Adapting the MPAS Dynamical Core for Applications Extending Into the Thermosphere

J. B. Klemp and W. C. Skamarock

1National Center for Atmospheric Research, Boulder, CO, USA

Abstract
To extend the nonhydrostatic global Model for Prediction Across Scales (MPAS) for deep-atmosphere (geospace) applications, we have modified the model equations and numerics to include variable atmospheric composition and (potentially large) molecular viscosity and thermal conductivity. The split-explicit numerical integration techniques in MPAS remain stable in idealized test cases for atmospheric domains extending into the upper thermosphere and continue to provide an efficient numerical framework for nonhydrostatic simulations. Variations in the atmospheric constituents influence the dynamical equations by altering the heat capacity and ideal gas constants. These feedbacks require little alteration of the dynamical equations although our testing reveals that the amplitude of disturbances may be sensitive to even small variations in the thermodynamic coefficients. Although the potential temperature is no longer formally conserved for adiabatic flow, it remains effective as a prognostic thermodynamic variable in the model equations. Molecular viscosity and thermal conductivity are dominant influences in the upper thermosphere and are represented implicitly in the model numerics. Because of the large magnitude of these terms, their treatment, though stable, may significantly underrepresent the true magnitude of their damping effects. Further consideration of these deep-atmosphere extensions to MPAS will be explored in more realistic simulations of thermospheric dynamics.

Plain Language Summary
Typically weather and climate models focus on simulating the atmosphere throughout the troposphere and stratosphere. However, atmospheric disturbances in these regions can also impact important physical processes at much higher altitudes, even extending into the upper thermosphere (~500 km). The Model for Prediction Across Scales (MPAS) was designed to simulate a broad range of atmospheric phenomena, from cloud scale up to global scale. Here, we modify the model and test its viability for deep-atmosphere applications that include the thermosphere. This raises new challenges for the model numerics due to the extreme variation in the atmospheric parameters, such as density, for example, that decreases by ~12 orders of magnitude between the surface and the upper thermosphere. The variability of the constituents of the atmosphere must now be included in the model as well as influences such as molecular viscosity and thermal conductivity, which are negligible in the lower atmosphere. In simulating idealized test cases in a simplified version of MPAS, we demonstrate that numerical integration of the model equations continues to provide a stable and efficient framework for applications in the thermospheric environment that include small scale atmospheric processes.

1. Introduction

It is well known that important physical processes in the thermosphere (approximately 90 – 500 km) can be significantly influenced by weather-produced disturbances in the lower atmosphere, particularly through the vertical propagation and dissipation of internal gravity waves (Miyoshi et al., 2014). Consequently, in modeling the behavior of the whole earth atmosphere, there is increasing need for whole atmosphere models that directly couple shallow and deep atmospheric processes (R. Roble, 2000; Liu et al., 2010; Akmaev, 2011). In seeking to more accurately represent the influences of tropospheric forcing on upper atmospheric circulations, it is also beneficial to accommodate nonhydrostatic influences that are potentially significant at smaller scales (Akmaev, 2011; Deng & Ridley, 2014; Ridley et al., 2006). The Model for Prediction Across Scales (MPAS) is a global nonhydrostatic model that has proven to be robust and efficient in simulations for a wide range of weather applications (Skamarock et al., 2012, 2014, 2018; Schwartz, 2019). In this study, we investigate the viability of extending the MPAS equations and numerics to effectively simulate the dynamics of the atmosphere from the surface to the upper regions of the thermosphere (~500 km).
In recent modifications to the MPAS dynamical core, Skamarock et al. (2020) have removed the shallow-atmosphere approximation and adapted the model numerics for the traditional deep-atmosphere equations (White et al., 2005) in which the depth of the atmosphere is not negligible in comparison to the radius of the earth. For this purpose, the MPAS equations and numerics were modified to use the actual geocentric distance \( r \) instead of the Earth radius \( r_e \) in the governing equations and the grid mesh configuration, to allow gravity to vary with height, and to include the full Coriolis force terms containing vertical velocity components in the momentum equations. With these augmentations to the dynamical core, the MPAS solver remains valid for applications extending into the lower thermosphere (~100–200 km).

Further extension of MPAS for use throughout the thermosphere raises additional challenges. The model numerics must accommodate extreme variations in the atmospheric parameters as the model domain may span 25–30 scale heights, with the density decreasing by ~12 orders of magnitude, and thermospheric temperatures that often reach 1,000–2,000 K. The numerical approach for integrating the prognostic equations in the current MPAS utilizes a split-explicit technique for integrating the prognostic equations in which the terms responsible for the propagation of acoustic and gravity-wave modes are advanced on smaller time steps (limited by the horizontal speed of sound), while the remaining terms and parameterized physics are stepped forward with a larger time increment appropriate for the physical modes of interest (Klemp et al., 2007; Skamarock et al., 2012). Thus, a basic question arises as to whether the split-explicit numerics used in the model integration remain viable when applied throughout the upper atmosphere.

In addition to issues related to the basic model numerics, a number of additional modifications to the MPAS dynamical equations and numerics are required to render the model potentially suitable for geospace applications. In the thermosphere, the composition of the atmosphere can no longer be considered independent of altitude; atmospheric constituents vary with scale heights inversely proportional to their molecular weight, and atomic ions become increasingly dominant. Changes in the atmospheric composition alter the thermodynamic properties such as heat capacity and the ideal gas constant, which also require modification of the thermodynamic equation. Although the kinematic viscosity and thermal diffusivity are negligible in the troposphere and stratosphere, these effects become dominant in the upper thermosphere.

To evaluate the viability of the MPAS model numerics with the inclusion of these deep-atmosphere modifications, herein we conduct our initial assessment in a 2-D vertical slab configuration on a flat earth before implementing these extensions in the full 3-D global MPAS code. Our emphasis is on assessing how this increased complexity can be accommodated while maintaining the accuracy and stability of the overall MPAS numerical framework. For this reason, we do not consider variations in the grid configuration with altitude, which have already been implemented in the full 3-D MPAS code (Skamarock et al., 2020). Confining our focus to the numerics for the basic dynamical system, we also defer any treatment of the added complexity of upper atmosphere chemistry and physics such as solar and Joule heating, ion drag, photoionization/photodissociation of molecules, etc.

We begin in Section 2 with a description of modifications of the dynamical equations to include variable atmospheric composition, molecular viscosity and thermal conductivity, and to improve the treatment of pressure gradients in deep-atmosphere applications. In Section 3, we explain how our split-explicit numerical integration technique is adapted to work effectively in deep-atmosphere environments, and we describe our initial method for including implicit treatment of the molecular viscosity and thermal conductivity terms. Testing of the model numerics is presented in Section 4 for idealized simulations in a 2-D slab configuration for an elevated oscillating heat source and for mountain wave simulations at several different horizontal scales. Summary remarks are included in Section 5.

