Accelerated convergence of convective simulations using boundary value problems

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WOW this is a really long sentence check out this abstract I'll just keep writing words to make this at least one line long so we know what the formatting looks like, ok?

I. INTRODUCTION

Natural convection occurs in the presence of disparate timescales. Granules on the solar surface overturn on the order of 10 minutes, whereas deep motions in the Sun are likely at low Mach number and constrained by the solar rotation rate of $\tilde{1}$ month. Despite these relatively short dynamical times, the scale of energy transport on the Sun occurs on the Kelvin-Helmholtz timescale of nearly 3×10^7 *years* [1]. As simulations aim to model natural convection by increasing into the high-Rayleigh Number (Ra) regime, where diffusive timescales are much longer than dynamical timescales [2], achieving converged simulations will require runs which span a greater number of convective timescales in order to thermally converge. Furthermore, with increasing Ra and decreasing diffusivities, motions become more turbulent and require finer grid meshes and smaller timesteps to resolve turbulent motions, meaning that achieving even one overturn timescale becomes a harder problem. These two effects combine to make thermally converging high-Ra, astrophysically interesting simulations intractable using modern numerical tools.

In studies of stratified convection where a convective layer lies between stable layers, studies have used the knowledge of Mixing Length Theory (MLT) to adjust the initial thermal profile of atmospheres to a state which is closer to the adiabat chosen by convection [7]. However, many studies of convection do not contain stable layers above and below the convection zone, and the presence of hard boundaries and the boundary layers that they form means that the proper adiabat cannot be known *a priori* until the simulation evolves the structure of the boundary layers.

The chosen boundary conditions at the upper and lower plates determine key quantities of the dynamics of the evolved state. Studies of incompressible, Boussinesq, Rayleigh-Bénard convection (RBC) often employ fixed temperature (Dirichlet) or fixed heat flux (Neumann) boundary conditions at both plates. Dirichlet conditions represent plates of infinite conductivity, whereas Neumann conditions model plates of finite conductivity. In both cases, choosing symmetric boundary conditions maintains overall system symmetry, and despite evolving towards different thermal structures, both types of conditions transport heat in the same manner [3].

Studies of convection which aim to model in astrophysical systems, such as the outer envelopes of low-to-moderate mass stars like the Sun, often employ a mixture of these two types of boundary conditions [4–6]. The flux at the lower boundary is fixed, modeling the constant energy generation of the stellar core, while the outer boundary condition is held at a fixed temperature, modeling the surface of a star which must output the energy generated internally. While this setup is a useful model for understanding natural systems, simulations which employ this setup often suffer from a long thermal relaxation as the atmosphere loses energy and approaches the adiabat chosen by the Dirichlet condition.

Here we present a method for using simple boundary value problems (BVPs), along with information about the evolved flow fields, to fast-forward the slow thermal evolution of convecting simulations. We run two sets of experiments: one in which we allow convective simulations to evolve for a full thermal timescale before taking measurements, and another in which we employ a fast-forwarding, BVP technique which occurs on dynamical timescales. We compare these two sets of simulations to show the validity of the BVP technique. Then, we use the BVP technique to run simulations at high Ra, in the regime where running for thermal timescales becomes computationally intractable.

II. EXPERIMENT

In our study, we adopt the Oberbeck-Boussinesq approximation. Here, the fluid has constant kinematic viscosity (ν), thermal diffusivity (κ), and coefficient of thermal expansion (α). We non-dimensionalize length by the layer height (L_z) , temperature by the (constant) initial temperature gradient across the layer (∇T_0), and time by the freefall timescale (L_z/v_{ff}, with $v_{\text{ff}} = \sqrt{\alpha g L_z^2 \nabla T_0}$, where g is uniform gravitational acceleration in the $-\hat{z}$ direction). The dimensionless Boussinesq equations governing the velocity $\boldsymbol{u} = u\hat{x} + v\hat{y} + w\hat{z}$, temperature $T = T_0 + T_1$, and reduced pressure ϖ are [8]

$$\nabla \cdot \boldsymbol{u} = 0, \tag{1}$$

$$\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u} \cdot \nabla \boldsymbol{u} = -\nabla \varpi + T_1 \hat{z} + \frac{\mathrm{Pr}}{\mathrm{Ra}} \nabla^2 \boldsymbol{u}, \tag{2}$$

$$\frac{\partial T_1}{\partial t} + \boldsymbol{u} \cdot \nabla (T_0 + T_1) = \frac{1}{\mathrm{Pr}\,\mathrm{Ra}} \nabla^2 T_1, \tag{3}$$

where the dimensionless control parameters are the Rayleigh and Prandtl numbers,

$$\mathrm{Ra} = \frac{g\alpha L^4 \left(\frac{dT}{dz}\right)_0}{\nu\chi} = \frac{(L\, v_{\mathrm{ff}})^2}{\nu\chi}, \qquad \mathrm{Pr} = \frac{\nu}{\chi}. \tag{4}$$

The dimensionless vertical extent of the domain is $z = [-1/2, 1/2]$, and at the boundaries we impose no-slip, impenetrable boundary conditions such that $w = u = v = 0$ at $z = \pm 1/2$. At the lower boundary, we employ a fixed flux condition such that $\partial T_1/\partial z = 0$ at $z = -1/2$, and we impose a fixed temperature condition $T_1 = 0$ at $z = 1/2$. Both horizontal directions are periodic and have equal aspect ratio, $\gamma = 4$, such that the horizontal coordinates $x, y = [0, \Gamma]$.

