1. Bounds on the transport of heat

Convection is ubiquitous in nature, occurring in the atmosphere, oceans, stars, and even in a coffee pot [1]. It has been studied both for its general application in such a variety of fields, and for the chaotic nature of the system itself (see [32], [22],[24],and [27] for some examples). The mathematically tractable problem of a fluid vertically constrained between two infinite (or periodic) plates was introduced by Lord Rayleigh in [32] and has since been explored in a variety of settings. For this simplified problem, it is of interest to consider an asymptotically strong driving force. In this asymptotic regime, turbulence is prevalent, and it is of interest to determine how different statistical properties of the flow depend on the strength of the driving force.

The goal of analysis, experiment, and numerical simulation has been to determine how relevant statistical properties of the flow depend on the driving force, and the physical setup of the system (see [2] for a comprehensive review of one such problem). The system can be specified by the boundary conditions on the temperature (fixed temperature, fixed flux, or mixed boundary conditions–see [44]), boundary conditions on the velocity (free-slip versus no-slip), the dimension of the box (2d or 3d), and in the case of periodic horizontal boundaries, the aspect ratio of the system. The fluid itself can be adequately described by the non-dimensional Prandtl number Pr which gives the ratio of the kinematic viscosity to the thermal diffusivity. A functional relationship between the transport of heat, a measure of the driving force, and these fundamental quantities is sought

The community has traditionally focused on Rayleigh Benard convection wherein the fluid is driven by an enforced temperature gradient that is specified by temperature boundary conditions on the top and bottom plates. The strength of this forcing is measured by the non-dimensional Rayleigh number Ra. The quantity of interest is the enhancement of heat transport due to convection, the non-dimensional Nusselt number Nu. It is generally agreed that at very large Ra, $\mathrm{Nu} \sim \mathrm{Ra}^{\gamma}$ however the precise values of γ are debated in the literature. Heuristic arguments based on well developed theories of turbulence yield contradictory results ranging from $\gamma = \frac{1}{3}$ to $\gamma = \frac{1}{2}$ with possible logarithmic corrective factors (see [23] and [20]).

1.1. **Rigorous Results.**

Rigorous bounds on the Nusselt number via a variational formulation were pioneered in [14] and later elaborated by [4]. Following the motivational work of Hopf in [13], Doering and Constantin [8] developed the so-called 'background method' for variational bounds on the transport of heat. This approach has been used for a fluid contained in a porous medium (see [29] and [9]), regular Rayleigh Benard convection as introduced in [8], and Rayleigh-Benard convection at infinite Prandtl number (see [7], [10], [11], and [38]). All of this work has focused on no-slip velocity boundaries which is realized experimentally, although the arguments implied in [23] and [20] do not specifically rely on this assumption. Following the numerics and asymptotic analysis in [28], [31], and [15], and in conjunction with Charles Doering (University of Michigan) I have developed a framework to also consider the case of free-slip boundaries in the context of the background method.

Following the ideas contained in [28], Professor Doering and I set up an enstrophy balance that occurs for free-slip boundary conditions in two dimensions. Recognizing that the vertical velocity can be bounded uniformly in terms of the enstrophy, allowed us to explicitly show that $\mathrm{Nu} \lesssim \mathrm{Ra}^{5/12}$ in this case, invalidating the argument that $\gamma = \frac{1}{2}$, unless it can be shown that such an argument relies on three-dimensional turbulence or no-slip boundary conditions (see [41] for details).

This fundamentally important result can be extended to three dimensions at infinite Prandtl number (where an enstrophy balance is implicit in the equations of motion), and also to the case of convection driven by an internal heat source, rather than an imposed temperature gradient (see [40]), so long as stress-free boundaries are present. The case of no-slip boundaries for internal heating at infinite Prandtl number (a case well-suited for simple model's of the earth's mantle) is also addressed in [39] where a framework for considering singular Hardy-Rellich type inequalities is discussed.

1.2. **Numerical Simulations.**

The rigorous results thus far obtained are only bounds on the solutions of the highly nonlinear Navier-Stokes equations. There is nothing said about whether these bounds are truly saturated, or if solutions exist that saturate said bounds, whether these solutions are stable enough to occur naturally. In order to truly explore the nature of convective turbulence accurately, highly resolved direct numerical simulations are essential (see [18] and others).