2. Modification of the Dynamical Equations for Deep-Atmosphere Applications

2.1. Representation of Pressure Gradients

In formulating the numerics for the dynamical equations for deep atmosphere applications, we recognize that with a terrain-following vertical coordinate \( \zeta = \zeta(y, z) \) based on geometric height the representation of vertical pressure gradients can be problematic since the pressure decreases exponentially with height and the depth of the model domain is many times greater than the density scale height. In addition to increased
numerical error, negative pressures can also arise if, for example, the hydrostatic equation is integrated vertically from the surface to balance the initial thermodynamic fields. For these reasons, we have altered the representation of pressure gradients in the dynamical equations, writing them in terms of \( \phi = \ln(p/p_0) \), which tends to vary more linearly with height and avoids the possibility of producing negative pressures. With this modification the vertical pressure gradient and buoyancy terms in the vertical momentum equation are represented simply as

\[
\frac{1}{\rho_m} \frac{\partial \phi}{\partial z} + g = \frac{1}{\rho_d} \left( \frac{\partial \phi}{\partial z} + g \rho_d \right) = \frac{p}{\rho_d} \frac{\partial \phi}{\partial z} + \frac{g}{\rho_d} R_d T_m
\]

(1)

where \( \rho_d \) is the density of dry air and \( \rho_m = \rho_d (1 + q_v + q_c + q_r + \cdots) \) is the full density, including moisture. Here, \( q_v = (q_v, q_c, q_r, \cdots) \) represents the mixing ratios of water vapor \( q_v \), cloud water \( q_c \), rain water \( q_r \), and any other moist species. The buoyancy term on the rhs of 1 has also been expressed in terms of temperature (following the second equal sign) using the ideal gas law \( p = R_d \rho_d T_m \), where \( T_m \) is the moist temperature \( T_m = [1 + (M_d / M_r) q_v] / T_r \), \( R_d \) is the gas constant for dry air, and \( M_d \) and \( M_r \) are the molecular weights of the dry air and water vapor \( q_v \), respectively. In this form, the initial fields in the model atmosphere can be readily balanced hydrostatically based on \( T_m \) through the vertical integration of the rhs of 1 set equal to zero, without jeopardy of producing negative pressures at high altitudes.

The horizontal pressure gradients are also cast in terms of \( \phi \) to improve the numerical accuracy, and are written in the form:

\[
\frac{1}{\rho_m} \nabla \cdot p = \frac{p}{\rho_m} \nabla \cdot \phi - \frac{p}{\rho_m} \frac{\partial \phi}{\partial z} \phi_H = \frac{p}{\rho_m} \nabla \cdot \phi + g \phi_H
\]

(2)

where \( \phi_H = \nabla \cdot \nabla z \) is a metric of the terrain-following vertical coordinate. The second term in the approximation to the horizontal pressure gradient in 2 has an alternative form to that in Klemp (2011) and Skamarock et al. (2012) that appears to improve the numerical accuracy, as discussed further in Appendix A.

### 2.2. Variable Atmospheric Composition

For shallow atmosphere models, dry air is composed primarily of nitrogen and oxygen and its composition is treated as constant in time and space. However, at altitudes above 100 km, diatomic nitrogen and oxygen begin decreasing rapidly with height, and free oxygen and other nominally trace molecules and ions become more dominant. The variations in atmospheric composition feed back into the dynamical equations by causing variations in the ideal gas constant \( R_d \) and heat capacity \( c_p \) for dry air, which are defined by:

\[
R_d = \frac{R^*}{M_d} = R^* \sum_{j=1}^{n} \omega_j M_j
\]

(3)

\[
c_p = \sum_{j=1}^{n} c_p \omega_j = R^* \sum_{j=1}^{n} \left( \frac{f_j}{2} + 1 \right) \omega_j M_j
\]

(4)

where \( M_j \) is the molecular weight of the dry air mixture, and \( R^* = 8.314 \) J/(Kmol) is the universal gas constant (product of the Boltzmann constant and the Avogadro constant). Here, the subscript \( j \) refers to the \( j \)th atmospheric constituent having a mixing ratio \( \omega_j \), molecular weight \( M_j \), and \( f_j \) molecular degrees of freedom. For the purpose of including the coupling of the dynamics with composition, we assume the atmosphere is comprised of nitrogen (\( N_2 \)), oxygen (\( O_2 \)), and free oxygen (\( O \)), which are the three major neutral constituents of the thermosphere (Dickinson et al., 1984). Since the mixing ratio for a constituent is defined as the density of the constituent divided by the density of dry air, \( \omega_{N_2} + \omega_{O_2} + \omega_O = 1 \).

### 2.3. Thermodynamic Equation

The potential temperature coupled with the dry-air density is utilized as a prognostic variable in MPAS as it is a conserved quantity for adiabatic flow in a shallow atmosphere with constant composition. This
representation also facilitates the formation of the vertically implicit numerics that is an essential aspect of the split-explicit numerical scheme (Klemp et al., 2007). However, in the deep atmosphere, as discussed above, the atmospheric composition is not constant, which alters the conservative properties of this formulation. This is illustrated by writing the internal energy equation

$$c_p \frac{dT}{dt} - R_d \frac{d \ln p}{dt} = Q$$

in terms of the potential temperature $\theta = T(p_0 / p)^\kappa = T / \pi$, which yields

$$\frac{d \ln \theta}{dt} = \frac{d \ln T}{dt} - \kappa \frac{d \ln p}{dt} - \frac{\ln p}{c_p} \frac{d \kappa}{dt} = \frac{Q}{c_p T} - \ln p \frac{d \kappa}{dt},$$

where $Q$ is the specific heating and $\kappa = R_d / c_p$. In the absence of diabatic heating ($Q = 0$), potential temperature is not conserved since $\kappa$ will vary due to variations in the atmospheric composition. This correction to the potential temperature equation has also been proposed for the WACCM-X 2.0 model for extension of the finite volume (FV) dycore to the deep atmosphere (Liu et al., 2018). Technically, the thermodynamic coefficients in $\kappa$ are not precisely constant even in the shallow atmosphere equations in the presence of moisture. However, these variations in $\kappa$ are typically less than a percent and are usually ignored (Emanuel, 1994). Since the atmospheric composition varies dramatically across the deep atmosphere, we retain this term to further assess its significance.

### 2.4. Deep Atmosphere Equation Set

The prognostic equations in MPAS for a shallow atmosphere are written in flux form using a height-based terrain-following vertical coordinate $\zeta = \zeta(x_H, z)$ as presented by Skamarock et al. (2012). As mentioned above, we do not consider here vertical variations of the grid-cell area that would arise in a deep atmosphere equations discretization on the globe. These metric adjustments have been derived and implemented in the full global MPAS code, as described by Skamarock et al. (2020). Flux variables are thus defined here using a transformation-adjusted dry density $\tilde{\rho}_d$, such that $\tilde{\rho}_d \cdot d\zeta$ represents the mass in a grid cell. In terms of the flux variables

$$V = \tilde{\rho}_d^2 = (U, V, W), \quad \Theta_m = \tilde{\rho}_d \Theta_m, \quad Q_j = \tilde{\rho}_d Q_j, \quad \Psi_j = \tilde{\rho}_d \Psi_j,$$

the nonhydrostatic equations can then be expressed as

$$\frac{\partial \Theta_m}{\partial t} = -(\nabla \cdot \Theta_m)\zeta - \Theta_m \phi \left[ \frac{\partial \tilde{\rho}_d \kappa}{\partial t} + \left( \nabla \cdot \nabla \kappa \right) \zeta \right] + \frac{1}{c_p} \nabla \cdot (k\nabla T) + F\Theta_m,$$

$$\frac{\partial \Psi_j}{\partial t} = -(\nabla \cdot \Psi_j)\zeta,$$

$$\frac{\partial Q_j}{\partial t} = -(\nabla \cdot Q_j)\zeta + FQ_j,$$

$$\frac{\partial V}{\partial t} = -(\nabla \cdot V)\zeta + FV, \quad \frac{\partial \Theta}{\partial t} = -(\nabla \cdot \Theta)\zeta + F\Theta,$$

$$\frac{\partial Q}{\partial t} = -(\nabla \cdot Q)\zeta + FQ,$$
The influences of turbulent mixing on the constituents are represented by the vertical eddy mixing term \( \psi \), which reflects the departures from diffusive equilibrium, such that \( \psi \) tends toward an equilibrium state (called aerostatic balance) in which the partial log pressure of each constituent \( \phi \) varies vertically in proportion to its molecular weight \( M_\phi \), such that \( \partial \phi / \partial z \rightarrow -gM_\phi / (\rho RT) \). The molecular diffusive transport term in (13) governs the rate at which the atmosphere relaxes toward this aerostatic balance. In this term, \( \alpha \) is a diagonal matrix that represents the relative diffusive rates of the constituents (Dickinson et al., 1984) and \( L \psi \), given by

\[
L \psi = \frac{\rho_0 D_0}{H_0} \frac{M_d}{M_{\phi_0}} \left[ H \frac{\partial}{\partial \zeta} \left( 1 - \frac{M_\phi}{M_d} \frac{H}{M_d} \frac{\partial M_d}{\partial \zeta} \right) \right] \psi,
\]

(14)

reflects the departures from diffusive equilibrium, such that \( L \psi = 0 \) corresponds to aerostatic balance. Here, \( H = R_e T / \rho \) is the scale height, \( D \) is a characteristic diffusion coefficient and the \( \phi_0 \) subscript refers to surface values, with \( D_0 = 2 \times 10^{-5} \) m\(^2\) s\(^{-1}\).

