A The Rayleigh-Bénard equations

A.1 Derivation

We begin with the Navier-Stokes equations for a 2D fluid whose density depends linearly on temperature in the Boussinesq approximation:

$$\left\{\begin{aligned} \text{Momentum:} \quad & \partial_t \boldsymbol{u} + (\boldsymbol{u}\cdot\boldsymbol{\nabla})\boldsymbol{u} = -\frac{1}{\rho_0}\boldsymbol{\nabla} p + \nu\nabla^2\boldsymbol{u} + g\alpha(T-T_0)\hat{\boldsymbol{z}} \\ \text{Thermal advection-diffusion:} \quad & \partial_t T + (\boldsymbol{u}\cdot\boldsymbol{\nabla})T = D_T\nabla^2 T \\ \text{Incompressibility:} \quad & \boldsymbol{\nabla}\cdot\boldsymbol{u} = 0 \end{aligned}\right. . \tag{1}$$

Here $\boldsymbol{u} = (u, 0, w)$ and $\boldsymbol{\nabla} = (\partial_x, 0, \partial_z)$.

(1) is cumbersome to solve numerically due to the presence of the pressure p, whose time derivative is not explicitly specified, and the incompressibility condition, which is not automatically satisfied by naïvely time-stepping the momentum equation.

Instead, one may use the fact that any divergence-free 2D vector field $\boldsymbol{u} = (u, 0, w)$ may be expressed in terms of a scalar streamfunction ψ as $\boldsymbol{u} = (-\partial_z\psi, 0, \partial_x\psi)$, which automatically satisfies $\boldsymbol{\nabla}\cdot\boldsymbol{u} = 0$. This leads to the vorticity-streamfunction representation of the Navier-Stokes equations, where the vorticity $\boldsymbol{\omega} \equiv \boldsymbol{\nabla}\times\boldsymbol{u}$ is simply $\nabla^2\psi\ \hat{\boldsymbol{y}}$. It may be shown that (1) is equivalent to

$$\left\{\begin{aligned} \partial_t\omega + (\boldsymbol{u}\cdot\boldsymbol{\nabla})\omega &= \nu\nabla^2\omega - g\alpha\partial_x T \\ \partial_t T + (\boldsymbol{u}\cdot\boldsymbol{\nabla})T &= D_T\nabla^2 T \\ \nabla^2\psi &= \omega \end{aligned}\right. . \tag{2}$$

Our numerical methods require us to recast (2) in flux form, i.e., $\partial_t\omega = \boldsymbol{\nabla}\cdot\boldsymbol{F}$ for some vector field $\boldsymbol{F}$ and similarly for T. This is easily done using the product rule for divergence combined with the incomprssibility constraint; for any scalar function ψ,

$$\boldsymbol{u}\cdot\nabla\psi = \boldsymbol{\nabla}\cdot(\boldsymbol{u}\psi) - \underbrace{(\boldsymbol{\nabla}\cdot\boldsymbol{u})}_{=0}\psi = \boldsymbol{\nabla}\cdot(\boldsymbol{u}\psi).$$

This leads to the flux-form Navier-Stokes equations in the vorticity-streamfunction representation,

$$\left\{\begin{aligned} \partial_t\omega &= \boldsymbol{\nabla}\cdot(\nu\boldsymbol{\nabla}\omega - \boldsymbol{u}\omega - g\alpha T\hat{\boldsymbol{x}}) \\ \partial_t T &= \boldsymbol{\nabla}\cdot(\nu\boldsymbol{\nabla}T - \boldsymbol{u}T) \\ \omega &= \boldsymbol{\nabla}\cdot(\boldsymbol{\nabla}\psi) \end{aligned}\right. . \tag{3}$$

The dynamical system (3) serves as the object of our parametrisation study.

