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Chapter 3

Rayleigh-Bénard convection

TODO: introductory paragraph – explain where this is going

3.1   Governing equations

Rayleigh-Bénard convection is the overturning motion of a fluid confined between two horizontal isothermal plates, the bottom plate being warmer than the top plate. The fluid is traditionally assumed to be incompressible, with density ρ related to temperature T by the linear equation of state

$$\rho = \rho_0[1 - \alpha(T - T_0)],$$

α being the volume coefficient of thermal expansion and ρ_0 and T_0 a reference density and temperature. Provided that the density variations are small ($\alpha(T - T_0) \ll 1$), one may employ the *Boussinesq approximation*, neglecting density variations everywhere except in their contribution to the weight force. This leads to the Boussinesq equations

$$\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u} \cdot \boldsymbol{\nabla} \boldsymbol{u} = -\frac{1}{\rho_0} \boldsymbol{\nabla} p' + \alpha(T - T_0)g\hat{\boldsymbol{z}} + \nu \nabla^2 \boldsymbol{u}, \tag{3.1}$$

$$\frac{\partial T}{\partial t} + \boldsymbol{u} \cdot \boldsymbol{\nabla} T = \kappa \nabla^2 T, \quad \text{and} \tag{3.2}$$

$$\boldsymbol{\nabla} \cdot \boldsymbol{u} = 0, \tag{3.3}$$

which represent the momentum balance, the conservation of energy and the assumption of incompressibility, respectively. The prognostic variables are the fluid velocity $\boldsymbol{u}$ and the temperature T (the pressure perturbation p' is implicitly determined by (3.3)). The parameters of the model are the kinematic viscosity ν and thermal diffusivity κ. $\hat{\boldsymbol{z}}$ is the upward unit vector. The Boussinesq approximation has led to the appearance of a buoyant force (per unit mass)

$$\alpha(T - T_0)g = \frac{\rho_0 - \rho}{\rho_0}g$$

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in the momentum equation, in agreement with Archimedes' principle. The reader is referred to Chandrasekhar (1961) for a detailed derivation of the Boussinesq equations; I have merely summarised the main assumptions and approximations involved.

In this work, I consider solutions of (3.1)–(3.3) in a two-dimensional domain $[0, d] \times [0, L]$ with Cartesian coordinates x and z, subject to no-slip, isothermal boundary conditions

$$\boldsymbol{u} = \boldsymbol{0}, \quad T = T_0 + \frac{\delta T}{2} \quad \text{at } z = 0 \text{ and} \tag{3.4}$$

$$\boldsymbol{u} = \boldsymbol{0}, \quad T = T_0 - \frac{\delta T}{2} \quad \text{at } z = d \tag{3.5}$$

on the top and bottom plates, and periodic boundary conditions

$$\boldsymbol{u}(x = 0) = \boldsymbol{u}(x = L) \quad \text{and} \quad T(x = 0) = T(x = L) \tag{3.6}$$

in the horizontal. δT is the constant temperature difference between the plates.

3.2 Nondimensionalisation and scale analysis

It is helpful to nondimensionalise the governing equations (3.1)–(3.6); this is not only useful for numerical work but also gives insight into the different flow regimes that are possible. A range of nondimensionalisations are used in fluid dynamics literature; I adopt a common one (see, e.g., Grötzbach 1983; Ouertatani et al. 2008; Stevens, Verzicco, and Lohse 2010) which is suitable for the turbulent convective regime.

The first step is to choose representative time, length and temperature scales. For low-viscosity, turbulent flow, a suitable time scale is the *free-fall time* t_0, which is the time for a fluid element with constant temperature $T = T_0 - \delta T$ to fall from the top plate to the bottom plate under the influence of buoyancy $(-g\alpha\delta T)$ alone. It is simple to show that

$$t_0 \sim \left(\frac{d}{g\alpha\delta T} \right)^{1/2},$$

ignoring a factor of $\sqrt{2}$. The obvious length and temperature scales are the plate separation d and temperature difference δT, respectively.