The influences of turbulent mixing on the constituents are represented by the vertical eddy mixing term in (13). Since the atmospheric constituents are found to be vertically well mixed below the vicinity of the
thermopause (~85 km), the eddy coefficient \( K_p \) is expected to decrease with height such that it has little influence above the middle mesosphere.

As mentioned above, we consider here only the three major atmospheric constituents that comprise the thermosphere, \( N_2 \), \( O_2 \), and \( O \). Since the sum of the mixing ratios \( \Psi \) must equal unity, we solve the prognostic Equation 13 for \( \Psi_{N_2} \) and \( \Psi_{O} \), and recover \( \Psi_{N_2} = 1 - \Psi_{O_2} - \Psi_{O} \) as a residual.

To illustrate the effect of the eddy diffusivity on the atmospheric constituents, we have integrated 13 for an atmosphere at rest, using a horizontally homogeneous vertical temperature profile adapted from a representative sounding from the WACCM-X 2.0 Model (Liu et al., 2018) as shown in Figure 1. The model top is set at 500 km with \( \Delta z = 2 \) km. The three atmospheric constituents \( N_2 \), \( O_2 \), and \( O \) are initialized in aerostatic balance and integrated for about 30 days, using an eddy mixing coefficient set (arbitrarily) at \( K_p = 2500 \cos^2(\frac{5 \pi z}{z_L}) \) \( \text{m}^2/\text{s} \) for \( z < z_L = 200 \) km. The resulting constituent profiles are displayed in Figure 2. Notice that in the initial aerostatically balanced state the mixing ratio of molecular oxygen decreases rapidly with height in the lower atmosphere while the nitrogen correspondingly increases.

This occurs because the density scale height for \( O_2 \) is smaller than that for \( N_2 \) due to its greater molecular weight. This behavior is obviously unrealistic and is removed by the vertical eddy mixing, which promotes well mixed constituents below about 100 km. The resulting vertical distribution of constituents in this simple idealization is qualitatively similar to the global mean mixing ratios obtained in the NCAR TCGM model for the thermosphere (Dickinson et al., 1984; Figure 4).

Figure 1 also displays the vertical profiles of the ideal gas constant \( R \) and the heat capacity \( c_p \) from 3 and 4 for the vertical distribution of the atmospheric constituents shown in Figure 2 that are associated with the temperature profile depicted in Figure 1. For these conditions \( R \) increases by about 80% from the surface to 500 km while \( c_p \) increases by about 30%.

Variations in the atmospheric composition may contain considerable additional complexity through the source \( S \) and removal \( R \) terms in 13 that govern the disassociation and recombination of the various atmospheric constituents. For our purposes in evaluating the numerics of the dynamical equations, we ignore these effects and include only the transport and diffusive processes for these constituents. Although changes in composition may have significant influences in regulating the behavior of the deep atmosphere, it is worth noting that the only feedbacks of atmospheric composition to the dynamical Equations 8–11 occur through variations in the thermodynamic coefficients \( R_j \) and \( c_p \) as defined in 3 and 4.

### 3. Numerical Integration of the MPAS Deep-Atmosphere Equations

The split-explicit numerical integration of the dynamical equations in the shallow-atmosphere MPAS is a fundamental component of the model numerics, and is thus a critical aspect to evaluate for deep-atmosphere configurations. In the split explicit formulation, the pressure gradient and buoyancy terms in 8 and 9 are stepped forward on the smaller acoustic time steps, along with the flux divergence terms in the potential temperature and density Equations 10 and 11. In evaluating these terms, the horizontal gradients are computed using explicit (forward-backward) numerics. However, using explicit numerics in the vertical direction would
typically impose severe restrictions on these acoustic time steps. Therefore, numerical efficiency is achieved by writing the vertical pressure gradient, buoyancy, and vertical flux divergence terms implicitly and solving within each vertical column by inverting a simple tridiagonal matrix. (See Klemp et al., 2007 for further details.) Thus the restriction on the acoustic time step should be limited only by the horizontal sound wave propagation on the horizontal grid. On these acoustic time steps, the prognostic variables are cast as perturbations from the most recent full time step. In this manner, essentially all of the slow-mode contributions to these terms are evaluated on the large time steps using a third order Runge-Kutta integration scheme. With these numerics, the model equations can be integrated on large time steps comparable to hydrostatic thermospheric models such as the TGCM (Dickinson et al., 1981) and WACCM-X (Liu et al., 2018), which use time steps on the order of 5 min, in comparison to the nonhydrostatic GITM that is limited to a 2 s time step due to its fully explicit time integration (Ridley et al., 2006).

Although we have written the pressure gradient terms in 8 and 9 in terms of \( \phi = \ln(p / p_0) \) as discussed in Section 2.1 to improve their numerical accuracy, this representation is applied only to the portion of the terms advanced on the large time steps. Thus, the pressure gradient terms in the small time step equations do not need to be altered from their form in the shallow-atmosphere implementation; they are the same as in Equations 13–16 presented in Klemp et al. (2007) except that reference profile variables in the vertical momentum Equation 14 are replaced by the full variables at time \( t \). Since the small time step variables are expressed as perturbations from the most recent large time step, the specific numerics used in representing the small time step terms have little impact on the overall accuracy of the numerical integration. Additional terms that have been included for deep atmosphere applications are accommodated in the large time step calculations.

The density-coupled mixing ratios for the atmospheric constituents 13 are advanced in flux form over the Runge-Kutta time steps in a similar manner to the moist constituents 12. After completing the Runge-Kutta steps, \( R_d \) and \( c_p \) are updated to the new time level using 3 and 4, respectively. The variability in \( \kappa = R / c_p \) directly influences the potential temperature \( \Theta_m \) through the second term on the rhs of 10. This is evaluated following the update of the thermodynamic coefficients using the expression

\[
F_{\Theta m}^{t+\Delta t} = -\rho \partial_{\phi} \Theta_m^{t+\Delta t} \left[ \frac{\zeta^{t+\Delta t} \kappa^{t+\Delta t}}{\Delta t} - \frac{\zeta^t \kappa^t}{\Delta t} + \left( \nabla \cdot \mathbf{V} \right) \right],
\]

and applied as a forcing term in the next time step for \( \Theta_m \). Here, the overbar indicates an average between times \( t \) and \( t + \Delta t \), and \( \mathbf{V} \) is the momentum that has been time-averaged over the acoustic steps, which is also used to advect the density weighted scalars to maintain consistency with the numerics of the continuity equation. Although the term in 15 is quite small, the integration is sensitive to the specific numerical representation of this term. For example, in the flux divergence term in 15, representing \( \kappa \) at either time \( t \) or \( t + \Delta t \) (instead of averaging in time) can occasionally promote an numerical instability in the numerical integration.