In this light, I have been working with Benson Muite (University of Michigan) and Hans Johnston (University of Massachusetts, Amherst) to design numerical algorithms that can perform extremely high resolution simulations of convective turbulence. These algorithms are being tested against published codes to ensure the accuracy of the final result. With the assistance of Peter van Keken (University of Michigan, Department of Geology) and Cian Wilson

(Columbia University) a set of benchmarks has been developed for infinite Prandtl number convection that verify the need for extreme resolutions.

The code developed at the University of Michigan by Professor Muite relies on a pseudo-spectral approach using a Chebyshev discretization in the vertical direction, while Professor Johnston has implemented a compact finite difference approach. The correspondence of results between these two different algorithms verifies the overall accuracy of each code. Both sets of code have been developed with the ability to interchange boundary conditions and forcing terms easily, making it possible to simulate highly turbulent states under many different circumstances. This will allow for a comprehensive set of numerical experiments that can be used to gather valuable information on the statistical properties of convective turbulence.

My role in this group has been primarily as a facilitator, communicating to the numerical analysts what quantities in the turbulent flow are physically significant, and coordinating the same with the geophysical community. I have also been involved in testing the code at different stages, ensuring that each different type of discretization provides the same results by testing against well established manufactured codes. Along with Professor Muite I have had the privilege of mentoring Brandon Cloutier (University of Michigan), an undergradute student, as he has begun performing simulations of internal heating driven convection at infinite Prandtl number.

1.3. **Future Work.** The Hardy-Rellich type inequalities considered in [39] can be further utilized to extend the work of [44] and [11] to the case of convection driven by an imposed temperature gradient, but with mixed thermal boundary conditions at infinite Pr. For fixed flux, I can show that $\gamma = 1/3$, but with a different logarithmic correction than that found in [11]. With the help of Ralf Wittenberg (Simon Frasier University) I am extending this result to mixed thermal boundary conditions akin to those used in [44].

The variety of exponents γ that are indicated from rigorous bounds indicate that the asymptotically strong transport of heat due to convective turbulence depends strongly on the boundary conditions. With all these results, the case of stress-free, fixed-flux boundary conditions has not been addressed. To date there are no rigorous bounds for this particular set of boundary conditions, including $\gamma = 1/2$. The best result that can be shown rigorously is that $\gamma \leq 1$ which is significantly different than any proposed scaling law. Using the background method to produce an improvement on this particular case is a priority that I intend to pursue with the assistance of Ralf Wittenberg, relying first on numeric computations akin to those performed in [31] as a guide.

In addition to the physically relevant problems discussed here, it is valuable to consider applications of these methods to similar problems where the background method may be utilized to a greater extent. These include, but are not limited to: surface tension driven (Benard-Marangoni) convection (see [12]), convection with temperature dependent viscosity (as a more realistic application to mantle convection), and internal heating in the presence of variable heat generation.

The nature of these systems allows for bounds on the heat transport either from above or below, but not both. This is because the conductive solution always exists (albeit unstably) and provides a lower (upper) limit to the heat transport. Numerical simulations and experiments are then thought to provide the stable solutions that will optimize the heat transport in some sense, and theoretically should saturate the rigorous bounds. Another way to approach this, is to consider near-analytic solutions that are expressed asymptotically. In [6] just such a solution is constructed for stress-free boundaries at finite Prandtl numbers. The resultant estimate of the Nusselt number indicates that $Nu \sim Ra^{1/3}$. While this result is not a rigorous solution of the equations, it does give a pseudo-lower bound on the 'ultimate' state of convection with stress-free boundaries.

I propose to follow the framework outlined in [6] to consider varying boundary conditions, in particular no-slip velocities on the top and bottom plates. While significant differences are not expected, a thorough investigation of this problem may yield some insight into the apparent differences that the velocity boundary conditions have on the rigorous bounds as explained above.

