EFFICIENT ATMOSPHERIC MODEL EQUILIBRIUM SEARCHING AND ASSESSMENT

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1. INTRODUCTION

Climate models are increasingly important to the hunt for life outside our solar system. Upcoming space telescopes (e.g., James Webb Space Telescope) will require weeks or months of integration time in order to probe an exoplanetary atmosphere (Cowan et al. 2015). Any target selected must be thoroughly vetted to ensure the best chance for recovering spectral features of a potentially habitable world.

One-dimensional radiative-convective models provide an efficient method for exploring and understanding the potential climate states of an exoplanet. Such one-dimensional models typically search for an equilibrium atmospheric state given a set of boundary conditions (e.g., the host stellar flux incident on the world) and assumptions about the atmospheric composition (e.g., a composition that is fixed or defined by thermochemical equilibrium). Commonly, an equilibrium climate solution is one that adjoins a convective adiabat in the deep atmosphere to a radiative zone in the upper atmosphere. The task of the one-dimensional climate model is, then, to seek out the radiative-convective boundary that yields an equilibrium climate solution.

Many of the most widely-adopted one-dimensional radiative-convective climate models (McKay et al. 1989; Kasting et al. 1993; Marley et al. 1996) are written in programming language standards that are now out-of-date. Thus, modern packages designed to enable parallelization of computational models cannot be straightforwardly applied to these legacy tools. Here, we explore techniques for increasing the computational efficiency of one-dimensional radiative-convective models. Critically, these techniques do not require implementation of sophisticated parallel-computing algorithms, and are designed to be adopted into legacy models.

2. MODEL DESCRIPTION

For our investigations, we adopt the Marley-Saumon-Fortney one-dimensional brown dwarf and exoplanet climate model (Marley et al. 1996; Fortney et al. 2008). This tool produces a temperature-pressure profile for an atmosphere in radiative-convective equilibrium, and also provides visible and infrared spectra at coarse resolution. The model incorporates numerous parameters potentially affecting climate and habitability, such as host stellar effective temperature and size, planet orbital distance, fraction of cloud coverage, and the condensable species (e.g., water) contained in those clouds.

Myriad input parameters provide flexibility when producing model atmospheres, but one challenging effect is that, in some circumstances, a range of potential near-equilibrium solutions are possible. Ensuring the resulting models are nearest to equilibrium, and thus physically realistic, is critical in evaluating the success of any atmospheric model. Moreover, each model run and corresponding evaluation requires significant computation.

A simple case to model is a free-floating (i.e., not orbiting a star) cloud-free brown dwarf. Typical compute time, given an uninformed guess for the initial atmospheric thermal structure, is 10 minutes. If we vary any one boundary condition (e.g., internal heat flux) N times, then we require N times as much compute time. If, for example, we use 6 different initial internal heat fluxes for a brown dwarf thermal structure grid, then we require one compute hour to execute.

More complicated models (e.g., a Jupiter-type planet with partial surface coverage by clouds formed from several condensing species) can take roughly an hour for a single model run (again, given an uninformed initial guess for the atmospheric state).

To provide a sense for what takes place during a model run, let us consider the initial steps. Our model begins with an initial user-provided "guess" as to where a radiative-convective boundary exists. This boundary describes the place in an atmosphere (usually in the upper troposphere) where the atmosphere thins enough to become less opaque to infrared energy, and radiation becomes the dominant method of heat transfer (Catling & Kasting 2017). If the initial guess does not lead to a solution, the model tries again using a nearby level.

Once a solution is found that is valid, the model is said to have converged. Success is mediated by a predefined error tolerance that comes into play during convergence checking. Unsurprisingly, the degree of error tolerance has a direct impact on compute time: a more forgiving error tolerance ensures arriving at a converged model in less time.

3. APPROACH

We explored several novel approaches to both searching for equilibrium solutions within a one-dimensional radiative-convective modeling framework and for testing the quality of these solutions. Instead of searching for the radiative-convective boundary level by level, we initially explored a parallelized approach that tested every potential radiative-convective boundary simultaneously. In other words, for a model with $N_{\rm lvl}$ levels, we launched $N_{\rm lvl}$ separate model runs with the initial radiative-convective boundary guess moved sequentially up through the atmosphere. This, and subsequent, tests were performed on the Northern Arizona University "Monsoon" computing cluster.

Our new multi-level simultaneous exploration approach makes use of the Message Passing Interface standard which enables communication between "ranks" (tasks) executing in parallel. Rather than each rank acting entirely independently, we designed them to check in with a master process which would assign work and receive model results. Thus, for example, a rank that rapidly finds an acceptably-converged solution can then indicate that other ranks need not continue their search, thereby reducing model runtime.

We describe two newly formulated metrics for quantifying model output quality. These metrics are based on model "physicality", where the best-converged solutions will obey energy conservation and will have lapse rates that do not exceed the adiabatic lapse rate. We record all input parameters and their resulting outputs (be they converged solutions or failed runs) in order to identify patterns. These data help to locate new and unexpected trends, and can also be used to inform machine-learning algorithms aimed at more intelligently selecting initial guesses.

Finally, we demonstrate our new approach through applications to both Super-Earth and Mini-Neptune exoplanets (i.e., planets between the size of Earth and Neptune which orbit stars outside our solar system). Such worlds are the most commonly found class of exoplanet to date, and represent exciting categories of exoplanets not found in our Solar System.

4. CONCLUSIONS

Climate models are critical to our search for life outside our solar system, but many well established models rely on out-of-date programming standards and techniques. Adopting streamlined approaches to modernizing legacy code will, in turn, enable new insight into climate model performance and results. Here, metrics for quantifying model quality will prove essential. Application of these ideas, for example, enables efficient and accurate explorations of Super-Earth and Mini-Neptune climate states.

5. ACKNOWLEDGEMENTS

This work was supported by a grant through NASA's Exoplanets Research Program. Computational analyses were run on Northern Arizona University's Monsoon computing cluster, funded by Arizona's Technology and Research Initiative Fund.

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