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Schwarzschild or Ledoux: composition gradients are fragile

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ABSTRACT

This will be an abstract.

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1. INTRODUCTION

- Observations tell us that we don't understand the mixing near convective boundaries.
- One fundamental question is: what stability criterion should be used? Define Schwarzschild and Ledoux boundaries.
- Section II of Kaiser et al. (2020) contains an excellent description of the difference between schwarzschild and ledoux criteria, mentions the fact that simulations that start at ledoux evolve towards schwarzschild. They note that the long-term behavior is understood, but short-timescale behavior needs more work.
- Georgy et al. (2021) compute models using the Schwarzschild and Ledoux criterion; they find that both criterion produce similar results on the main sequence but noticeably different tracks on the post-MS, and that the Ledoux criterion tracks are a somewhat better fit than the Schwarzschild.
- Naive implementation e.g., in Paxton et al. (2013) run into problems in the context of MLT logic.

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- These naive implementations also are at odds with simulations: high entrainment rates (citations), and entrainment theories suggest that ledoux-stable but schwarzschild-unstable regions should be fully mixed (Fuentes & Cumming 2020), more citations.
- Furthermore, Gabriel et al. (2014) point out that a naive use of the Ledoux criterion is logically inconsistent within the framework of mixing length theory.
- New algorithms (Paxton et al. 2018, 2019) have been developed which handle boundaries self-consistently and essentially make Schwarzschild and Ledoux criterion the same.
- This theoretical discussion has occurred in the context of theoretical arguments and 1D models, but convection is a three-dimensional process.
- Fundamental, simple experiments which demonstrate the efficacy of these new algorithms, and whether convection prefers the Schwarzschild or Ledoux stability criterion, are lacking.
- Many high-resolution simulations of convection in stellar contexts have measured instantaneous entrainment rates achieved in 1D-motivated setups

(Meakin & Arnett 2007; Woodward et al. 2015; Jones et al. 2017; Cristini et al. 2019; Andrassy et al. 2020), but these simulations generally do not run for enough convective overturn times (hundreds or thousands) to detect appreciable changes in the location of the convective boundary due to entrainment. These simulations have also shown the convective boundary moving beyond the initial Ledoux boundary, but generally do not show the final state of this evolution.

- In this work, we present a simple three-dimensional experiment that demonstrates that regions that are stable by the Ledoux criterion are fragile, and that, at late times, the Ledoux and Schwarzschild criterion both find the same edge of the convection zone.

2. THEORY

- The stability of a convective region can instantaneously be determined using the Schwarzschild criterion,
$$y_S = \nabla_{\rm rad} - \nabla_{\rm ad}, \tag{1}$$
or the Ledoux criterion,
$$y_L = \nabla_{\rm rad} - \nabla_{\rm L}, \tag{2}$$
with the unstable convection zone contained within the region where $y < 0$ (see e.g., section 2 of Paxton et al. 2018).

- The *instantaneous* stability changes over the course of many convective freefall times, and stellar evolution timesteps generally span many convective overturn times.

- The goal of this work is to find if y_S and y_L evolve toward the same value, and whether they evolve toward the initial boundary as determined by y_S or y_L.

- We will study a numerical simulation with three layers: a convective layer $y_s < 0$ and $y_L < 0$, a "semiconvective" (see section 4 of Paxton et al. 2013) (Salaris & Cassisi 2017) layer with $y_S < 0$ but $y_L > 0$ (which is stable to ODDC Garaud 2018), and a fully stable layer with $y_L > 0$ and $y_S > 0$.

- While "semiconvective" layers are often unstable to doubly-diffusive instabilities in stellar regimes (Moore & Garaud 2016), our purpose in this work is to demonstrate that regardless of whether these layers are doubly-diffusive unstable, they are entrained and destroyed by neighboring convective zones.

3. RESULTS

- We simulate a three-layer system with X properties using the Dedalus pseudospectral solver. We refer the reader to appendices A and B for details of the model assumptions, setup, and numerical methods.

- In figure **??** we show volume visualizations of instantaneous dynamics near the beginning, during the entrainment phase, and in the evolved state of one of these simulations. Here is a description of the things to look for in these visualizations. I should write this before I decide which things to put into this figure.