The viscosity and diffusivity terms in 8–10 require some special treatment. Because the molecular viscosity and thermal conductivity are relatively constant throughout the atmosphere, the kinematic viscosity \( \nu = \mu / \rho_g \) and the thermal diffusivity \( K_d = k_c / (\rho_g c_p) \) increase exponentially with height in inverse proportion to the density, such that these terms become dominant in their influences on \( \nu \) and \( \Theta_m \) in the upper thermosphere. Because of their large magnitude, these terms must be computed implicitly to maintain stability. At present, this is accommodated with incremental updates through directional splitting. At the beginning of each large time step the diffusion terms are evaluated implicitly, first in the vertical and then in the horizontal. The tendencies from these updates are then combined with the tendencies from the remaining terms in the equations in completing the time step.

This approach is easy to implement and produces the desired effect of strong damping in the upper thermosphere. However, it raises the question as to whether these terms are being treated with sufficient accuracy. Setting aside the issue of evaluating the terms with incremental updates, consider the influence of a basic one-dimensional damping term

\[
\sigma^{t+\Delta t} = \sigma^t + \nu \Delta t \frac{\partial^2}{\partial z^2} \left[ \frac{(1 + \epsilon)}{2} \sigma^{t+\Delta t} + \frac{(1 - \epsilon)}{2} \sigma^t \right]
\]

(16)

KLEMP AND SKAMAROCK
for a prognostic variable $\sigma$. Assuming good spatial resolution, the Fourier representation for a single vertical wave number $\sigma = \hat{\sigma} z^2 A \exp(ikz)$ yields an amplification factor $A$ per time step given by

$$ A = \frac{2 - (1 - \epsilon)\gamma}{2 + (1 + \epsilon)\gamma}, $$

(17)

where $\gamma = \nu k^2 \Delta z$. Since $\gamma \gg 1$ in the upper thermosphere, writing (16) as second order centered in time (Crank-Nicholson) with $\epsilon = 0$ results in an amplification factor $A$ that just oscillates in time as $A \to -1$. For this reason, we evaluate these damping terms with forward centering in time (first order) such that $\epsilon = 1$. Although this yields significant damping per time step ($A \to \gamma^{-1}$), it is much less than the correct analytic value given by $A = \exp(-\gamma)$. The deficiencies of Crank-Nicolson for large values of $\gamma$ are discussed by Osterby (2003), who also proposes several alternatives besides forward centering to reduce Crank-Nicolson oscillations. If more accurate treatment of the molecular viscosity and thermal conductivity is needed in thermospheric applications, further measures, such as temporal substepping, could be considered.

Because atmospheric quantities such as pressure and density may vary by many orders of magnitude across a deep-atmosphere domain, we expect that numerically integrating the equation set 8–13 will require double precision calculations. In practice, we have found that double precision is needed when the model top is significantly greater than about 200 km to avoid the appearance of small scale noise in the model fields.

In the current implementation of MPAS for shallow atmospheres, the thermodynamic variables in the governing equations are cast in terms of perturbations ($\rho_d$, $\mu'$, $\Theta_m$) from a representative reference sounding ($\tilde{\rho}_d$, $\tilde{\mu}$, $\tilde{\Theta}_m$) to reduce truncation and roundoff errors in the numerics (Klemp et al., 2007). However, for deep-atmosphere applications, the perturbations variables might typically become large in comparison to their reference values, thus negating much of the motivation for their implementation (and further obviated by the use of double precision). Thus, double precision and the discrete Equations 8–13 employing full variables are used in obtaining the results reported in this paper.

### 4. Idealized Test Simulations

#### 4.1. Elevated Heating/Cooling Function

For an initial test of the model numerics, we simulate the 2-D atmospheric response in a non-rotating framework ($f = 0$) to an oscillating heating/cooling source term located in the middle thermosphere. The model domain has a depth $z_t = 500$ km and is initialized using a horizontally homogeneous sounding with the temperature profile shown in Figure 1 and no mean wind. For the localized oscillating heating function for temperature $Q_h$, we specify:

$$ Q_h = C_h \sin \left( \frac{\pi t}{3600} \right) \cos \left( \frac{\pi L_q}{2} \right) \text{ (Ks}^{-1} \text{) for } L_q \leq 1, $$

(18)

where the heating rate is $C_h = 0.015$ Ks$^{-1}$ and the radial nondimensional distance $L_q$ from the center of the heating function at $(x_c, z_c)$ is given by

$$ L_q = \left( \left( \frac{x-x_c}{10 \Delta x} \right)^2 + \left( \frac{z-z_c}{10 \Delta z} \right)^2 \right)^{1/2}. $$

(19)

The heating function is centered at $z_c = 300$ km, with $x_c$ located in the middle of the model domain. For this heating function, the thermal forcing oscillates with a period of 2 h.

Because the influences of the molecular viscosity $\mu$ and thermal conductivity $k_t$ become large in the thermosphere, we tested the model numerics with several configurations for the model dissipation. We first simulated the case with $\mu = k_t = 0$ to observe the inviscid response. Since this case will produce significant reflection of gravity waves from the rigid lid upper boundary, we also ran the test case with $\mu = k_t = 0$ but included a gravity wave absorbing layer near the model top. The absorbing layer is specified as proposed by (Klemp et al., 2008), in which a vertically implicit Rayleigh damping term is applied to $w$ in the vertical momentum equation with a coefficient
Including a gravity wave absorbing layer above \( 400 \text{ km} \) and \( 0.1 \text{ s}^{-1} \). For the final test configuration, we ran with no absorbing layer but specified \( \mu \) and \( k_c \) at their appropriate atmospheric values as described by Liu et al. (2010) for the WACCM model:

\[
\mu = (4.03\psi_{O_2} + 3.42\psi_{N_2} + 3.9\psi_{O}) T^{-0.69} 10^{-7} \text{ kg(ms)}^{-1}
\]

\[
k_c = [56.0(\psi_{O_2} + \psi_{N_2}) + 75.9\psi_{O}] T^{0.69} 10^{-5} \text{ J(mKs)}^{-1},
\]

where \( T \) is the temperature in degrees Kelvin. The stability of the vertical diffusion term due to the kinematic viscosity \( \nu = \mu / \rho_d \) is constrained by the dimensionless coefficient \( K_c = \nu \Delta t / \Delta z^2 \). Using explicit numerics for this term, stability nominally requires that \( K_c < 0.25 \). For the model configuration in this test case, \( K_c \) achieves this threshold of 0.25 at about 160 km and continues to increase with height to about 300 at \( z_d = 500 \text{ km} \) due to the large decreases in density, confirming the necessity to use implicit numerics. The same considerations apply to the mixing due to the thermal conductivity.

For each of these cases, we set the horizontal and vertical mesh spacings to \( \Delta x = 20 \text{ km} \) and \( \Delta z = 2 \text{ km} \), respectively, and integrated the split-explicit model numerics with a large time step \( \Delta t = 80 \text{ s} \) and a smaller acoustic time step \( \Delta \tau = \Delta t / 6 \) out to 24 h. These integrations exhibit good stability with no additional explicit filters besides those specifically included as modifications in this test case. For this temperature sounding (Figure 1), the speed of sound increases by a factor of 2.8 from the surface to the top of the model domain (347–986 m s\(^{-1}\)), such that the horizontal acoustic Courant number at upper levels is about 0.65.

In treating the atmospheric composition, we avoid the complication of spinning up the atmosphere from an aerostatic balance by initializing the constituents with vertical profiles that approximate those shown by the solid lines in Figure 2.