A.2 Nondimensionalisation

The system (3) contains 12 dimensional parameters (3 independent variables, 5 dependent variables and 4 constants), spanning 3 physical dimensions (length, time and temperature). According to the Buckingham π theorem, the relationships may be re-expressed in terms of $12-3=9$ dimensionless parameters. These are found using the method of repeating variables, where the repeating variables are chosen to be ν, g and α:

$$\begin{aligned} &\tilde{t} = t\left(\frac{g^2}{\nu}\right)^{1/3}, && \tilde{\omega} = \omega\left(\frac{\nu}{g^2}\right)^{1/3}, && \tilde{x} = x\left(\frac{g}{\nu^2}\right)^{1/3}, \\ &\tilde{z} = z\left(\frac{g}{\nu^2}\right)^{1/3}, && \tilde{u} = \frac{u}{(\nu g)^{1/3}}, && \tilde{w} = \frac{w}{(\nu g)^{1/3}}, \\ &\tilde{T} = \alpha T, && \tilde{D_T} = \frac{D_T}{\nu} \equiv \mathrm{Pr}^{-1}, && \tilde{\psi} = \frac{\psi}{\nu}, \end{aligned}$$

where Pr is the Prandtl number.

Rewritten in terms of the dimensionless parameters, the dimensionless form of (3) is

$$\partial_t \omega = \boldsymbol{\nabla} \cdot (\boldsymbol{\nabla}\omega - \boldsymbol{u}\omega - T\hat{\boldsymbol{x}}) \tag{4a}$$
$$\partial_t T = \boldsymbol{\nabla} \cdot (\mathrm{Pr}^{-1}\boldsymbol{\nabla}T - \boldsymbol{u}T) \tag{4b}$$
$$\omega = \boldsymbol{\nabla} \cdot (\boldsymbol{\nabla}\psi) \tag{4c}$$

where we have dropped the tildes.

A.3 Finite difference discretisation

While many numerical methods exist for solving partial differential equations, we opt for a simple finite difference approach in order to facilitate the separation of the system into "resolved" and "unresolved" parts later. Figure 1 shows the grid that we shall use.

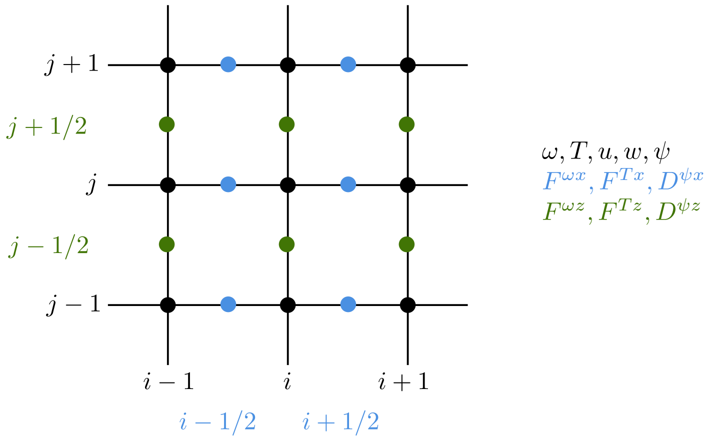

Figure 1: The grid used for the finite difference solution. The key on the right indicates which of the three staggered sub-grids each variable is defined on.

Define the vorcitity flux in (4a) as

$$\boldsymbol{F}^{\omega} = \boldsymbol{\nabla}\omega - \boldsymbol{u}\omega - T\hat{\boldsymbol{x}},$$

with components

$$F^{\omega x} = \partial_x \omega - u\omega - T,$$
$$F^{\omega z} = \partial_z \omega - w\omega.$$