Making the substitutions $p'/\rho_0 \to \pi$ and $T - T_0 \to \theta$ in (3.1)–(3.6) and expressing all variables in units of t_0, d and δT leads to the dimensionless equations

$$\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u} \cdot \boldsymbol{\nabla} \boldsymbol{u} = -\boldsymbol{\nabla}\pi + \left(\frac{\text{Pr}}{\text{Ra}} \right)^{1/2} \nabla^2 \boldsymbol{u} + \theta\hat{\boldsymbol{z}}, \tag{3.7}$$

$$\frac{\partial \theta}{\partial t} + \boldsymbol{u} \cdot \boldsymbol{\nabla}\theta = (\text{Ra}\,\text{Pr})^{-1/2} \nabla^2\theta, \quad \text{and} \tag{3.8}$$

$$\boldsymbol{\nabla} \cdot \boldsymbol{u} = 0, \tag{3.9}$$

which are solved in the domain $[0, \Gamma] \times [0, 1]$ with boundary conditions

$$\boldsymbol{u} = \boldsymbol{0}, \quad \theta = +\frac{1}{2} \qquad \text{at } z = 0, \tag{3.10}$$

$$\boldsymbol{u} = \boldsymbol{0}, \quad \theta = -\frac{1}{2} \qquad \text{at } z = 1, \tag{3.11}$$

$$\boldsymbol{u}(x = 0) = \boldsymbol{u}(x = \Gamma) \quad \text{and} \quad \theta(x = 0) = \theta(x = \Gamma). \tag{3.12}$$

There are three dimensionless parameters: the aspect ratio of the domain

$$\Gamma \equiv \frac{L}{d},$$

the *Prandtl number*

$$\mathrm{Pr} \equiv \frac{\nu}{\kappa}$$

which measures the relative importance of viscosity (momentum diffusivity) and thermal diffusivity, and the *Rayleigh number*

$$\mathrm{Ra} \equiv \frac{g\alpha d^3 \delta T}{\kappa \nu}.$$

The Rayleigh number can be interpreted as the ratio of the time scale for thermal transport by conduction to the time scale for thermal transport by convection. It determines the importance of diffusion for the evolution of $\boldsymbol{u}$ and θ; inspection of (3.7) and (3.8) indicates that low Ra implies strong diffusion and high Ra weak diffusion. Stability analysis (see, e.g., Chandrasekhar (1961) and the seminal work by Lord Rayleigh (1916)) reveals that there exists a critical Rayleigh number (dependent on boundary conditions but of order 10^3), below which the equations have a stable equilibrium with the fluid at rest and a linear conductive temperature profile. Above the critical Rayleigh number, the equilibrium is unstable and small perturbations lead to the formation of a regular series of steady convection cells. If the Rayleigh number is increased much further (Le Quéré (1991) cites $\mathrm{Ra} \approx 2 \times 10^8$), the solution becomes unsteady and increasingly turbulent. This work is concerned with the turbulent regime, since Rayleigh numbers for atmospheric deep moist convection can be as large as 10^{22} (Chillà and Schumacher 2012).

3.3 Large-eddy simulation

In Chapter 5 I will compare the output of a parametrised low-resolution model of (3.1)–(3.12) to the output of the unparametrised base model (i.e., the control). However, it was found in the early stages of this work that unparametrised low-resolution models were prone to numerical instability, preventing the obtainment of a suitable control solution. This is to be expected; at high Rayleigh numbers, when dissipation is weak, the solutions develop large gradients near small-scale features that cannot be properly resolved by coarse models, causing them to crash. To be more precise, the energy spectra of turbulent flows exhibit an *energy cascade* whereby energy is transferred from larger-scale motions to smaller-scale motions; only at sufficiently small scales is energy removed from the system by the dissipative terms in the equations (Pope 2000). In coarse models where these smallest scales are not resolved, excess energy accumulates at the highest resolved wavenumbers.

I choose to stabilise the numerical model by artificially introducing additional dissipative terms that act on the smallest scales, modelling the energy transfer to unresolved motions in what is effectively a simple parametrisation. This is known as *large-eddy simulation* or LES. There are many options when it comes to choosing the additional terms, but for the sake of simplicity I adopt the Smagorinsky model, the oldest and simplest. As it happens, the Smagorinsky model was originally proposed in the context of atmospheric modelling, by Smagorinsky (1963). The following description of the model follows Pope (2000).