The time series for the maximum vertical velocity for these three test simulations are displayed in Figure 3. In each of these cases, the flow achieves a nearly steady 2 h periodicity, consistent with the thermal forcing period, by the end of the 24 h integration. As expected, the strongest response occurs in the inviscid case. The perturbations amplify with increasing height above the forcing level, and are then reflected from the rigid lid upper boundary, as is evident in the plots of the vertical velocity and perturbation temperature at \( t = 24 \text{ h} \) in Figures 4a and 4b. Including a gravity wave absorbing layer above \( z_d = 400 \text{ km} \), the maximum vertical velocity in the upward propagating branch of the disturbance below 400 km is constrained to be 500 km.

Including the molecular viscosity and thermal conductivity terms, the perturbations produced by the thermal forcing are strongly damped. The periodic oscillations become essentially steady by 6 h, with significant amplitude only in the immediate vicinity of the forcing (Figures 4e and 4f). Notice that the contour intervals for the vertical velocity and temperature in Figures 4e and 4f are an order of magnitude smaller than in Figures 4a–4d.

### 4.2. Mountain Waves

For a mountain wave test case, we are faced with the complication that the wave amplitude increases with increasing height in proportion to the inverse square root of density. For the temperature sounding in Figure 1 this would result in an amplification factor of \( \approx 5 \times 10^3 \) between the surface and a height of 500 km. This amplification is largely offset in the mid to upper thermosphere by the molecular viscosity and thermal conductivity, which produce strong dissipation at these altitudes. To test the viability of the numerics for...
Figure 4. (a, c, e) Vertical velocity in m s\(^{-1}\) and (b, d, f) temperature perturbations in K at \(t = 24\) h for the elevated thermal forcing case. (a, b) inviscid with no upper absorbing layer; (c and d) inviscid with upper absorbing layer; (e and f) with molecular viscosity and thermal conductivity and no upper absorbing layer.
domains extending through the thermosphere, we first consider deep atmosphere mountain wave solutions in the absence of molecular viscosity and thermal conductivity. For this purpose, we specify an admittedly artificial vertical eddy mixing that is large enough to keep the waves below overturning amplitudes at high altitudes. This eddy mixing combines a small constant coefficient with a Richardson number $R_i$ dependent local eddy mixing that loosely follows the scheme proposed by Hong et al. (2006) for free atmosphere diffusion:

$$K_{m} = K_{b} + \ell^2 f(R_i) \frac{\partial u}{\partial z},$$

where

$$R_i = \frac{g}{\theta} \left[ \frac{\partial u}{\partial z} \right]$$

and

$$f(R_i) = \frac{1}{(1 + cR_i)^2}. \quad (24)$$

Here, we set the length scale $\ell = \Delta z$ and define $c = 0.2$, which is smaller than in Hong’s formulation in order activate the local eddy mixing over a broader range of Richardson numbers. The constant background eddy mixing is set at $K_b = \beta \Delta z^2 / \Delta t$ to control small scale noise in the simulation while allowing the local eddy mixing to stabilize the wave structure in regions of small Richardson number.

The mountain wave simulations are conducted for a horizontally homogeneous atmosphere characterized by the temperature sounding displayed in Figure 1 and a uniform wind $U = 50$ ms$^{-1}$. The top of the domain is again set at $z_t = 500$ km with a constant vertical grid size of $\Delta z = 2$ km and a gravity wave absorbing layer applied above 400 km as described in the previous section. This vertical resolution is appropriate given that waves generated in this atmosphere will have a vertical wavelength $(\pi U / N)$ that ranges between about 14 and 40 km over the depth of the domain.

The mountain terrain is defined as the frequently used bell-shaped mountain:

$$h(x) = \frac{a^2 h_m}{(x - x_i)^2 + a^2}. \quad (25)$$

where $h_m = 100$ m and $a$ is the mountain half width. The horizontal resolution is set to $\Delta x = a / 5$ and the domain width $(300a \Delta x)$ is sufficiently large that the periodic lateral boundary conditions do not adversely affect the results. The equations are integrated using a time step in seconds of four times the horizontal grid size in kilometers and six acoustic sub-steps per time step. As in the previous test case, we initialize the atmospheric constituents with vertical profiles similar to those shown in Figure 2, which are close to diffusive equilibrium.

Introducing the terrain into the horizontally homogeneous atmosphere at the initial time produces unbalanced disturbances that propagate away from the mountain. In mountain wave simulations, these disturbances typically diminish rapidly during the transient response and do not adversely affect the evolving wave structure. However, for the very deep atmospheric domain in our simulations these acoustic disturbances can amplify rapidly as they propagate upward into the thermosphere, producing spurious results and often numerical instability. These disturbances are particularly troublesome in the absence of molecular viscosity and thermal conductivity. To damp out initially induced perturbations, we include Rayleigh damping terms in the prognostic equations at early times to constrain deviations from their initial state. These terms have the form:

$$\frac{\partial \sigma}{\partial t} = \cdots - 0.02 \frac{U t}{8a} \exp \left( - \frac{U t}{8a} \right) (\sigma - \sigma_0) \quad (26)$$

for a prognostic variable $\sigma$ having a value $\sigma_0$ in the initially undisturbed state. This procedure appears to work well for these idealized mountain wave simulations, but leaves open the question of how best to deal with these initial disturbances (if necessary) in real-atmosphere simulations.

In conducting these mountain wave test simulations, we consider different horizontal scales of motion by specifying several different mountain half-widths $a$. Setting $a = 100$ km, the wave response should be hydrostatic $(a N / U \sim 20)$ and rotational effects should be weak $(af / U = 0.2)$. At this scale the group velocity
of the waves should be nearly vertical, and this behavior is confirmed in Figure 5a, which displays the vertical velocity at an integration time of about 3 days. By this time, the wave structure is essentially steady with the wave amplitude concentrated directly above the terrain. To control small-scale noise in this simulation, we have specified the dimensionless constant eddy mixing to be $\beta = 0.03$. (The triangular shape at bottom of Figure 5 and subsequent figures are included only to indicate the location of the mountain, which is actually only 100 m in height.)

At larger horizontal scales rotational influences become stronger and the waves propagate downstream as they progress upward. This is apparent in the vertical velocity field in Figure 5b for the simulation with $a = 500$ km at about 16 days, in which the wave train extends noticeably downstream at upper levels. This wave structure is not completely steady at this time as it is slowly progressing farther downstream with time.

For this simulation we are able to reduce the constant vertical mixing to $\beta = 0.005$, which permits the Richardson number dependent portion of the eddy mixing to play a more significant role in influencing the wave structure. The spatial distribution of the mixing coefficient $mK$, displayed in Figure 6a, reveals that this dissipation is active throughout the wave train, with the maximum dimensionless value reaching $K_m \Delta t / \Delta z^2 = 0.24$.

To avoid an artificial spinup of the atmospheric constituents from an aerostatic balance, for these simulations we initialized these constituents with vertical profiles close to those depicted by the solid lines in Figure 2. Since the molecular diffusive transport and vertical eddy mixing terms are nearly in balance, perturbations of the constituents are modified primarily by advective transport (as confirmed by comparison with a simulation in which the diffusive transport and eddy mixing terms are turned off). Figure 6b illustrates the pertur-

**Figure 5.** Vertical velocity for uniform ($U = 50$ m s$^{-1}$) flow past a 100 m bell-shaped mountain with an absorbing layer above 400 km and with no molecular viscosity or thermal conductivity. The temperature sounding corresponds to the profile in Figure 1. The mountain half-width is (a) $a = 100$ km, and (b) $a = 500$ km.
bations in the ideal gas constant $R'$ that result from the variations in these constituents. Notice that the perturbations in $R'$ are confined primarily to the layer between about 150 and 350 km, which is consistent with the region in which most of the variations in the mean profile for $R$ occur (see Figure 1). Although the maximum deviations from the initial profile in Figure 1 are less than one percent (also true for $c_p$, not shown), even these small variations in the thermodynamic properties can have a noticeable effect on the results. For example, holding $R$ and $c_p$ fixed at their initial values, the simulated wave amplitude for this $a = 500$ km case increases by about 30%. Since the molecular diffusive transport and vertical eddy mixing terms in the atmospheric constituent Equation 13 produce a small amount of vertical redistribution of constituents during the integration, the perturbations in $R$ shown in Figure 6b are displayed as the deviation from the undisturbed vertical profile far from the mountain.