I have been involved in testing the aforementioned numerical algorithms that are meant to provide direct numerical simulations of highly turbulent convection. Currently we are accumulating enough data from different sources to provide a set of benchmark problems and data so other models can be compared with these well-resolved and agreed upon results. Once this initial step is completed, the availability of computational resources via the Teragrid will allow myself and the other investigators to consider the asymptotic scaling of statistical quantities for traditional Rayleigh-Benard convection under a variety of boundary conditions, as well as the adaptation of the code to internal heating driven convection, Benard-Marangoni convection, and possibly variable viscosity convection as well. This will provide a believable set of highly resolved simulations that are of interest to the community.

In the past two years, I have been made aware of the numerical discovery of a rather unique mode of convection. In two dimensional Rayleigh-Benard convection with moderately large Rayleigh numbers (typically $Ra \sim 10^8$) with periodic boundary conditions, several different numerical codes (personal communication with Hans Johnston, Glenn Flierl, David Goluskin and Charles Doering) have indicated the presence of a semi-stable horizontal shear mode of convection in which the temperature is nearly conductive, and the horizontal velocity dominates the vertical. I will consider linear stability of this state to determine the precise stability of the shear mode, as well as the effect it has on the transport of heat. I will also explore the possibility of asymptotically constructing such a solution.

2. VERIFICATION OF CLIMATE MODELS

Weather and climate prediction is at the fundamental level, a matter of fluid dynamics. The driving force behind climate and/or weather is the circulation of the gases that make up the air we breathe. The spatial scales involved, particularly in climate models, vary from meter length waves that are influenced by anthropogenic influences to large scale circulations on the order of thousands of kilometers. Temporally the climate is also influenced by time scales ranging from seconds to thousands of years. This presents a major problem for the climate modeling community that requires a sound verification of each model's results. Finite limitations on computational resources make it impossible to resolve all scales, either temporal or spatial, forcing the interested scientist to consider heuristic (and often ad-hoc) engineering practices that are meant to imitate the unresolved processes. The question is whether these imitations of the sub-grid scale processes are physically relevant, and lead to a realistic simulation.

Some of these sub-grid scale processes are modeled through physical parameterizations where simplifying assumptions allow for quick calculations to simulate the net effect of such small scales. Apart from the so-called 'physics' component of the model, is the discretization of the equations that are thought to represent the motion of the dry atmosphere. This 'dynamical core' is the component of the model that relies on fundamental numerical and physical considerations derived directly from the principles of fluid mechanics. Each dynamical core of necessity has sub-grid scales that are not resolved, and are not taken care of by the physics routines, and so dissipative processes must be added to the model (see [17] for a comprehensive description of these processes). The addition of dissipation is model dependent, and the effects may vary, but the careful quantification of said effects is necessary to understand the impact of these processes on climate prediction.

I have been working with James Kent (University of Michigan, Atmospheric Oceanic and Space Sciences) under the direction of Christiane Jablonowski (University of Michigan, AOSS) and Richard B. Rood (University of Michigan, AOSS) in an effort to quantify the effects of these unresolved processes at the subgrid level. Using a combination of test case problems for dynamical cores (see [16] for the description of some test cases), techniques gained from numerical analysis, and effective collaboration with model designers, we have begun to quantify the effect of these forms of added dissipation and their potential feedbacks on the prediction of climate and weather.

2.1. Explicitly added diffusion.

One of the most straightforward forms of dissipation is adding an explicit diffusive term to the equations of motion. This approach is traditionally well accepted as a representation of the eddy viscosity for the unresolved scales (see [30] and [17]). In practice, the coefficients of viscosity are empirically tuned to maintain a desired slope in the kinetic energy spectrum (see [34] for one example). This somewhat ad-hoc representation of the eddy viscosity is also applied in the form of a hyper-diffusion operator of fourth, sixth or even eighth order with the corresponding coefficients chosen to emulate the desired slope of the kinetic energy spectrum. Most of these considerations are without regard to the method of discretization applied to the model, and neglect to take into account the impact that such a diffusive process may have via an explicit time-stepping scheme.

In [43] we considered the impact of a specific type of explicit dissipation called divergence damping, and the effective numerical stability constraints imposed on the viscous damping coefficient via the explicit time-stepping utilized in the finite volume dynamical core of NCAR's CESM1.0 model. These results include a careful analysis of the impact of a polar Fourier type filter (necessary for the latitude-longitude grid used by CAM-FV) on the stability of the scheme.