The variables u, ω, T are defined on the black grid in Figure 1. $F^{\omega x}$ is defined on the horizontally staggered blue grid and always has a half-integer first index. $F^{\omega z}$ is defined on the vertically staggered green grid, with a half-integer second index. The reason for the staggering will become clear when we define the "resolved" and "unresolved" variables in the next section. With this in mind, we approximate the derivatives using central differences, giving

$$F^{\omega x}_{i+1/2,j} = \frac{\omega_{i+1,j} - \omega_{ij}}{\Delta x} - u_{i+1/2,j}\omega_{i+1/2,j} - T_{i+1/2,j},$$
$$F^{\omega z}_{i,j+1/2} = \frac{\omega_{i,j+1} - \omega_{ij}}{\Delta z} - w_{i,j+1/2}\omega_{i,j+1/2},$$

where Δx and Δz are the grid spacings. These expressions are slightly problematic due to terms like $u_{i+1/2,j}$ that are indexed halfway between grid points, but the issue is easily resolved by approximating these terms as averages of the neighbouring points:

$$
\begin{aligned}
F^{\omega x}_{i+1/2,j} &= \frac{\omega_{i+1,j} - \omega_{ij}}{\Delta x} - \frac{(u_{ij} + u_{i+1,j})(\omega_{ij} + \omega_{i+1,j})}{4} + \frac{T_{ij} + T_{i+1,j}}{2}, \\
F^{\omega z}_{i,j+1/2} &= \frac{\omega_{i,j+1} - \omega_{ij}}{\Delta z} - \frac{(w_{ij} + w_{i,j+1})(\omega_{ij} + \omega_{i,j+1})}{4}.
\end{aligned} \tag{5}
$$

Similarly, the components of the temperature flux in (4b),

$$
\boldsymbol{F}^T = \mathrm{Pr}^{-1} \boldsymbol{\nabla} T - \boldsymbol{u} T,
$$

have the finite difference approximations

$$
\begin{aligned}
F^{Tx}_{i+1/2,j} &= \mathrm{Pr}^{-1} \frac{T_{i+1,j} - T_{ij}}{\Delta x} - \frac{(u_{ij} + u_{i+1,j})(T_{ij} + T_{i+1,j})}{4}, \\
F^{Tz}_{i,j+1/2} &= \mathrm{Pr}^{-1} \frac{T_{i,j+1} - T_{ij}}{\Delta z} - \frac{(w_{ij} + w_{i,j+1})(T_{ij} + T_{i,j+1})}{4}.
\end{aligned}
$$

Now, the finite difference approximation of the vorticity equation (4a) becomes

$$
\begin{aligned}
\partial_t \omega_{ij} &= (\boldsymbol{\nabla} \cdot \boldsymbol{F}^{\omega})_{ij} \\
&= \frac{F^{\omega x}_{i+1/2,j} - F^{\omega x}_{i-1/2,j}}{\Delta x} + \frac{F^{\omega z}_{i,j+1/2} - F^{\omega z}_{i,j-1/2}}{\Delta z},
\end{aligned} \tag{6}
$$

and similarly for the temperature equation (4b),

$$
\begin{aligned}
\partial_t T_{ij} &= (\boldsymbol{\nabla} \cdot \boldsymbol{F}^{T})_{ij} \\
&= \frac{F^{Tx}_{i+1/2,j} - F^{Tx}_{i-1/2,j}}{\Delta x} + \frac{F^{Tz}_{i,j+1/2} - F^{Tz}_{i,j-1/2}}{\Delta z}.
\end{aligned}
$$

The finite difference form of the Poisson equation (4c) is constructed by defining the components of the streamfunction gradient,

$$
\begin{aligned}
D^{\psi x} i+1/2, j &= \frac{\psi_{i+1,j} - \psi_{ij}}{\Delta x}, \\
D^{\psi z} i, j+1/2 &= \frac{\psi_{i,j+1} - \psi_{ij}}{\Delta z}.
\end{aligned} \tag{7}
$$

The Poisson equation then becomes

$$
\omega_{ij} = \frac{D^{\omega x}_{i+1/2,j} - D^{\omega x}_{i-1/2,j}}{\Delta x} + \frac{D^{\omega z}_{i,j+1/2} - D^{\omega z}_{i,j-1/2}}{\Delta z}. \tag{8}
$$

A.4 Resolved and unresolved variables

So far, we have derived a numerical method to solve the Rayleigh-Bénard system (4) on a grid. However, in order to develop a parametrisation, we will need to express it in terms of a set of large-scale “resolved” variables and a set of sub-grid-scale “unresolved” variables. Zacharuk et al. (2018) demonstrate a simple approach where the resolved variables are average values of the original variables across several neighbouring grid cells and the unresolved variables are the corresponding residuals at each point. They considered a 1D system, but we now generalise the method to 2D.