At smaller horizontal scales, nonhydrostatic effects begin to influence the mountain wave structure. This is evident in our test simulation for $a = 25$ km shown in Figure 7a after 1 day, conducted with $\beta = 0.027$ and with no molecular viscosity or thermal conductivity. Due to the nonhydrostatic influences, the wave energy propagates downstream as it progresses upward, contributing to the significant downstream extent of the waves. Here the conditions that contribute most to the nonhydrostatic response are located at the levels of smaller atmospheric stability in the upper thermosphere (due to the high temperatures). Thus, the downstream refraction of the waves are strongest at levels above 200 km.

As mentioned above, the influences of molecular viscosity and thermal conductivity become large in the upper thermosphere and absorb most of the gravity wave energy propagating up from below. This is illustrated in the physically more realistic simulation for $a = 25$ km displayed in Figure 7b with the molecular viscosity and thermal conductivity specified according to 21 and 22. In this case the wave amplitude is confined almost entirely below about 200 km, removing any need for an artificial damping layer to absorb wave energy approaching the upper lid of the domain. Below about 150 km, the viscosity and conductivity have little effect on the mountain waves, and the vertical velocity fields in Figures 7a and 7b below this level are essentially the same. (Note that the contour interval in Figure 7b is only one fifth the interval shown in Figure 7a.)

For the mountain wave test cases discussed above, the mean wind speed was set at a uniform $U = 150$ ms$^{-1}$, which enabled testing of the model numerics for mountain waves propagating into the upper thermosphere in the absence of the large dissipation produced by molecular viscosity and thermal conductivity. However, the actual horizontal winds in the upper thermosphere can often reach several hundred meters per second, particularly during geomagnetically disturbed periods (Akmaev, 2011).

To test the model numerics in the presence of stronger thermospheric winds, we reran these mountain wave cases specifying a mean wind $U = 50 + 250\sin^2(\frac{5\pi z}{z_e})$ ms$^{-1}$, as displayed in Figure 8a. With significant increases in the wind speed, the character of the mountain waves is correspondingly altered, as is evident from the linear inviscid dispersion equation for the individual Fourier components (approximated for the anelastic steady-state equations with constant coefficients)

![Diagram](image_url)
where $N$ is the Brunt-Väisälä frequency and $k$ and $\ell$ are the horizontal and vertical wave numbers, respectively (Klemp & Lilly, 1980). For a given $k$, as $U$ increases, the vertical wave number $\ell$ decreases as the denominator in 27 increases. In addition, the nonhydrostatic influences increase [through the numerator in 27] while the rotational influences decrease [through the denominator in 27]. Since the vertical wave length increases significantly as $U$ approaches $300$ ms$^{-1}$ in the upper thermosphere, vertical diffusion is much less effective in dissipating vertically propagating wave energy. Thus, it is not practical to simulate this case using only the eddy mixing 23 to control the wave amplitude. For this reason, we only simulate these cases with the inclusion of molecular viscosity and thermal conductivity. Although the mountain waves are almost completely damped out below the middle thermosphere in the cases with a constant $U = 50$ ms$^{-1}$, with the stronger horizontal winds shown in Figure 8a the waves can penetrate much farther into the thermosphere due to their greater vertical wave length. With these stronger winds, we find that numerical stability can be maintained by reducing the large time step from $\Delta t = 4 \Delta x$ (km) to $\Delta t = 2.5 \Delta x$ (km), while acoustic time step remains unchanged ($\Delta t = \Delta x / 4$).

For the case with a mountain half width $a = 25$ km, we set $\beta = 0.04$ in the eddy mixing formulation 23 to constrain the wave amplitude in the lower mesosphere where the molecular viscosity and thermal conductivity have little influence. The resulting vertical velocity for the steady state mountain waves is displayed in Figure 8b. At these horizontal scales, the stronger nonhydrostatic influences cause much of the wave

\[ \ell^2 = k^2 \frac{N^2 - k^2 U^2}{k^2 U^2 - \ell^2}. \]  
(27)

Figure 7. As in Figure 5b except for a mountain half-width $a = 25$ km (a) with no molecular viscosity $\mu$ or thermal conductivity $k$, and (b) with $\mu$ and $k$, as defined in 21 and 22.
response to become evanescent above the middle mesosphere as $a/NU \to 0.8$ (Klemp & Lilly, 1980). Thus, most of the wave energy is trapped in the lower mesosphere, which displaces the wavefield downstream from the mountain.

Increasing the mountain half width to $a = 100$ km, the stationary waves penetrate further into the upper mesosphere, as shown in Figure 8c. The nonhydrostatic influences become significant as $U$ increases with height and as waves are turned toward the horizontal, they are absorbed by the molecular viscosity and thermal conductivity. This behavior is in contrast to that for this case with $U = 150$ ms$^{-1}$ where wave structure was strongly hydrostatic (Figure 5a).

With a mountain half width further increased to $a = 500$ km, the waves regain a strong hydrostatic character, propagating to the top of the model domain where they are attenuated by the absorbing layer, which is included above $z = 400$ km. For this case, the constant portion of the vertical eddy mixing coefficient has been reduced to $\beta = 0.025$. Rotational influences are greatly reduced from those apparent in the $U = 50$ ms$^{-1}$ case (Figure 5b); the propagation of energy is nearly vertical and the waves remain directly above the mountain terrain. Note that in Figure 8, the scaling for the horizontal $x$ axes are expanded by a factor of 2 from those in Figures 5–7 for the $U = 50$ ms$^{-1}$ cases to better display the wave structure.

When the waves have the capability to propagate to high altitudes, the kinematic viscosity and thermal diffusivity can influence the structure of the waves in addition to dissipating them. In a detailed analysis of the linear dispersion characteristics in the presence of kinematic viscosity and thermal diffusivity, Vadas and Fritts (2005) confirmed that the waves with the largest vertical wave lengths dissipate at the highest altitudes. They found that as these diffusive influences increase with height, the intrinsic frequency decreases and causes the vertical wave length to decrease, and with sufficiently large diffusion the wave may be reflected. For this case with $a = 500$ km, the large vertical wave length resulting from the strong horizontal winds allows the waves to propagate to the top of the simulated domain. However, it is difficult...
to distinguish the relative influences of the increasing winds with height and the increasing dissipation on the wave structure.

5. Summary
Adapting MPAS for applications that extend well into the thermosphere requires some significant modifications to the model equations and the model numerics. As mentioned in the Introduction, some of these extensions have been implemented in MPAS by Skamarock et al. (2020) in removing the shallow atmosphere approximations from the model equations applied to the sphere. With these modifications the MPAS equations use the actual geocentric distance from the center of the Earth to allow the mesh configuration and gravity to vary with height and include the full Coriolis terms in the momentum equations. To adapt MPAS for model domains that span a large number of vertical scale heights, we have further modified the model numerics and generalized the model equations to include variable composition, and potentially large molecular viscosity and thermal conductivity.

