Contents

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TODO: epigraph

Chapter 5

Evaluation of the parametrised model

5.0.1 Thermal properties

Two more definitions are necessary before proceeding. First, the Nusselt number measures the 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 Chillà and Schumacher (2012), I use the definition (before nondimensionalisation)

$$\mathrm{Nu}(z,t) \equiv \frac{\langle wT \rangle_{A,t} - \kappa \partial \langle T \rangle_{A,t} / \partial z}{\kappa \delta T / d} \tag{5.0.1}$$

where $\langle \cdot \rangle_{A,t}$ denotes averaging over time and the horizontal plane at height z, and $w = \boldsymbol{u} \cdot \hat{\boldsymbol{z}}$ is the vertical velocity. The rate of heat transport in the numerator has two terms: advection $\langle wT \rangle_{A,t}$ and conduction $-\kappa \partial \langle T \rangle_{A,t} / \partial z$. The denominator $\kappa \delta T / d$ is the rate of heat transport for a linear conductive temperature profile with the fluid at rest.

Another important quantity is the thickness δ_T of the *thermal boundary layer* at each plate where large temperature gradients exist. Chillà and Schumacher (2012) define δ_T as follows: if, on average, the fluid temperature changes with height from $+\delta T/2$ at the lower plate to 0 (the mean value in the well-mixed interior) over a distance δ_T, then

$$\left. \frac{\partial \langle T \rangle_{A,t}}{\partial z} \right|_{z=0} \approx -\frac{\delta T}{2\delta_T}.$$

But if one considers the definition of the Nusselt number (5.0.1) at $z = 0$, the advection term $\langle wT \rangle_{A,t}$ vanishes due to the $\boldsymbol{u} = \boldsymbol{0}$ boundary condition and

$$\mathrm{Nu}(z=0) = -\frac{d}{\delta T} \left. \frac{\partial \langle T \rangle_{A,t}}{\partial z} \right|_{z=0}.$$

Thus,

$$\delta_T = \frac{d}{2\,\mathrm{Nu}(z=0)}. \tag{5.0.2}$$

5.0.2 Resolution dependence of numerical solutions

TODO: s.sherwood: Might be important to further explain here that you will regard this as the ("warts and all") dynamical system you want to emulate at a coarser representation. This avoids the issue of whether this hig-res is a perfect solution of the fluid equations or not (it doesn't have to be, although for robustness we want it to be relatively insensitive to small changes in dx).

The first basic requirement for a parametrisation testbed is a reasonably accurate high-resolution model to treat as truth. The next requirement is a truncated coarse model which posesses systematic biases relative to truth that might reasonably be improved by parametrising the unresolved subgrid-scale dynamics. In this section, I review relevant literature on numerical solutions of the Rayleigh-Bénard problem with the aim of establishing the nature of the biases that might be expected. Practically, the following questions must be answered:

- What resolution is necessary for a converged solution?
- Which quantities are most sensitive to insufficient resolution?

Theoretical resolution requirements for accurate simulations

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

$$h \leq \pi\eta = \pi \left(\frac{\nu^3}{\langle\epsilon\rangle}\right)^{1/4} \tag{5.0.3}$$

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

$$\epsilon(\boldsymbol{x}, t) \equiv \frac{\nu}{2} \sum_{ij} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)^2 \tag{5.0.4}$$

(Chillà and Schumacher 2012). The inequality (5.0.3) 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 using the thermal boundary layer thickness (5.0.2), and one asks how many grid points are necessary in this layer. Grötzbach did not give a theoretical argument to derive this number but claimed that 3 points are sufficient for turbulent flows. 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 $\mathrm{Ra} = 2 \times 10^9$ and $\mathrm{Pr} = 0.7$). 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.

Resolution-dependence tests and consequences of under-resolution

Performing numerical experiments for a 3D fluid layer, Grötzbach found that RMS velocity and 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. He concluded that condition (5.0.3) was overly restrictive and recommended (for $\mathrm{Pr} > 0.59$) the simplified, approximate version

$$h \lesssim 5.23\,\mathrm{Pr}^{-1/4}\mathrm{Ra}^{-0.3205}.$$

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 (5.0.3) 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 (5.0.3) 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., (5.0.3) was satisfied). However, they found that the horizontally averaged or local kinetic energy dissipation rate (5.0.4) and the corresponding thermal dissipation rate

$$\epsilon_T(\boldsymbol{x}, t) \equiv \kappa \sum_i \left(\frac{\partial T}{\partial x_i} \right)^2 \tag{5.0.5}$$

were much more sensitive, with their convergence requiring even stricter conditions than (5.0.3).

In summary, conditions on the mean grid spacing and number of grid points in the thermal boundary layer exist to guide high-resolution simulations. It is known that the Nusselt number and kinetic and thermal dissipatiom rates are sensitive to under-resolution, so the statistics of these quantities could serve as metrics for evaluating parametrisation performance.

5.1 Summary

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