The structure of the domain is shown in Figure 2, which is essentially Figure 1 with the addition of a new red grid. As previously discussed, the original variables ω, T, ψ, etc. are defined on the black grid, which we shall call the “fine” grid. Points on the fine grid are enumerated by lowercase indices (i, j), beginning with $(0, 0)$ at the bottom-left corner. We then construct a “coarse” grid (red), whose spacing is n times larger than the fine grid (n is an integer). Points on this grid are enumerated by uppercase indices (I, J),

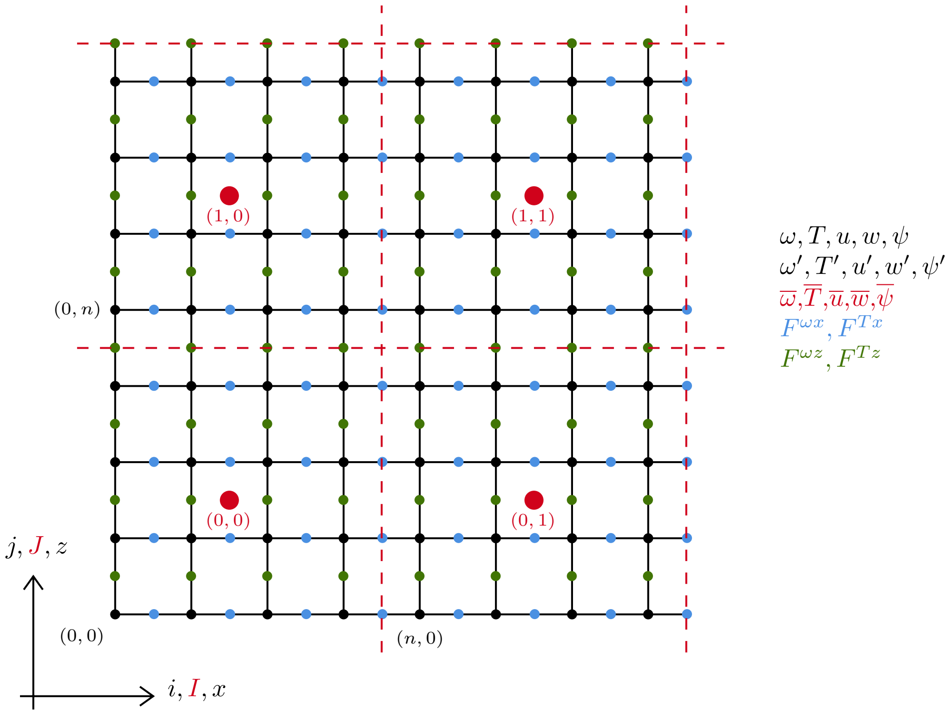

Figure 2: The grid used for the finite difference solution, showing an example where the coarse grid spacing is $n = 4$ times larger than the fine spacing.

and the $(0, 0)$ point on the coarse grid lies at $((n-1)/2, (n-1)/2)$ on the fine grid. Figure 2 has $n = 4$ as an example.