- In figure **??** we show horizontally- and time-averaged profiles of the initial state of the simulation, during the entrainment phase, and in the evolved state. Here's an in-depth description of what's plotted. Here's what you should take away from each panel of the plots.

- In figure **??**, we plot a Kippenhahn-like diagram of the simulation. The orange region is the convection zone, the green region is Ledoux-stable but Schwarzschild-unstable, and the purple region is both Schwarzschild and Ledoux stable. The line at the top of the orange region determines the boundary of the convection zone according to y_L, and the line at the bottom of the purple region determines the CZ boundary according to y_S. While these lines start at different heights, convection entrains low-composition fluid according to a classic $\sqrt{t}$ entrainment law until these criteria are the same.

4. CONCLUSIONS

- We simulated X.

- These simulations demonstrate that the Schwarzschild criterion provides a good estimate of the boundary of the unstable convection zone.

- This analysis ignores secondary effects (e.g., convective penetration Anders et al. 2021, because we designed our experiments to minimize these effects).

- These results provide evidence from 3D dynamical simulations that modern implementations of MLT (Paxton et al. 2018, 2019) which are more logically consistent (Gabriel et al. 2014) are more accurate.

- Our results demonstrate that while the Ledoux criterion is the proper *instantaneous* criterion for the boundary of convective regions, entrainment will erode stable composition gradients at convective boundaries. For stages in stellar evolution where $t_{\rm conv} \ll t_{\rm evolution}$, stellar evolution codes should use the Schwarzschild boundary; for stages where $t_{\rm conv} \lesssim t_{\rm evolution}$, future 3D numerical simulations should develop a more complete and parameterized theory of entrainment at convective boundaries, following the work of e.g., Turner (1968); Fuentes & Cumming (2020).

- Many Ledoux-stable but Schwarzschild-unstable regions in stars are unstable to ODDC (overstable doubly-diffusive convection), which has been theoretically described well in local models (Mirouh et al. 2012; Wood et al. 2013; Xie et al. 2017); these results are reviewed in Garaud (2018), applied to main sequence stellar cores in Moore & Garaud (2016), and should be included in stellar models.

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APPENDIX

A. MODEL & INITIAL CONDITIONS

In this work we study the simplest possible system: incompressible, Boussinesq convection with a composition field and a height-varying background radiative conductivity, similar to that used in Fuentes & Cumming (2020); Anders et al. (2021). These equations are

$$\boldsymbol{\nabla}\cdot\boldsymbol{u} = 0, \tag{A1}$$

$$\partial_t\boldsymbol{u}\cdot\boldsymbol{\nabla}\boldsymbol{u} = -\frac{1}{\rho_0}\boldsymbol{\nabla}p + \frac{\rho_1}{\rho_0}\boldsymbol{g} + \nu\boldsymbol{\nabla}^2\boldsymbol{u}, \tag{A2}$$

$$\partial_t T + \boldsymbol{u}\cdot\boldsymbol{\nabla}T + w\nabla_{\rm ad} + \boldsymbol{\nabla}\cdot[-\kappa_{T,0}\boldsymbol{\nabla}\overline{T}] = \kappa_T\boldsymbol{\nabla}^2 T', \tag{A3}$$

$$\partial_t C + \boldsymbol{u}\cdot\boldsymbol{\nabla}C = \kappa_{C,0}\boldsymbol{\nabla}^2\overline{C} + \kappa_C\boldsymbol{\nabla}^2 C', \tag{A4}$$

$$\frac{\rho_1}{\rho_0} = -|\alpha|T + |\beta|C. \tag{A5}$$

Here, $\boldsymbol{u}$ is the vector velocity, T is the temperature, C is the composition, ρ_0 is the constant background density, p is the kinematic pressure which enforces Eqn. A1, ρ_1 are density fluctuations which act only on the buoyant term, and α and β are the thermal and compositional expansion coefficients, and $\nabla_{\rm ad}$ is the adiabatic gradient. Diffusive terms are controlled by the kinematic viscosity ν, as well as the thermal diffusivity κ_T and compositional diffusivity κ_C. On the horizontally-invariant ($n_x = 0$ and $n_y = 0$) mode, we use a height-depended thermal diffusion coefficient $\kappa_{T,0}$ (which allows $\nabla_{\rm rad}$ to vary with height) and a lower compositional diffusivity $\kappa_{C,0} < \kappa_C$ to ensure that the evolution of the mean composition profile is due to advection rather than diffusion.