It is easiest to first rewrite (3.7) and (3.8) in index notation (with implied summation over repeated indices). The modified equations read

$$\frac{\partial u_i}{\partial t} + u_j \partial_j u_i = -\partial_i \pi + \left(\frac{\mathrm{Pr}}{\mathrm{Ra}}\right)^{1/2} \partial_j \partial_j u_i + \theta \delta_{iz} + \partial_j \tau_{ij} \quad \text{and} \tag{3.13}$$

$$\frac{\partial \theta}{\partial t} + u_j \partial_j \theta = (\mathrm{Ra}\,\mathrm{Pr})^{-1/2} \partial_j \partial_j \theta + \partial_j F_j, \tag{3.14}$$

where the new terms are highlighted in red and δ_{ij} is the Kronecker delta symbol. τ_{ij} is known as the *residual stress tensor* and F_j is known as the *residual heat flux*. The residual stress tensor is given by

$$\tau_{ij} = 2\nu_{\mathrm{sgs}} S_{ij}^*,$$

where

$$\nu_{\mathrm{sgs}} = (C_S \Delta)^2 \sqrt{2 S_{ij} S_{ij}}$$

is the so-called *eddy viscosity* and

$$S_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$$

is the *strain rate tensor*. S_{ij}^* is the deviatoric part of the strain rate tensor given by

$$S_{ij}^* = S_{ij} - \frac{1}{3}S_{kk}\delta_{ij};$$

in fact, for incompressible flows $\frac{1}{3}S_{kk} = \partial_i u_i = 0$ so $S_{ij}^* = S_{ij}$. $\Delta \equiv 2(\Delta x \Delta z)^{1/2}$ is a filter width depending on the *local* grid spacings Δx and Δz, and $C_S = 0.17$ is the Smagorinsky constant.

It is known that the Smagorinsky model introduces too much artificial dissipation near walls in bounded flows such as Rayleigh-Bénard convection (Pope 2000). This is remedied by redefining the eddy viscosity to be

$$\nu_{\mathrm{sgs}} = (C_S \Delta)^2 (1 - e^{-z^+/A^+})^2 \sqrt{2 S_{ij} S_{ij}},$$

where the *van Driest damping function* $1 - e^{-z^+/A^+}$ attenuates the viscosity near the walls. The damping function depends on

$$z^+ \equiv \frac{\min(z, 1-z)}{\delta_\nu},$$

the distance to the nearest wall normalised by the viscous length scale δ_ν. It is conventional to choose $A^+ = 26$. TODO: explain measurement of delta-nu

The residual heat flux is similarly modelled as

$$F_j = \kappa_{\mathrm{sgs}} \partial_j \theta,$$

where it is assumed that the *eddy diffusivity* κ_{sgs} is equal to the eddy viscosity ν_{sgs} (as in Vreugdenhil and Taylor 2018, for example).

3.4 Model configuration

The nondimensionalised Boussinesq equations (3.7)–(3.12) are solved numerically using Dedalus (v3), a spectral code built in Python (Burns et al. 2020). Spectral methods represent the solution of a partial differential equation as a linear combination of linearly independent basis functions, solving for the coefficients of the basis function expansion rather than the values of the solution in real space. The resolution of the model is thus set by choosing the number of basis functions used. This work uses a Fourier (sine/cosine) basis in the horizontal direction and a basis of Chebyshev polynomials (of the first kind) in the vertical direction. The Fourier basis has the special property that all linear combinations respect the periodic boundary conditions. Timestepping is performed using a second-order Runge-Kutta scheme. The complete model source code is publicly available TODO: data availability.

The Rayleigh number was set to 10^9, a value at which the flow was found to be unsteady and feature transient eddies. The aspect ratio of the domain was $\Gamma = 8$ and the Prandtl number was set to 1 for simplicity.

TODO: link to animations

3.5 Choice of resolution: literature

The next important step is to choose the resolution of the fine and coarse models. The fine model will serve as "truth", providing the training dataset to which the parametrisation model will be fitted and the test dataset against which the parametrised coarse model will be evaluated. Its resolution should therefore be high enough that the (yet-to-be-)chosen evaluation metrics are relatively insensitive to small changes

in resolution (i.e., there should be near-convergence of long-term statistics). Note, however, that neither a perfect solution of the fluid equations nor perfect agreement with real-world experimental measurements are necessary; the fine model merely serves as a reference dynamical system whose behaviour I aim to reproduce by parametrising the coarse model. In order to create a worthwhile parametrisation problem, the coarse model's resolution should therefore be low enough that it exhibits statistically significant biases relative to the fine model, as measured by the chosen evaluation metrics. However, as explained in § 3.3, the coarse model must still be numerically stable so that it can provide an unparametrised control solution.

