

## Background and Motivation

The need for ground to exosphere General Circulation Models (GCMs) were specified for the first time by [redacted] in 2000 [4]. These models, commonly known as the whole atmosphere models, are needed for a more accurate study of the relevant physical and chemical interactions, climate change, climate response to solar variability, space weather, and the interpretation of global observations [2, 4]. Two decades following the work of [redacted] whole atmosphere modeling has developed into an active and fast growing area of research. Currently, there is a strong push for representation of the lower atmosphere in space weather models of the upper atmosphere [1, 5]. For accurate simulation of the region between the Sun and the Earth, the impacts from the lower atmosphere need to be taken into account in addition to the atmospheric impacts from the solar output and magnetosphere [1-3]. This is extremely influential in the future development of the whole atmosphere models which will be focusing increasingly more on geospace applications. This focus stems from our society becoming more and more dependent on advanced technology which can be vulnerable to space weather.

Geospace applications require atmospheric models with tops in excess of 500 km, well into the upper thermosphere. In these regions the accuracy of the hydrostatic and shallow atmosphere approximation becomes problematic. However, whole atmosphere models are usually built from existing (GCMs), which are generally based on the shallow-atmosphere and hydrostatic approximation [1, 5-7]. Some examples of currently available whole atmosphere models based on these assumptions include: the Whole Atmosphere Model (WAM) [8, 9], the Whole Atmosphere Community Climate Model with thermosphere and ionosphere extension (WACCM-X) [2, 3], and the Ground to topside model of the Atmosphere and Ionosphere for Aeronomy (GAIA) [10, 11].

The hydrostatic approximation means that a number of terms will not be taken into account as a result of assuming a balance between the gravity and gradient in pressure. These terms include: Coriolis, centrifugal acceleration, and ion drag [12]. The hydrostatic assumption becomes problematic for very fast processes (comparable or shorter than the atmosphere buoyancy period) and processes with large vertical scales (comparable or larger than scale height) [13].

The shallow-atmosphere approximation allows us to neglect the terms related to the spherical curvature of the atmosphere and the variations of the gravitational field [14]. In addition, the contribution of the horizontal component of the Earth's angular velocity to the Coriolis acceleration is neglected [13]. These neglected terms impact the accuracy of the models. For example, the results of a scale study by [redacted] and [redacted] in 1995 showed that for diabatically driven flows in the tropics and planetary-scale flows the neglected terms of the Coriolis acceleration might be in the order of 10% [15]. This is not a small error considering the need, for example, for the precise prediction of satellite orbits.

Moreover, the systematic errors introduced by approximations may accumulate over time and lead to significant accuracy problems. This is especially important for the large-scale circulations of the middle and upper atmosphere [13]. Hence, there is an increasing need for whole atmospheric models with nonhydrostatic and deep-atmosphere dynamical core.

## Proposed Research and Scientific Questions

WACCM-X, developed by the High Altitude Observatory (HAO) at NCAR, extends from the Earth surface to the exobase (~600 km). However, the dynamical framework of this model is based on the hydrostatic and shallow atmosphere assumption [2, 3]. As previously explained, these assumptions need to be relaxed. Recently, NCAR's Model for Prediction Across Scales-Atmosphere (MPAS-A) [16], which solves the nonhydrostatic equations, has been extended to enable the integration of deep-atmosphere equations [17].

**I propose to further extend MPAS-A's deep atmosphere, nonhydrostatic numerical capabilities to be used as the dynamical core by WACCM-X.** This would allow me to address the following scientific questions during my ASP fellowship:

**(1) How do gravity waves propagate in the thermosphere?** Gravity waves are a major driver of the middle and upper atmosphere circulation and variability. In addition, they play an important role in the transport of chemical

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constituents. By performing high resolution and nonhydrostatic whole atmosphere simulations, the gravity wave distribution, seasonal variation, and their effect in the thermosphere can be studied. Selection of a non-hydrostatic dynamical core affects the modeled gravity wave spectrum. This will create the means to explore their implications on medium and small-scale traveling atmospheric/ionospheric disturbances.

