorhandener thermischer Wolken abnimmt und erst dann zunimmt, wenn der durch Scherung dominierte Bereich erreicht ist.

In Kapitel 5 haben wir eine Variation der Fluideigenschaften durch eine Änderung der Prandtl-Zahl zu unserem Parameterraum hinzugefügt. Sowohl Flüssigkeiten, als auch Gase werden für Anwendungen der thermischen Scherkonvektion verwendet und ihre Fluideigenschaften spielen eine sehr wichtige Rolle. Damit konnte nachgewiesen werden, dass die Prandtl-Zahl in der Tat einen starken Einfluss auf die Strömungsdynamik unseres Systems hat. Bei Hochleistungswärmetauschern, die normalerweise geschmolzene Salze oder Silikonöle verwenden, oder auch in der Ozeandynamik ist die Prandtl-Zahl hoch und daher der Impulstransport zwischen den Wänden stark, was zu einer größeren Auswirkung der Wandscherung auf die Strömungsstrukturen führt. Dies ist bei niedrigen Prandtl-Zahlen viel weniger ausgeprägt, wie zum Beispiel bei flüssigen Metallen, die zur Kühlung in Kernreaktoren verwendet werden.

Kapitel 6 nähert sich dem Thema der gescherten thermischen Konvektion aus der Sicht verschiedener Visualisierungstechniken. In diesem Kapitel haben wir ein interaktives Visualisierungs-Framework verwendet, um die Daten zu untersuchen, die durch die numerischen Simulationen erzeugt wurden, die wir für die vorhergehenden Kapitel durchgeführt hatten. Um das Volume-Rendering bei solch groß angelegten Daten zu nutzen, sind bestimmte Techniken, wie z.B. ein Parallel-Computing-Ansatz mit einem Supercomputing-Cluster, notwendig, um diese Visualisierungen praktikabel zu machen. Die Ergebnisse unseres Volume-Rendering sind in mehreren Abbildungen dieser Dissertation zu finden, einschließlich der Vorder- und Rückseite.

Diese Dissertation ist ein wesentlicher Schritt zum besseren Verständnis der thermischen Konvektion in großem Maßstab. Durch die Untersuchung von Superstrukturen konnte eine bessere Vorstellung von den notwendigen Simulationsgrößen für zukünftige numerische Simulationen der thermischen Konvektion gewonnen werden. Diese Untersuchung über die gescherte RB-Konvektion legte den Grundstein für eine Erweiterung der Grossmann-Lohse-Theorie für den Wärmetransport im Fall der gescherten thermischen Konvektion, die universell das Verhalten des Wärmetransports in Form der Nusselt-Zahl als Funktion des thermischen Antriebes, der Wandscherung und der Fluideigenschaften beschreiben könnte. Mit der Arbeit an verschiedenen Visualisierungstechniken wurden die notwendigen Ressourcen entwickelt, um zukünftiger Forschung den Zugang zu modernsten Werkzeugen zur Visualisierung auch von sehr großen Datensätzen zu ermöglichen und damit eine völlig neue Perspektive zur Untersuchung der turbulenten Fluidodynamik zu erschaffen.

Samenvatting

Turbulente thermische convectie is, in alle vormen, een veel voorkomend fenomeen in ons dagelijks leven. Niet alleen voor kleine toepassingen, maar ook op grote schaal is thermische convectie onze dagelijkse metgezel. Ongeveer 70 procent van onze aarde is bedekt met water, dus spelen de oceanen een grote rol in het karakter van onze planeet en het klimaatsysteem van de aarde is er sterk mee verbonden. In dit proefschrift is het gedrag van grootschalige structuren bestudeerd met behulp van directe numerieke simulaties.

In hoofdstuk 1 is het ontstaan van superstructuren in zeer turbulente Rayleigh-Bénard (RB) convectie in domeinen die horizontale lengtes bereikten tot $\Gamma = 128$ keer de afstand tussen de boven- en onderplaat toegelicht. In de afgelopen decennia werd in de meeste experimenten de focus gelegd op relatief kleine aspect ratio's om zeer grote Rayleigh-getallen te bereiken. De structuren in veel natuurlijke gevallen van convectie zijn echter erg groot. In dit hoofdstuk is ook aangetoond dat voor zeer grote Rayleigh-getallen bepaalde domein formaten nodig zijn om de statistiek volledig te laten convergeren. We hebben aangetoond dat integrale grootheden zoals warmtetransport een aspect ratio van ten minste $\Gamma = 4$ vereisen, waarbij de integrale lengte schaal ($\Gamma = 32$) en de piekpositie van de temperatuur- en turbulente kinetische energiesignatuur ($\Gamma = 64$) nog grotere domeinen nodig hebben om te convergeren.