With the above constraints in mind, § 3.5.1 will review the guidelines that have been established in the literature for producing well-resolved simulations of Rayleigh-Bénard convection. § 3.5.2 will then review the metrics that are known to be sensitive to under-resolution; these may be used to experimentally determine appropriate resolutions for the fine and coarse models, and later (in Chapter 5) to evaluate parametrisation performance.

3.5.1 Resolution guidelines

Grötzbach (1983) is recognised as the first to formulate resolution requirements for accurate simulations of Rayleigh-Bénard convection (Chillà and Schumacher 2012; Scheel, Emran, and Schumacher 2013). He identified separate constraints on the mean (i.e., averaged in each spatial direction) grid spacing and the vertical spacing near the plates; I first discuss the former. Grötzbach reasoned that a numerical model that neglects subgrid-scale effects must have a geometric mean grid spacing $h = (\Delta x \Delta y \Delta z)^{1/3}$ such that

$$h \leq \pi\eta = \pi \left(\frac{\nu^3}{\langle\epsilon\rangle} \right)^{1/4} \tag{3.15}$$

where $\eta \equiv (\nu^3/\langle\epsilon\rangle)^{1/4}$ is the *Kolmogorov length*, the universal smallest relevant length scale for general turbulent flow, and $\langle\epsilon\rangle$ is the spatial and temporal average of the kinetic energy dissipation rate defined by

$$\epsilon(\boldsymbol{x},t) \equiv \frac{\nu}{2} \sum_{ij} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)^2 \tag{3.16}$$

(Chillà and Schumacher 2012). The inequality (3.15) between h and η can be understood using the Nyquist-Shannon theorem, which states that a sampling frequency $f \geq k/\pi$ is needed to unambiguously reconstruct a signal with maximum wavenumber k; substituting $f = 1/h$, $k = 1/\eta$ leads to the claimed relation.

Grötzbach recognised that the above reasoning was only valid for the mean grid spacing; large gradients in temperature and velocity near the top and bottom plates require finer resolution in those regions. The notion of nearness can be formalised by considering the thickness of the *thermal boundary layer*, the region at each plate where large temperature gradients exist. Consider a Taylor series expansion of the horizontally- and time-averaged dimensionless temperature profile about $z = 0$; recalling the boundary condition (3.10), this reads

$$\langle\theta\rangle_{A,t} \approx \frac{1}{2} + \left. \frac{\partial\langle\theta\rangle_{A,t}}{\partial z} \right|_{z=0} z + O(z^2).$$

The thermal boundary layer thickness δ_T is defined (see, e.g., Chillà and Schumacher 2012) as the height at which, to first order, the temperature reaches the mean value in the well-mixed interior of the domain (i.e., zero for this problem). It follows that

$$\delta_T = -\frac{1}{2} \left(\left. \frac{\partial\langle\theta\rangle_{A,t}}{\partial z} \right|_{z=0} \right)^{-1}. \tag{3.17}$$

One then asks how many grid points must be within the thermal boundary layer. Grötzbach claimed that 3 points are sufficient for turbulent flows but did not give a theoretical argument to derive this

number. Shishkina et al. (2010) presented a theoretical argument based on the (experimentally and numerically justified) assumption of laminar *Prandtl-Blasius* flow conditions in the boundary layer and were able to calculate the minimum number of grid points (e.g., 9 for Ra $= 2 \times 10^9$ and Pr $= 0.7$). The results agreed with criteria derived in previous numerical experiments. Importantly, the results of Shishkina et al. allow *a priori* determination of vertical resolution requirements, potentially bypassing the time-consuming and expensive process of iteratively running simulations, checking their convergence and updating the resolution.