The "resolved" variables, denoted by overbars $(\bar{\cdot})$, are defined on the coarse grid. The value of a resolved variable (e.g., $\bar{\omega}$) at point (I, J) is the average value of the orignal variable (e.g., ω) over an n-by-n subset of the fine grid, centred on the coarse grid point. In Figure 2 with $n = 4$, the value at each red point is the average across a 4×4 set of black points, delimited by dashed red lines. Mathematically, the resolved vorticity values (for example) are defined as

$$\bar{\omega}_{IJ} = \frac{1}{n^2} \sum_{m,p=-(n-1)/2}^{(n-1)/2} \omega_{i(I)+m,j(J)+p}, \tag{9}$$

where $i(I) = nI + (n-1)/2$ and $j(J) = nJ + (n-1)/2$.

The "unresolved" variables, denoted by primes, are defined on the fine grid. The value of, say, ω'_{ij} is the residual of ω_{ij} with respect to the corresponding coarse average value:

$$\omega'_{ij} = \omega_{ij} - \bar{\omega}_{I(i),J(j)}, \tag{10}$$

where $I(i) = \lfloor i/n \rfloor$ and $J(j) = \lfloor j/n \rfloor$ ($\lfloor \cdot \rfloor$ is the floor function.)

The first step is to take the time derivative of (9) and substitute the expression for $\partial_t \omega_{ij}$ from (6):

$$\begin{aligned}\partial_t \bar{\omega}_{IJ} &= \frac{1}{n^2} \sum_{m,p=-(n-1)/2}^{(n-1)/2} \partial_t \omega_{i(I)+m,j(J)+p} \\ &= \frac{1}{n^2} \sum_{m,p=-(n-1)/2}^{(n-1)/2} \left[\frac{F^{\omega x}_{i(I)+m+1/2,j(J)+p} - F^{\omega x}_{i(I)+m-1/2,j(J)+p}}{\Delta x} \right.\end{aligned}$$

$$+\frac{F^{\omega z}_{i(I)+m,j(J)+p+1/2}-F^{\omega z}_{i(I)+m,j(J)+p-1/2}}{\Delta z}\Bigg].$$

The utility of the staggered grids now becomes clear; the fluxes in the interior are cancelled, leaving only the fluxes at the boundaries:

$$\begin{aligned}
\partial_t\bar\omega_{IJ} &= \frac{1}{n^2}\Bigg[\sum_{p=-(n-1)/2}^{(n-1)/2}\frac{F^{\omega x}_{i(I)+n/2,j(J)+p}-F^{\omega x}_{i(I)-n/2,j(J)+p}}{\Delta x} \\
&\qquad+\sum_{m=-(n-1)/2}^{(n-1)/2}\frac{F^{\omega z}_{i(I)+m,j(J)+n/2}-F^{\omega z}_{i(I)+m,j(J)-n/2}}{\Delta z}\Bigg]. \\
&= \frac{1}{n^2}\sum_{m=-(n-1)/2}^{(n-1)/2}\Bigg[\frac{F^{\omega x}_{i(I)+n/2,j(J)+m}-F^{\omega x}_{i(I)-n/2,j(J)+m}}{\Delta x} \\
&\qquad+\frac{F^{\omega z}_{i(I)+m,j(J)+n/2}-F^{\omega z}_{i(I)+m,j(J)-n/2}}{\Delta z}\Bigg].
\end{aligned}\tag{11}$$

The first term in the sum is the net horizontal flux into the $n\times n$ region belonging to $\bar\omega_{IJ}$, and the second term is the net vertical flux. We have essentially employed a discrete form of the divergence theorem.

The next step, which we do not write out explicitly, is to substitute the expressions (5) for the fluxes into (11). This expresses $\partial_t\bar\omega_{IJ}$ in terms of ω, u, w, T. Finally, inserting the decompositions $\omega=\bar\omega+\omega'$, $u=\bar u+u'$, etc. leads to an expression for $\partial_t\bar\omega_{IJ}$ that has the form

$$\partial_t\bar\omega_{IJ}=S_{\bar\omega}(\bar\omega,\bar u,\bar w,\bar T)+C_{\bar\omega}(\omega',u',w',T')+X_{\bar\omega}(\bar u,u',\bar w,w').\tag{12}$$