Allowing the atmospheric constituents to vary can have potentially significant influences on the model dynamics. These feedbacks occur through changes in the ideal gas constant $R$ and the heat capacity $c_p$, which depend solely on the relative concentrations of these constituents. With variable thermodynamic coefficients, potential temperature is no longer strictly conserved for adiabatic flow. Nevertheless, in our numerical testing with MPAS it appears that potential temperature can still be effectively used as a prognostic variable with an additional term that accounts for the variability in $\kappa = \frac{R}{c_p}$.

The height-based hybrid terrain-following coordinate in MPAS seems well suited for deep atmosphere domains, and avoids the complications that arise in a pressure-based vertical coordinate when gravity becomes a function of height. Also, the split-explicit numerical integration used in MPAS appears to remain viable in the limited deep atmosphere testing we have conducted across a range of horizontal scales and that includes the influences of variable atmospheric composition. As expected, the presence of molecular viscosity and thermal conductivity in the mid and upper thermosphere strongly damps disturbances propagating up from the lower atmosphere. However, it is interesting to see in our mountain wave simulations that waves having large horizontal wave lengths can penetrate throughout the thermosphere in the presence of strong thermospheric winds that promote large vertical wave lengths that are not as strongly damped by the molecular viscosity and thermal conductivity.

There are a number of issues that may require further consideration. In writing the governing Equations 8–13 we have incorporated simplifying approximations as discussed above that will require further scrutiny in our continuing efforts to improve the accuracy of the modeling system. We have also mentioned that the numerical integration appears to be sensitive to the specific numerics used to represent the variations in the thermodynamic coefficients in the potential temperature equation. While the numerics described by 15 appear to maintain numerical stability for this feedback, further testing may be needed to determine whether this treatment is sufficiently robust. Another issue is the rapid growth of acoustic disturbances that arise in our deep-atmosphere mountain wave test cases when the terrain is introduced at the initial time. While including Rayleigh damping at early times in the simulation appears to remove these disturbances, it remains unclear if these initial imbalances will be an even larger problem in real data simulations with much larger amplitude terrain. Also, as discussed above, the large values of molecular diffusivity and thermal conductivity in the upper thermosphere make it difficult to accurately represent these damping influences. Although implicit representation of these terms maintains numerical stability, the magnitude of damping in the current implementation may significantly under represent their true influences. Further consideration of these issues will be explored in more realistic simulations of thermospheric dynamics, and with the inclusion of appropriate thermospheric physics.

Appendix A: Numerical Treatment of the Horizontal Pressure Gradient
To improve the accuracy of the numerics employed in MPAS, Klemp (2011) introduced an extension of the traditional and hybrid terrain-following height coordinates to progressively smooth the coordinate surfaces with increasing height to more rapidly remove the influences of the smaller scale terrain features. Testing
this modified vertical coordinate in a 2-D vertical slab configuration for idealized resting atmosphere simulations confirmed that artificial circulations arising from numerical inaccuracies in the horizontal pressure-gradient term could be significantly reduced. For these resting atmosphere experiments, the horizontal pressure gradient in the terrain-following coordinate \( \zeta(x, z) \) was represented in the conservative form suggested by Klemp et al. (2007) with second order finite differencing on a staggered C grid:

\[
\zeta \nabla \rho \cdot p = \nabla \zeta (z_{\rho} p) - \partial \zeta (z_{H} p) = \delta_{H} (z_{\rho} p) - \delta_{H} (z_{H} p^{\varepsilon} H).
\]  

(A1)

Here, \( \nabla \) and \( \nabla \zeta \) refer to the divergence operator along constant \( z \) and \( \zeta \) surfaces, respectively. Elsewhere the \( \zeta \) subscript represents vertical differentiation while the \( H \) subscript denotes horizontal differentiation at constant \( \zeta \). The discrete form of the pressure-gradient operator is given in the second part of A2, where the appropriate C-grid spatial averaging is represented by overbars. \( z_{H} \) and \( z_{\zeta} \) represent the metrics of the vertical coordinate transformation in this notation.

The resting atmosphere test case presented by Klemp (2011) was configured to promote a significant artificial circulation using the basic terrain-following vertical coordinate in order to emphasize the significant improvement that could be achieved with a smoothed hybrid coordinate. Shortly after implementing the initial numerical formulation for MPAS (Skamarock et al., 2012) with the horizontal pressure gradients represented as in A1, we revisited the numerics for these pressure gradients to improve their numerical accuracy. Recognizing that the numerical error in A1 is aggravated by the significant spatial averaging in the vertical adjustment term (last term in A1), we rewrote the horizontal pressure gradient as

\[
\zeta \nabla \rho \cdot p = \zeta \nabla \zeta \rho \cdot p - z_{H} \partial \zeta \rho \cdot p = \zeta^{H} \delta_{H} \rho \cdot p + g z_{H} \bar{\rho}_{m}^{H},
\]  

(A2)

where we have used the hydrostatic equation \( \partial \zeta \rho \cdot p = -g \bar{\rho}_{m} \) to approximate the \( \partial \zeta \rho \cdot p \) term. Here, \( \bar{\rho}_{m} \) is the full moist density times the coordinate metric \( z_{\zeta} \). This approximation appears to work well, since even for nonhydrostatic flow, the hydrostatic vertical pressure gradient is the dominant component of the full vertical pressure gradient.

As a modification to A2, it is possible to retain the full vertical pressure gradient in the vertical adjustment term for the horizontal pressure gradient in terrain-following coordinates. This is accomplished by just adding and subtracting the buoyancy (\( g \bar{\rho}_{m} \)) in the full expression and rearranging the terms to yield:

\[
\zeta \nabla \rho \cdot p = \zeta^{H} \delta_{H} \rho \cdot p + g z_{H} \bar{\rho}_{m}^{H} - z_{H} \left( \partial \zeta \rho \cdot p + g \bar{\rho}_{m}^{H} \right).
\]  

(A3)

This formulation is the same as A2 with the addition of the last term in A3, which represents the nonhydrostatic correction to the vertical pressure gradient. Although this term contains significant averaging [as in the last term in A1], it is averaging only the nonhydrostatic adjustment to the pressure gradient, computed with the same numerical representation as used for the vertical pressure-gradient/buoyancy terms in the vertical momentum equation. Thus, this term vanishes numerically for hydrostatic flow.

To illustrate the reduction in horizontal pressure gradient errors with our revised numerical formulation A2, we have recomputed the Klemp (2011) resting atmosphere test case for the basic terrain-following coordinate using the two formulations A1 and A2. The maximum vertical velocities, displayed in Figure A1, show that the artificial circulations induced by numerical errors in the horizontal pressure gradient term have been reduced by more than an order of magnitude using the new formulation. Although nonhydrostatic effects contribute significantly in this test case (500 m horizontal grid), the results using either A2 or A3 are virtually indistinguishable (not shown). Based on this and other testing, we adopted the simpler A2 for the MPAS numerics. With this improved pressure gradient formulation, the magnitude of the perturbations produced for this test case are more comparable to other more recent numerical simulations of this test case (cf. Shaw & Weller, 2016; Weller & Shahrokhi, 2014).

In Section 3, we mentioned that for the deep atmosphere we are solving the equations in terms of the full thermodynamic variables instead of perturbations from a reference sounding. One potential benefit in adopting the use of perturbation variables is the reduction of truncation errors in computing the horizontal
pressure gradients. For this resting atmosphere test case, we simulated the artificial circulations produced by the horizontal pressure gradient term computed using either the full thermodynamic variables or perturbation variables and found the results to be nearly identical (Figure A1).