In hoofdstuk 2 zijn grootschalige structuren in turbulent RB convectie verder geanalyseerd. Hier hebben we de grootschalige circulatie (GSC) geïsoleerd doormiddel van een voorwaardelijke middelingstechniek, dit maakte het mogelijk om de statistiek te evalueren onafhankelijk van het aantal GSC's en hun oriëntatie. We rapporteren dat statistische gegevens zoals de grenslaagdikte en wind Reynold-getallen niet sterk afwijken van resultaten in een beperkt gebied bij $\Gamma = 1$, hoewel de convectie rollen convergeren naar een significant grotere omvang in ons $\Gamma = 32$ domein. De voorwaardelijke middelingstechniek staat ons ook toe om lokaal gedrag van de statistiek in de pluim impact en uitwerppgebied te onderzoeken. We hebben laten zien dat er een grote mate van warmtetransport is bij de platen bij het optreden van GSC en slechts een kleine mate van warmtetransport bij het terugtreden in de bulk stroming. Door het berekenen van het Reynolds afschuifgetal en interpoleren richting de kri-

tieke waarde van $Re_s^{crit} \approx 420$, hebben we voorspelt dat de transitie naar het uiterste systeem verwacht wordt bij $Ra_{crit} \approx \mathcal{O}(10^{15})$ voor een onbegrensde geometrie, wat overeenstemming is met voorgaande experimentele observaties.

In het verdere verloop van dit proefschrift hebben we een extra drijvende kracht toegevoegd aan de stroming. In hoofdstuk 3 worden stromingen gedreven door drukgradiënten (Poiseuille stroming) en door wandafschuiving (Couette stroming). Hier is onze simulatie voor Couette-RB stroming vergeleken met een externe simulatie voor Poiseuille-RB stroming.

Wanneer wandafschuiving wordt toegevoegd aan zuivere turbulente thermische convectie worden de voorheen vrijwel tweedimensionale thermische pluimen geforceerd omgezet in een driedimensionale toestand. Afhankelijk van de relatieve hoeveelheid wandafschuiving in relatie tot de thermische forcing kunnen verschillende stromingsregimes worden onttrokken. In hoofdstuk 4 hebben we een breed parametergebied van verschillende thermische forcing en wandafschuiving laten zien. In dit hoofdstuk hebben we simulaties van Couette-RB stroming in een groot en erg lang rechthoekig domein uitgevoerd, en konden we drie verschillende stromingsregimes vinden. In het thermisch gedomineerde regime is de wandafschuiving bijna verwaarloosbaar en de stromingsdynamiek is zeer vergelijkbaar met pure thermische convectie. Als de afschuiving toeneemt komt de stroming in een overgangsregime terecht waar de grootschalige structuren de eerder genoemde verschuiving naar een driedimensionale toestand plaats vindt. Dit resulteert in dunne convectie rollen die zich strekken over de volle lengte van het domein in de richting van de wandafschuiving. Wanneer de afschuiving sterk genoeg is om het gehele stoomveld te domineren, wordt het afschuiving gedomineerde stelsel bereikt waar de langwerpige convectie rollen beginnen te meanderen. We hebben ontdekt dat bij het starten van een pure thermische convectie en het toevoegen van wandafschuiving, de warmtetransport eerst afneemt door de verstoringen en uiteenvallen van de huidige thermische pluimen, waarna het alleen toeneemt zodra het afschuivingsregime is bereikt.

In hoofdstuk 5 hebben we variatie van de vloeistof eigenschappen aan onze parameters toegevoegd doormiddel van een aanpassing in het Prantl-getal in onze parameter ruimte. Zowel vloeistoffen als gassen worden regelmatig gebruikt voor de toepassing van afgeschoven thermische convectie en hun vloeibare eigenschappen zijn daarbij van groot belang. We hebben aangetoond dat het Prandtl-getal inderdaad een sterke invloed heeft op de stromingsdynamiek van ons systeem. Voor krachtige warmtewisselaars, die meestal werken op basis van gesmolten zouten of siliconenolie, of bij oceaan dynamiek is het Prandtl-

getal hoog en daarom is het momentumtransport tussen de wanden sterk, wat leidt tot een groter effect van wandafschuiving op de stromingsstructuren. Dit is in veel mindere mate van toepassing bij lage Prandtl-getallen, bijvoorbeeld bij vloeibare metalen die worden gebruikt bij het koelen van kernreactors.