3.5.2   Metrics sensitive to under-resolution

Performing numerical experiments for a 3D fluid layer, Grötzbach found that the RMS velocity and the *Nusselt number* were the most sensitive quantities to insufficient mean grid spacing, but even they increased "only slightly" above the values obtained from well-resolved simulations. The dimensionless Nusselt number measures the instantaneous rate of (vertical) heat transport across a horizontal plane at height z, normalised by the purely conductive rate that would exist if the fluid were at rest (Verzicco and Camussi 1999). Following Kooij et al. (2018), I define

$$\mathrm{Nu}(z,t) \equiv \sqrt{\mathrm{Ra}\,\mathrm{Pr}}\langle w\theta \rangle_A - \left\langle \frac{\partial \theta}{\partial z} \right\rangle_A \tag{3.18}$$

where $\langle \cdot \rangle_A$ denotes averaging over the horizontal plane at height z, and $w = \boldsymbol{u} \cdot \hat{\boldsymbol{z}}$ is the vertical velocity. Notice that the heat transport has contributions from both advection (the first term) and conduction (the second term). Authors frequently consider the vertically-averaged value

$$\langle \mathrm{Nu}(z,t) \rangle_z = \sqrt{\mathrm{Ra}\,\mathrm{Pr}}\langle w\theta \rangle_{A,z} + 1$$

and/or the time-averaged value, which is is independent of height due to energy conservation,

$$\langle \mathrm{Nu}(z,t) \rangle_t = \langle \mathrm{Nu}(z,t) \rangle_{z,t} = \sqrt{\mathrm{Ra}\,\mathrm{Pr}}\langle w\theta \rangle_{A,z,t} + 1.$$

Later work also supports the finding that the Nusselt number is sensitive to under-resolution. Even studying only steady-state convective solutions at moderate Rayleigh number, Le Quéré (1991) found that the maximum and minimum Nusselt numbers were most sensitive to changes in resolution and had the largest uncertainty among existing benchmark solutions. Other studies have used the convergence of the Nusselt number as an indicator that the spatial resolution is sufficient to produce an accurate solution (Ouertatani et al. 2008).

Stevens, Verzicco, and Lohse (2010) performed 3D simulations in a finite cylindrical cavity with the aim of reconciling the apparent disagreement between the Nusselt numbers in previous numerical studies and experimental observations. They found that agreement with experiment could be achieved, but only by using a much higher resolution than the previous studies. They offered the physical explanation that horizontally under-resolved simulations produce insufficient thermal diffusion, leading to systematic overestimation of the buoyancy of convective plumes near the side-walls of the cylinder; this results in Nusselt numbers that exceed experimentally observed values. This led them to conclude that the two criteria of Grötzbach (1983)—for mean grid spacing and for the vertical spacing near the upper and lower plates—are not independent; the definition $h = (\Delta x \Delta y \Delta z)^{1/3}$ in (3.15) allows the horizontal spacing to remain relatively coarse near the plates, provided the vertical spacing is small. Since fine horizontal resolution is also necessary to accurately capture the dynamics of the thin plumes, they proposed that (3.15) be applied with $h = \max(\Delta x, \Delta y, \Delta z)$ instead.

Some more recent work, however, casts doubt on the notion that the Nusselt number is sensitive to under-resolution and that its convergence is a good indicator that the flow is well-resolved. In assessing the performance of several published computational fluid dynamics codes on the Rayleigh-Bénard problem in a cylindrical cavity, Kooij et al. (2018) identified one higher-order code that reproduced the theoretically predicted scaling of Nu as a function of Ra even when the flow was deliberately under-resolved. On the

other hand, the presence of numerical artefacts in the instantaneous temperature field near the bottom plate was a clear indicator of insufficient resolution.

Scheel, Emran, and Schumacher (2013) performed similar high-resolution simulations for a cylindrical cavity and also found that the Nusselt number, among other global transport properties, were "fairly insensitive to insufficient resolution, as long as the mean Kolmogorov length [was] resolved" (i.e., (3.15) was satisfied). However, they found that the horizontally averaged or local kinetic energy dissipation rate (3.16) and the corresponding thermal dissipation rate

$$\epsilon_T(\boldsymbol{x}, t) \equiv \kappa \sum_i \left(\frac{\partial T}{\partial x_i} \right)^2 \tag{3.19}$$

were much more sensitive, with their convergence requiring even stricter conditions than (3.15).

3.6 Choice of resolution: experiment

§ 3.5 showed that simulations must satisfy certain grid spacing conditions in order to be accurate, and presented several metrics that are sensitive to under-resolution. I now perform numerical experiments and use these conditions and metrics to determine appropriate resolutions for the fine and coarse models in the parametrisation study that will follow.

TODO: describe experiments and present results

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