The first term, $S_{\bar\omega}$, describes the self-interactions of the resolved variables. The second term, $C_{\bar\omega}$, couples the resolved variables to the unresolved ones. The third term, $X_{\bar\omega}$, consists of cross terms such as $\bar u\omega'$ (arising from the nonlinear term $(u_{ij}+u_{i+1,j})(\omega_{ij}+\omega_{i+1,j})$ in (5)) that cannot be separated into self-interaction and coupling terms. The aim of parametrisation is to estimate $C_{\bar\omega}$ and $X_{\bar\omega}$, only having knowledge of the resolved variables.

A similar decomposition can be performed for the temperature equation (4b), giving an expression of the form

$$\partial_t\bar T_{IJ}=S_{\bar T}(\bar\omega,\bar u,\bar w,\bar T)+C_{\bar T}(\omega',u',w',T')+X_{\bar T}(\bar u,u',\bar w,w').\tag{13}$$

Like (12), the Poisson equation for $\bar\omega$ can be expressed as a net flux,

$$\begin{aligned}
\bar\omega_{IJ} &= \frac{1}{n^2}\sum_{m=-(n-1)/2}^{(n-1)/2}\Bigg[\frac{D^{\psi x}_{i(I)+n/2,j(J)+m}-D^{\psi x}_{i(I)-n/2,j(J)+m}}{\Delta x} \\
&\qquad+\frac{D^{\psi z}_{i(I)+m,j(J)+n/2}-D^{\psi z}_{i(I)+m,j(J)-n/2}}{\Delta z}\Bigg],
\end{aligned}$$

which can also be reduced to self-interaction and coupling terms:

$$\bar\omega_{IJ}=S_{\bar\psi}(\bar\psi)+C_{\bar\psi}(\psi').\tag{14}$$

There is no cross-term for the Poisson equation.

A.5 Solution algorithm

Once appropriate boundary conditions have been formulated, (6)–(8) may be solved directly to obtain a "truth" solution on the fine grid. Given the fields ω, u, w, T at the current time step, the values at the next time step are determined by the following procedure:

1. Using (6), update ω at each point with the simple forward Euler method $\omega_{ij}(t+\Delta t) = \omega_{ij}(t) + \Delta t \cdot \partial_t \omega_{ij}(t)$.
2. Using (7), update T at each point.
3. Given $\omega(t+\Delta t)$ use standard numerical linear algebra methods to solve the Poisson equation (8) for $\psi(t+\Delta t)$.
4. Calculate $u(t+\Delta t) = -\partial_z \psi(t+\Delta t)$ and $w(t+\Delta t) = \partial_x \psi(t+\Delta t)$.

The parametrised solution for the resolved variables is similar, but requires additional estimation steps:

1. Estimate the coupling terms $C_{\bar{\omega}}$ and $X_{\bar{\omega}}$ that appear in (12).
2. Using (12), update $\bar{\omega}$ at each point.
3. Estimate the coupling terms $C_{\bar{T}}$ and $X_{\bar{T}}$ that appear in (13).
4. Using (13), update $\bar{T}$ at each point.
5. Estimate the coupling term $C_{\bar{\psi}}$ that appears in (14).
6. Given $\bar{\omega}(t+\Delta t)$, solve the Poisson equation (14) for $\psi(t+\Delta t)$.
7. Calculate $\bar{u}(t+\Delta t) \approx -\partial_z \bar{\psi}(t+\Delta t)$ and $\bar{w}(t+\Delta t) \approx \partial_x \bar{\psi}(t+\Delta t)$.

References

Zacharuk, M., S. I. Dolaptchiev, U. Achatz, and I. Timofeyev (2018). "Stochastic subgrid-scale parametrization for one-dimensional shallow-water dynamics using stochastic mode reduction". *Quarterly Journal of the Royal Meteorological Society* **144**(715), 1975–1990. DOI: 10.1002/qj.3396.