Hoofdstuk 6 behandelt het onderwerp van afgeschoven thermische convectie uit het oogpunt van verschillende visualisatietechnieken. In dit hoofdstuk hebben we gebruik gemaakt van een interactief visualisatiekader om de gegevens verkregen uit de numerieke simulaties uit de eerdere hoofdstukken te bestuderen. Om volumerendering toe te passen op data van zo'n grote schaal zijn bepaalde technieken, zoals het gebruik van parallel computergebruik met behulp van een supercomputer-cluster, nodig om deze vorm van visualisatie rendabel te maken. De resultaten van onze volumerenderingen zijn te vinden in verschillende figuren in dit proefschrift, evenals op het voor- en achterkant.

Dit proefschrift is een significante stap naar een beter begrip van thermische convecties op grote schaal. Door de studie van superstructuren hebben we een beter idee verkregen over de benodigde domeingroottes voor toekomstige numerieke simulaties van thermische convectie. Ons onderzoek naar RB convectie heeft een basis gelegd voor het uitbreiden van de Grossmann-Lohse theorie voor warmtetransport in het geval van wandafschuiving. Dit kan gebruikt worden om het gedrag van warmtetransport in de vorm van het Nusselt-getal $Nu(Ra, Pr, Re_w)$ universeel uit te leggen als een functie van thermische dwang, wandafschuiving en vloeistof eigenschappen. Met ons werk aan verschillende visualisatietechnieken hebben we de benodigde middelen ontwikkeld die nodig zijn voor toekomstige onderzoeken, om zo toegang te krijgen tot geavanceerde hulpmiddelen die nodig zijn om zelfs zeer grote data sets te visualiseren waardoor het mogelijk wordt om turbulente stromingsdynamiek vanuit een compleet nieuw perspectief te bestuderen.

About the author

Alexander Georg Emanuel Blass was born in Wiesbaden, Germany, on January 2nd, 1990. He received his high school diploma in Wiesbaden and then studied Mechanical and Process Engineering at Technische Universität Darmstadt with special courses in flight mechanics and flight propulsion. After receiving his bachelor's degree, he moved to the University of Wisconsin - Madison, USA, to study Engineering Mechanics. During that time he developed an affinity for fluid dynamics and turbulent structures and also followed classes in astrodynamics and rocket propulsion. In 2016 he obtained his master's degree and moved to the Netherlands, where he joined the Physics of Fluids group at the University of Twente, and started his doctoral studies on the topic of direct numerical simulations of sheared Rayleigh-Bénard turbulence under the supervision of Prof. Detlef Lohse, Prof. Roberto Verzicco, and Dr. Richard Stevens. His research interests include turbulent flows, geophysical convection, and high-performance visualization techniques.

Scientific output

Publications

2018

- Richard J.A.M. Stevens, **Alexander Blass**, Xiaojue Zhu, Roberto Verzicco, and Detlef Lohse
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- **Alexander Blass**, Roberto Verzicco, Detlef Lohse, Richard J.A.M. Stevens, and Dominik Krug
Flow organization in laterally unconfined Rayleigh-Bénard turbulence
Journal of Fluid Mechanics (Under review)

Invited and selected talks

- Max-Planck-Center Meeting,
Göttingen, Germany. (January 2019)
- 71th APS Division of Fluid Dynamics Meeting,
Atlanta, USA (November 2018)
- European Fluid Mechanics Conference,
Vienna, Austria. (September 2018)
- International Conference on Rayleigh-Bénard Turbulence 2018,
Enschede, The Netherlands. (May 2018)
- J. M. Burgers Center for Fluid Dynamics CFD Contact Group Meeting,
Delft, The Netherlands (*Invited*). (March 2018)
- 70th APS Division of Fluid Dynamics Meeting,
Denver, USA. (November 2017)
- Department of Mathematics and Department of Engineering Physics,
University of Wisconsin - Madison,
Madison, USA (*Invited*). (November 2017)
- Physics of Fluids Group, University of Twente,
The Netherlands. (November 2017)
- EUROMECH Turbulent superstructures in closed and open flows,
Erfurt, Germany. (July 2017)

Poster contributions

- Visit of the German and Dutch Ambassadors,
Enschede, The Netherlands. (February 2019)