**(2) What are the nonhydrostatic effects missing in the current models?** Comparison of nonhydrostatic and hydrostatic dynamical cores will allow the assessment of the impact of nonhydrostatic cores on various spatial and temporal scales. Previous studies have shown that nonhydrostatic models can resolve sound and gravity waves more accurately [5-7]. Hence, relaxing the hydrostatic approximation entirely would be beneficial for whole atmosphere modeling by admitting potentially important acoustic waves and successfully reproducing high-frequency gravity wave dissipation.

### Methods

The dynamical core of MPAS-A has already been extended to address deep atmosphere geometry and full Coriolis and curvature terms as presented in reference [17]. These are the necessary steps in the evolution of this nonhydrostatic solver to applications requiring higher model tops. However, a number of other modifications to the MPAS-A dynamical equations are required to render the model potentially suitable for geospace applications. MPAS-A requires the addition of molecular viscosity and diffusion in order to stabilize artificial wave growth. This is due to the significant effect of viscosity in the thermosphere. In addition, above the turbopause (~105 km), the molecular weight of species determines its dynamical evolution. Hence, each species should have its own set of dynamical equations to be solved. Molecular diffusion is also affected by the variable gravity, which in turn modifies the atmospheric scale heights. Thus, the dynamical core has to be reformulated to properly model the individual species, and a correction has to be added to the thermal equation.

**My first task is to implement the generalization of the equations of state and thermodynamics in MPAS-A to take into consideration the variable species in the thermosphere. The second task would be the addition of molecular viscosity and diffusion in MPAS-A.** An initial study of this has been presented in the 2019 Mesoscale and Microscale Meteorology (MMM) annual report [18], where a 2-D MPAS prototype model has been created, which incorporates these extensions. I plan to implement these changes in the full MPAS-A model, which will allow me to address the scientific questions posed in the previous section as follows:

**Question (1):** I will examine the propagation and impact of gravity waves from realistic tropospheric sources up into the thermosphere by studying molecular viscosity effects on the waves, the penetration height of waves, their global distribution and seasonal variation, and their impact on thermosphere circulation.

**Question (2):** I will study the differences between WACCM-X with the current hydrostatic dynamical core and WACCM-X with MPAS-A. Such comparative analysis of the differences will reveal the nonhydrostatic effects that have been missing in the current models.

### Relevance to NCAR's Research and Strategic Plan

My proposed research is well aligned with NCAR's Strategic Plan which embraces a whole geospace model [19]. It also fits well with the primary goal of the System for Integrated Modeling of the Atmosphere (SIMA) project of conducting frontier science simulations in climate, weather and geospace research using a unified modeling system [20]. More specifically, the proposed research enhances and complements current efforts in the HAO, MMM, and the Climate and Global Dynamics (CGD) laboratories. Working at the disciplinary intersection of these vibrant communities will provide me, as an early career scientist, invaluable collaborative opportunities. I will benefit greatly from working with [REDACTED] (HAO) on the WACCM-X developments. Similarly, I hope to collaborate with [REDACTED] (MMM) and [REDACTED] (MMM) on the MPAS-A adaptation. The CGD staff will also be important collaborators in this project.

This fellowship will allow me to be part of a collaborative cohort, mentored by leading NCAR scientists, and benefit from the breadth of science and training happening at NCAR. I believe the ASP fellowship will help me

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become the independent and influential scientist that I aspire to be.

### Relevance of Previous Research Experience

Modeling the atmosphere and its interactions with other components of the Earth and geospace systems requires multi-physics and multiscale simulation. Using coupled simulations instead of one standalone platform allows for the best way to deal with the difference in time scale and mesh requirements, the use of the best numerical method for each model, and the advantage to build upon legacy codes. Working on a multi-disciplinary PhD thesis, entitled "Development and Validation of an Aero-thermo-Elastic Analysis and Design Platform" [21, 22], has provided me with this experience. In this work I successfully coupled a 3D finite-volume Navier-Stokes solver (NSU3D) [23-26] with a 3D finite-element thermoelastic solver (AStrO) [21, 22, 27-30]. I had to obtain a strong understanding of the physics and numerical analysis, to successfully couple these solvers for tackling engineering design problems. This experience has given me the ability to work across models, scales and disciplines to solve problems with very similar characteristics to those found in whole atmosphere earth system modeling. Moreover, my multidisciplinary background in Electrical Engineering, Space System Engineering, and Computational Fluid Dynamics, provides me with a unique set of skills which positions me well for this proposed research and with NCAR's interdisciplinary research mission.

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