A. The Boundary Value Problem

The Boussinesq BVP is simply the time-stationary, horizontally- and time- averaged equations of hydrostatic balance and energy conservation,

$$\frac{\partial}{\partial z} \langle \varpi \rangle = \langle T_1 \rangle \hat{z}, \tag{5}$$

$$\frac{\partial}{\partial z} \langle w T_1 \rangle = \frac{1}{\mathrm{PrRa}} \frac{\partial^2}{\partial z^2} \langle T_1 \rangle, \tag{6}$$

where $\langle A \rangle$ represents a time- and horizontally averaged profile of the quantity A. These equations arise from taking time- and horizontal- averages of Eqns (2-3) and neglecting terms that vanish due to symmetry in the evolved flows. Convective flows are perturbations around a thermal profile defined by these equations in the proper evolved state.

In Boussinesq RBC, the thermal structure of the atmosphere is fully determined by the specification of the convective flux, $F_{conv} = \langle w T_1 \rangle$. If this profile is known, then T_1 and ϖ can be found under the proper specifications of boundary conditions. Under the choice of mixed thermal boundary conditions, the initial atmosphere contains more thermal energy ($\propto T$) than the evolved adiabatic solution. As the atmosphere adjusts to be nearly isothermal in the interior, it must evolve towards the (cold) temperature value specified at the upper boundary. The evolution of the atmosphere results in an asymmetric flux profile during the slow thermal evolution of the atmosphere. Furthermore, under our nondimensionalization, the convective flux (and the flux at the upper boundary layer) are O(1) during the convective transient, whereas the flux entering the atmosphere at the lower boundary is $\mathrm{O}(\mathrm{Ra}^{-1/2})$, so the asymmetry of the fluxes becomes increasingly pronounced as Ra is increased into the turbulent realm.

In order to find the evolved temperature profile of the atmosphere using the Boussinesq BVP equations, the evolved profile of the convective flux must be properly specified. In order to construct this profile, we acknowledge that the evolved solution will in flux equilibrium, carrying the amount of the flux entering through the bottom. Thus, the steady-state profile of the convective flux can be approximated as

$$F_{\mathrm{conv,\ steady}} = F_{\mathrm{bot}} \frac{\langle w T_1 \rangle}{\langle w T_1 - \kappa \partial_z (T_0 + T_1) \rangle} = F_{\mathrm{bot}} \frac{\langle F_{\mathrm{conv,\ IVP}} \rangle}{\langle F_{\mathrm{tot,\ IVP}} \rangle}. \tag{7}$$

Or, put simply, the steady state convective flux is retrieved by properly removing the asymmettry from the flux profile.

In our Boussinesq BVPs, we solve Eqns. (5-6), substituting $\langle w T_1 \rangle = F_{\mathrm{conv,\ steady}}$ as defined in eqn. (7) to retrieve the proper vertical profile of T_1 and ϖ. We then update the mean horizontal value of T_1 and ϖ in a corresponding IVP, and continue to timestep forward with the newly adjusted atmosphere.

In essence, solving the BVP is equivalent to saying that even though the magnitude of flux through the system is not initially correct, the system appropriately picks out the ratios

$$f_{\mathrm{conv}} = \frac{F_{\mathrm{conv}}}{F_{\mathrm{tot}}} \qquad f_{\mathrm{cond}} = \frac{F_{\mathrm{cond}}}{F_{\mathrm{tot}}}. \tag{8}$$

in the convective, transient state, but the total amount of flux is too large until the system reaches the proper isotherm.

B. Numerics

We utilize the Dedalus[1] pseudospectral framework [9] to time-evolve (1)-(3) using an implicit-explicit (IMEX), third-order, four-step Runge-Kutta timestepping scheme RK443 [10]. The temperature field is decomposed as $T = T_0(z) + T_1(x, y, z, t)$ and the velocity is $\boldsymbol{u} = w\hat{\boldsymbol{z}} + u\hat{\boldsymbol{x}} + v\hat{\boldsymbol{y}}$. In our 2D runs, $v = 0$. Variables are time-evolved on a dealiased Chebyshev (vertical) and Fourier (horizontal, periodic) domain in which the physical grid dimensions are 3/2 the size of the coefficient grid. Domain sizes range from 32x128 coefficients at the lowest values of Ra to 1024x4096 coefficients at Ra $> 10^9$ in 2D.