2.2. Test case development and tracer transport.

The integration of climate models requires the accurate advection of several (sometimes on the order of one hundred [21]) chemical constituents that have dramatic impacts on the predictive value of a forecast. As such, the ability of a dynamical core to accurately transport passive tracers is vital. In [19] several different tracer transport algorithms are tested via some complicated test cases, to determine the relative accuracy of each algorithm. These tests are used to highlight a deficiency in the number of vertical model levels used in the current model utilized in CESM1.0.

Potential vorticity in the absence of frictional forces and moisture, is preserved, and hence qualifies as an interesting instrument to gauge the consistency between a model's tracer advection algorithm, and it's integration of the dynamical variables. [42] identifies just such a test problem, providing various quantitative means for measuring the differences between dynamics and tracer advection.

2.3. **Future Work.** Extension of the work initiated in [19] will be pursued to further 2 and 3 dimensional advection test cases of increasing complexity, to test the ability of numerical algorithms to not only maintain accuracy in the presence of simple flows, but to maintain conservation of key properties. For example a simple test case with two non-interacting rotational cells simulates a barrier that a passive constituent should not pass through. Initial testing indicates that some overly diffusive advective algorithms allow significant amounts of the tracer to leak from one cell to the other, creating a non-physical transfer across the barrier. In addition to this, the conservation of tracer variance in the presence of highly deformational, nonlinear flows and extensions of [25] to three dimensions are being explored.

Working with Paul Ullrich (University of Michigan, AOSS) and Mark A. Taylor (Sandia National Laboratories), I have performed a stability analysis of the explicitly added diffusive operator for the CAM Spectral Element (CAM-SE) model (see [35], [37] and [36] as well as [26]). Testing of the validity of this analysis as well as the stability of the advective operator currently implemented in CAM-SE is being performed at this time. It is expected that time-step adjustments to ensure diffusive instabilities do not appear, will be implemented in the developed CAM-SE code in the future.

An aspect of dynamical cores that is near-universal across all modeling platforms is the implementation of a 'sponge layer' at the model top. In reality, it is difficult to place a top on the earth's atmosphere as it becomes exponentially thinner, and truthfully satisfies some type of free-surface boundary condition. In application however, it is necessary to place an artificial top to an atmospheric model. To avoid the possible reflection of waves from this artifact, an increase in the dissipative characteristics of the model is carried out near the top of the model. For instance, CAM-SE and CAM-EUL (the eulerian or pseudo-spectral) models all employ a fourth order hyper-diffusion on the horizontal components of momentum throughout the model, except in the upper most layers where a second order diffusion operator is employed. Such an abrupt change in the order of the equations may lead to negative effects. I intend to explore these possible effects in great detail, in particular how these might alter the results of [5] for the existence and uniqueness of solutions to the hydrostatic equations.

The impact of the dissipative forces used in the dynamical core of a model are not well understood with regard to the interplay with the physics parameterizations that are used in full model runs meant for climate prediction. Using the simple physics parameterization developed in [33] we can test the impact of dissipative mechanisms on the consequent physical characteristics of the model. In addition, differences in how the dissipation is applied to the dynamical variables, and passive tracers through the advection algorithm, will be considered. CAM-SE is particularly well-suited for this exploration, as the tracers and dynamic variables can be treated separately, and there are extensive possibilities for the interplay between the physics-dynamics coupling.

In relation to the study performed in [42], it was found that for nonlinear flow, it is highly unlikely that a dynamical core can maintain consistency between dynamics and tracers. This is not entirely unexpected as the nonlinear term in the momentum equation, when discretized implies that potential vorticity is no longer conserved, i.e. the discretized advection equation for potential vorticity is no longer equivalent to the momentum and conservation of energy equations. While this has been alluded to for two dimensional turbulence (see [3]) this effect of discretization has not been quantified for 3d. I will pursue further exploration of this phenomena, and a quantifiable measure of the 'consistency' of a model in the presence of strongly nonlinear flow, questioning whether this is a feasible trait for global circulation models to have.

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