We nondimensionalize Eqns. A1-A5 according to

$$\begin{aligned} &T^* = (\Delta T)T, \qquad C^* = (\Delta C)C, \qquad \partial_{t^*} = \tau_{\rm ff}^{-1}\partial_t, \qquad \boldsymbol{\nabla}^* = L_s^{-1}\boldsymbol{\nabla}, \qquad p^* = \rho_0 u_{\rm ff}^2\varpi, \\ &\boldsymbol{u}^* = u_{\rm ff}\boldsymbol{u} = \frac{L_s}{\tau_{\rm ff}}\boldsymbol{u}, \qquad \tau_{\rm ff} = \left(\frac{L_s}{|\alpha|g\Delta T}\right)^{1/2}, \qquad \kappa_{T,0}^* = (L_s^2\tau_{\rm ff}^{-1})\kappa_{T,0}. \end{aligned} \tag{A6}$$

For convenience, here we define quantities with $*$ (e.g., T^*) as being the "dimensionful" quantities of Eqns. A1-A5. Henceforth, quantities without $*$ (e.g., T) are dimensionless. Here, L_s is the length scale of the initial Schwarzschild-unstable convection zone and $\tau_f f$ is the buoyant freefall timescale. The temperature and composition are set by the destabilizing radiative temperature gradient $\Delta T = L_s(\partial_z T + \boldsymbol{\nabla}_{\rm ad})$ and the stabilizing composition gradient ($\Delta C =$

$L_s \partial_z C$). Within this nondimensionalization, the dynamical control parameters are

$$\mathcal{P} = \frac{u_{\rm ff} L_s}{\kappa_T}, \qquad \mathrm{R}_0 = \frac{|\alpha|\Delta T}{|\beta|\Delta C}, \qquad \mathrm{Pr} = \frac{\nu}{\kappa_T}, \qquad \tau = \frac{\kappa_C}{\kappa_T}, \qquad \tau_0 = \frac{\kappa_{C,0}}{\kappa_T} \tag{A7}$$

The dimensionless equations of motion are

$$\boldsymbol{\nabla} \cdot \boldsymbol{u} = 0 \tag{A8}$$

$$\partial_t \boldsymbol{u} + \boldsymbol{u} \cdot \boldsymbol{\nabla} \boldsymbol{u} = -\boldsymbol{\nabla} \varpi + (T - \mathrm{R}_0^{-1} C)\hat{z} + \frac{\mathrm{Pr}}{\mathcal{P}} \boldsymbol{\nabla}^2 \boldsymbol{u} \tag{A9}$$

$$\partial_t T + \boldsymbol{u} \cdot \boldsymbol{\nabla} T + w \nabla_{\rm ad} + \boldsymbol{\nabla} \cdot [-\kappa_{T,0} \boldsymbol{\nabla} \overline{T}] = \frac{1}{\mathcal{P}} \boldsymbol{\nabla}^2 T'., \tag{A10}$$

$$\partial_t C + \boldsymbol{u} \cdot \boldsymbol{\nabla} C = -\frac{\tau_0}{\mathcal{P}} \boldsymbol{\nabla}^2 \overline{C} + \frac{\tau}{\mathcal{P}} \boldsymbol{\nabla}^2 C'. \tag{A11}$$

We define the thermal and compositional gradients

$$\nabla_{\rm T} \equiv -\frac{\partial T}{\partial z}, \qquad \nabla_{\rm C} \equiv -\mathrm{R}_0^{-1} \frac{\partial C}{\partial z}, \tag{A12}$$

and stability is determined by the sign of the Brunt-Väisälä frequency,

$$N^2 = N^2_{\rm structure} + N^2_{\rm composition}, \text{ with } N^2_{\rm structure} = -(\nabla_{\rm T} - \nabla_{\rm ad}),\ N^2_{\rm composition} = \nabla_{\rm C}, \tag{A13}$$

where $N^2 > 0$ is buoyantly stable, so the stability criterion is $\nabla_{\rm C} - (\nabla_{\rm T} - \nabla_{\rm ad}) > 0$, as in stellar models (Salaris & Cassisi 2017).