As initial conditions, we fill T_1 with random white noise whose magnitude is $10^{-6}(\text{Ra Pr})^{-1/2}$. This ensures that the initial perturbations are much smaller than the evolved convective temperature perturbations, even at large Ra. We filter this noise spectrum in coefficient space, such that only the lower 25% of the coefficients have power.

In 2D, there are often multiple steady state solutions (e.g., 2-roll and 3-roll solutions) which have slightly different flow properties (heat transport, etc.). Even though the initial perturbations are very small, they shape the convective transient and thus determine the nature of the steady state convection, at least in the laminar regime. In order to ensure that our results are not biased by differences in flow structure, we ran the simulations using distinct random temperature perturbations so as to compare statistics in comparable flow fields. In 3D, rolls are nonstationary over convective timescales, and so these effects need not be considered there.

C. Results

We use the standard definition of the Nusselt number,

$$\text{Nu} = \frac{\left\langle wT - (\text{Ra Pr})^{-1/2}\nabla T\right\rangle}{\left\langle -(\text{Ra Pr})^{-1/2}\nabla T\right\rangle} = 1 + \frac{\langle wT\rangle}{-\Delta T}\sqrt{\text{Ra Pr}}, \tag{9}$$

where $\Delta T = T(z = 1/2) - T(z = -1/2)$ is the evolved temperature difference between the top and bottom plates. This form of the Nusselt number is valid even when the system is not yet in flux equilibrium, and reduces to the standard fixed flux definition of $\text{Nu} = [1 - \langle wT\rangle / P]^{-1}$ [3].

Here we talk about how the solutions are different, or similar. This includes:

1. Showing that the flow fields look similar
2. Showing how the temperature / flux profiles look similar/different
3. showing how Nu and Re scale with Ra in BVP / IVP.
4. showing how the PDFs of w, wT, and T change.

Then we need to make some comments about whether this is good or bad

Then we need to mention how the same thing can be done in stratified, just there you don't assume symmetrical boundary layers.

III. DISCUSSION & CONCLUSIONS

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[1] http://dedalus-project.org/

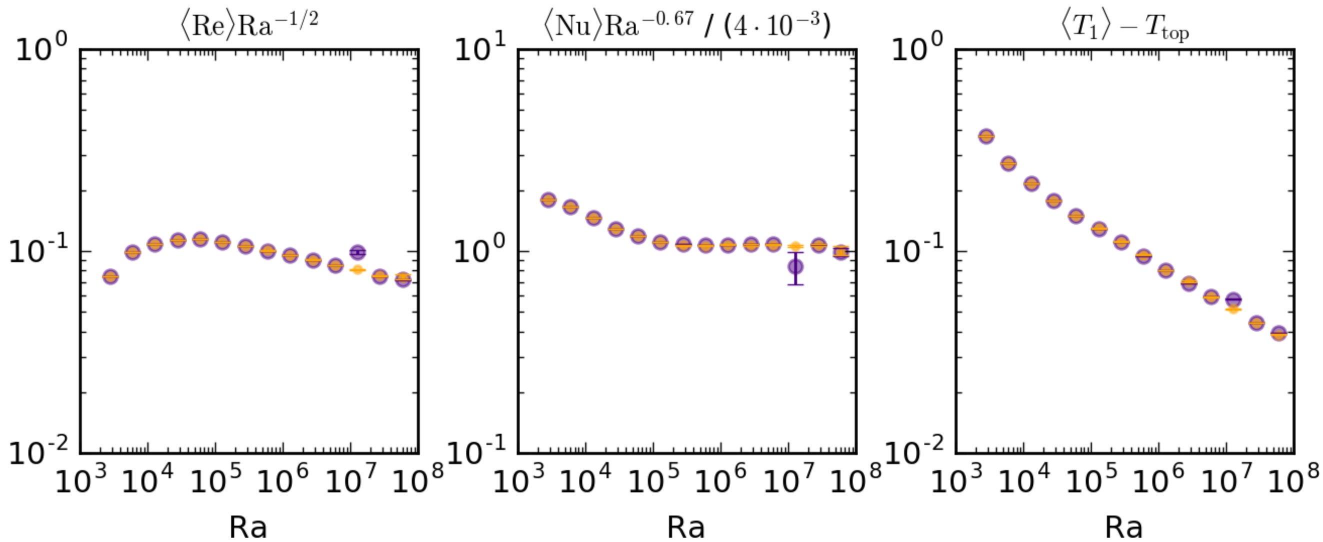

FIG. 1.

Appendix A: Table of Boussinesq Runs

Appendix B: Table of stratified runs

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