- Physics at Veldhoven,
Veldhoven, The Netherlands. (January 2019)
- Gallery of Fluid Motion,
71th APS Division of Fluid Dynamics Meeting,
Atlanta, USA. (November 2018)
- MESA+ Annual meeting,
Enschede, The Netherlands. (September 2018)
- JMBC Burgers Symposium,
Lunteren, The Netherlands. (June 2018)
- MESA+ Annual meeting,
Enschede, The Netherlands. (September 2017)
- Summer School on Complex Motion in Fluids,
Cambridge, United Kingdom. (September 2017)
- JMBC Burgers Symposium,
Lunteren, The Netherlands. (May 2017)

Video and picture contributions

- Gallery of Fluid Motion,
72th APS Division of Fluid Dynamics Meeting,
Seattle, USA. (November 2019)
- AFMS Photo and Video Competition,
Australian Fluid Mechanics Conference,
Adelaide, Australia. (December 2018)
- Scientific Visualization & Data Analytics Showcase,
Supercomputing 18,
Dallas, USA. (November 2018)
- Gallery of Fluid Motion,
70th APS Division of Fluid Dynamics Meeting,
Denver, USA. (November 2017)

- SURF Visualization Competition, Amsterdam, The Netherlands. (December 2017)

Awards and honors

- Science Communication Poster Prize, Veldhoven, The Netherlands. (January 2019)
- Second Price of the AFMS Video Competition, Adelaide, Australia. (December 2018)
- Third Price of the AFMS Photo Competition, Adelaide, Australia. (December 2018)
- Finalist of the Scientific Visualization & Data Analytics Showcase, Supercomputing 18, Dallas, USA. (November 2018)
- Finalist of the MESA+ Poster Competition, MESA+ Annual meeting, Enschede, The Netherlands. (September 2018)
- Winner of the SURF Visualization Competition, Amsterdam, The Netherlands. (December 2017)

Organization

- International Conference on Rayleigh-Bénard Turbulence, Enschede, The Netherlands. (May 2018)

Bachelor student supervision

- Pier Tabak (July 2018)
- Arnout Franken (June 2017)

Teaching experience

- Teaching assistant for the Master course “Turbulence” as part of the Applied Physics study in the years (2016/2017) and (2017/2018).

Peer review

- Peer reviewer for the Journal of Fluid Mechanics (JFM and JFM-Rapids).

Computational grants

- Cartesius, SURFsara, Amsterdam, The Netherlands. (2016-2020)
- PizDaint, CSCS, Lugano, Switzerland. (2016-2019)

Direct numerical simulations of Couette flow with unstable stratifications

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Fig. 1

Fig. 2

Direct numerical simulations of Rayleigh-Bénard flow (indicated by a Rayleigh number Ra) with induced wall shearing (indicated by a Reynolds number Re) have been performed. Large coherent thermal structures emerge from the heated plate and meander (Fig. 1). For flow dominated by thermal convection, big plumes are visible (Fig. 2). In between these two cases, intermediate regimes can be found, where the thermal plumes transition into long streaks that don't meander (Fig. 3,4).

Fig. 1: $Ra = 4 \times 10^6$; $Re = 8000$

Fig. 2: $Ra = 1 \times 10^8$; $Re = 0$

Fig. 3: $Ra = 2 \times 10^7$; $Re = 8000$

Fig. 4: $Ra = 4 \times 10^7$; $Re = 4000$

Fig. 3

Fig. 4

Figure S.1: Poster: JMBC Burgers Symposium 2017.

Direct numerical simulations of turbulent sheared thermal convection

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Simulations of Rayleigh-Bénard flow with induced wall shearing have been performed on a **6912x3456x384** grid. **Large coherent thermal structures** emerge from the heated plate and meander. The **vorticity formations** are visualized with the Q-criterion. The zooms show small-scale structures in the flow.

Figure S.2: Poster: Physics at Veldhoven 2019.

Figure S.3: Pictures [196] of an 8-part 3D-print of the meandering flow structures in a simulation of sheared thermal convection from chapter 4.

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When I look back at what had to come together from getting my high school diploma in my home town to ultimately completing this document, my dissertation in the field of applied fluid dynamics, so many people come to my mind without them this would not have been possible. Professors, teachers, colleagues, friends, and family. At this point I would like to thank all of you from my heart for what you have done for me. Below, I want to mention a number of people that have accompanied me on my scientific path and that deserve special credit.

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Alexander Blass
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