In this work, we study a three-layer model in $z = [0, 3]$. We want to construct a simulation with

$$N^2 = \begin{cases} -1 & z \leq 1 \\ R_0^{-1} - 1 & 1 < z \leq 2 \\ R_0^{-1} & 2 < z \end{cases}, \qquad N^2_{\rm composition} = \begin{cases} 0 & z \leq 1 \\ R_0^{-1} & 1 < z \leq 2 \\ 0 & 2 < z \end{cases}, \qquad N^2_{\rm structure} = \begin{cases} -1 & z \leq 1 \\ -1 & 1 < z \leq 2 \\ R_0^{-1} & 2 < z \end{cases} \tag{A14}$$

To achieve this, we set $\partial_z C = -\mathrm{R}_0 N^2_{\rm composition}$ and $\partial_z T = N^2_{\rm structure} - \nabla_{\rm ad}$, where we set $\nabla_{\rm ad} = 5[\mathrm{R}_0^{-1} - 2]$ as a constant so that $\nabla_{\rm ad} > 0$ for all values of R_0 studied. We furthermore enforce that $\nabla_{\rm T} = \nabla_{\rm rad}$ in the initial state, where

$$\nabla_{\rm rad} = -\frac{F_{\rm tot}}{\kappa_{T,0}}, \tag{A15}$$

is the radiative gradient and $F_{\rm tot}$ is the total vertical energy flux through the system. We set the total flux $F_{\rm tot} = -(1 + \nabla_{\rm ad})/\mathcal{P}$ and the convective flux $F_{\rm conv} = 1/\mathcal{P}$, so $\kappa_{T,0}(z) = -((1 + \nabla_{\rm ad})/\partial_z T)\mathcal{P}^{-1}$.

B. SIMULATION DETAILS & DATA AVAILABILITY

We time-evolve equations ?? using the Dedalus pseudospectral solver (Burns et al. 2020) using timestepper SBDF2 (Wang & Ruuth 2008) and safety factor 0.3. All fields are represented as spectral expansions of n_z Chebyshev coefficients in the vertical (z) direction and as (n_x, n_y) Fourier coefficients in the horizontal (x, y) directions; our domain is therefore horizontally periodic. We use a domain with an aspect ratio of two so that $x \in [0, L_x]$, $y \in [0, L_y]$, and $z \in [0, L_z]$ with $L_x = L_y = 2L_z$. The initial convection zone spans initially spans 1/3 of the domain depth and in the evolved state spans 2/3 of the domain depth, so it has an initial aspect ratio of 6 and a final aspect ratio of 3. To avoid aliasing errors, we use the 3/2-dealiasing rule in all directions. To start our simulations, we add random noise temperature perturbations with a magnitude of 10^{-6} to the initial temperature profile (discussed in ??).

Spectral methods with finite coefficient expansions cannot capture true discontinuities. In order to approximate discontinuous functions such as Eqns. A14, we must use smooth transitions. We therefore define a smooth Heaviside step function,

$$H(z; z_0, d_w) = \frac{1}{2}\left(1 + \mathrm{erf}\left[\frac{z - z_0}{d_w}\right]\right). \tag{B16}$$

where erf is the error function. In the limit that $d_w \to 0$, this function behaves identically to the classical Heaviside function centered at z_0. Throughout this work, we set $d_w = 0.05$.

A table describing all of the simulations presented in this work can be found in Appendix C. We produce figures ?? and ?? using matplotlib (Hunter 2007; Caswell et al. 2021). We produce figure ?? using TODO. All of the Python scripts used to run the simulations in this paper and to create the figures in this paper are publicly available in a git repository[1], and in a Zenodo repository (**?**).

C. TABLE OF SIMULATION PARAMETERS

Input parameters and summary statistics of the simulations presented in this work are shown in Table **??**.

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