As discussed in Section 2.1, for deep-atmosphere applications, representing pressure gradients in terms of gradients in \( \phi = \ln(p / p_0) \) instead of \( p \) provides increased accuracy in the model numerics. Although this benefit is primarily associated with the vertical pressure gradients, for consistency, the horizontal pressure gradient terms can also be expressed in terms of \( \phi \), as shown in Section 2.1, such that the counterpart to (A4) is the finite difference form of 2:

\[
\frac{\rho_d}{\rho_m} z_c \nabla_z p = \left( \frac{\rho_d}{\rho_m} p z_c \right)^H \delta H \phi + g z_c \frac{\rho_c}{\rho_d} \tag{A4}
\]

Here, we have included the ratio of the density of dry air to moist air \( \rho_d / \rho_m \) that multiplies the pressure gradient in the horizontal momentum Equation 8. Rerunning this resting atmosphere test case using \( \phi = \ln(p / p_0) \) for both the horizontal and vertical pressure gradients as expressed in (A4) and 1 yields results that are virtually identical to those shown in Figure A1 for the new version of \( p_c \).

**Data Availability Statement**

The MPAS model code is publicly available, and can be found in the Zenodo repository: https://zenodo.org/record/3241875. The test case simulations were conducted with a 2D slab version of the code, with modifications as documented in this paper.

**Acknowledgments**

Funding for this research was provided by the National Center for Atmospheric Research through support from the National Science Foundation under Cooperative Support Agreement AGS-0856145. The authors would like to thank the two anonymous reviewers for their insightful comments that improved the clarity of the paper. The National Center for Atmospheric Research is supported by the National Science Foundation.

**References**

Akmaev, R. A. (2011). Whole atmosphere modeling: Connecting terrestrial and space weather. *Reviews of Geophysics*, 49(4), RG4004. https://doi.org/10.1029/2011RG000364

Becker, E. (2001). Symmetric stress tensor formulation of horizontal momentum diffusion in global models of atmospheric circulation. *Journal of the Atmospheric Sciences*, 58, 269–282. https://doi.org/10.1175/1520-0469(2001)058<0269:sstfoh>2.0.co;2

Becker, E., & Burkhardt, U. (2007). Nonlinear horizontal diffusion for gcms. *Monthly Weather Review*, 135, 1439–1454. https://doi.org/10.1175/mwr3348.1

Deng, Y., & Ridley, A. J. (2014). Simulation of non-hydrostatic gravity wave propagation in the upper atmosphere. *Annales Geophysicae*, 32(4), 443–447. https://doi.org/10.5194/angeo-32-443-2014

Dickinson, R. E., & Ridley, E. C. (1972). Numerical solution for the composition of a thermosphere in the presence of a steady subsolar to-antisolar circulation with application to Venus. *Journal of the Atmospheric Sciences*, 29(8), 1557–1570. https://doi.org/10.1175/1520-0469(1972)029<1557:nsftco>2.0.co;2
Dickinson, R. E., Ridley, E. C., & Roble, R. G. (1981). A three-dimensional general circulation model of the thermosphere. *Journal of Geophysical Research: Space Physics, 86*(A3), 1499–1512. https://doi.org/10.1029/JA086iA03p01499

Dickinson, R. E., Ridley, E. C., & Roble, R. G. (1984). Thermospheric general circulation with coupled dynamics and composition. *Journal of the Atmospheric Sciences, 41*(2), 205–219. https://doi.org/10.1175/1520-0469(198402)41<205:tgctcm>2.0.co;2

Dutton, J. A. (1966). *The ceasless wind: an introduction to the theory of atmospheric motion*. New York, New York: Dover Publications.

Emanuel, K. A. (1994). Atmospheric convection. New York, New York: Oxford University Press.

Hong, S.-Y., Noh, Y., Dudhia, J., Noh, Y., & Dudhia, J. (2006). A New vertical diffusion package with an explicit treatment of entrainment processes. *Monthly Weather Review, 134*, 2318–2341. https://doi.org/10.1175/mwr3199.1

Klemp, J. B. (2011). A terrain following coordinate with smoothed coordinate surfaces. *Monthly Weather Review, 139*, 2163–2169. https://doi.org/10.1175/MWR-D-10-05046.1

Klemp, J. B., Dudhia, J., & Hassiottis, A. D. (2008). An upper gravity-wave absorbing layer for NWP applications. *Monthly Weather Review, 136*, 3987–4004. https://doi.org/10.1175/2008MWR2596.1

Klemp, J. B., & Lilly, D. K. (1980). Mountain waves and momentum flux. In *Orographic effects in planetary flows*, GARP publication series no. 23 (pp. 116–141). Geneva: ICSU/WMO.

Klemp, J. B., Skamarock, W. C., & Dudhia, J. (2007). Conservative split-explicit time integration methods for the compressible nonhydrostatic equations. *Monthly Weather Review, 135*, 2897–2913. https://doi.org/10.1175/mwr3440.1

Liu, H.-L., Bardeen, C. G., Foster, B. T., Lauritzen, P., Liu, J., Lu, G., et al. (2018). Development and validation of the whole atmosphere community climate model with thermosphere and ionosphere extension (waccm-x 2.0). *Journal of Advances in Modeling Earth Systems, 10*(2), 381–402. https://doi.org/10.1002/2017MS001232

Liu, H.-L., Foster, B. T., Hagan, M. E., Mcinerney, J. M., Maute, A., Qian, L., et al. (2010). Thermosphere extension of the whole atmosphere community climate model. *Journal of Geophysical Research: Space Physics, 115*(A12), A12302. https://doi.org/10.1029/2010JA015586

Miyoshi, Y., Fujiwara, H., Jin, H., & Shingawa, H. (2014). A global view of gravity waves in the thermosphere simulated by a general circulation model. *Journal of Geophysical Research: Space Physics, 119*(7), 5807–5820. https://doi.org/10.1002/2014JA019848

Osterby, O. (2003). Five ways of reducing crank-nicolson oscillations. *BIT Numerical Mathematics, 43*, 811–822. https://doi.org/10.1023/b:bitn.0000009942.00540.94

Roble, R. (2000). On the feasibility of developing a global atmospheric model extending from the ground to the exosphere (pp. 53–67). Washington DC American Geophysical Union Geophysical Monograph Series. https://doi.org/10.1029/GM123p0053

Roble, R. G., Ridley, E. C., & Dickinson, R. E. (1987). On the global mean structure of the thermosphere. *Journal of Geophysical Research: Space Physics, 92*(A9), 8745–8758. https://doi.org/10.1029/JA092iA09p08745

Schwartz, C. S. (2019). Medium-range convection-allowing ensemble forecasts with a variable-resolution global model. *Monthly Weather Review, 147*(6), 2997–3023. https://doi.org/10.1175/MWR-D-18-0452.1

Shaw, J., & Weller, H. (2016). Comparison of terrain-following and cut-cell grids using a nonhydrostatic model. *Monthly Weather Review, 144*(6), 2085–2099. https://doi.org/10.1175/mwr-d-15-0226.1

Skamarock, W. C., Duda, M., Ha, S., & Park, S.-H. (2018). Limited-area atmospheric modeling using unstructured mesh. *Monthly Weather Review, 146*(10), 3445–3460. https://doi.org/10.1175/MWR-D-18-0155.1

Skamarock, W. C., Klemp, J. B., Duda, M. G., Fowler, L. D., Park, S.-H., & Ringler, T. (2012). A multiscale nonhydrostatic atmospheric model using Centroidal Voronoi Tesselations and C-grid staggering. *Monthly Weather Review, 140*, 3090–3105. https://doi.org/10.1175/MWR-D-11-00215.1

Skamarock, W. C., Ong, H., & Klemp, J. B. (2020). A fully compressible nonhydrostatic deep-atmosphere-equations solver for MPAS. *Monthly Weather Review, 149*, 571–583. https://doi.org/10.1175/MWR-D-20-0286.1

Skamarock, W. C., Park, S.-H., Klemp, J. B., & Snyder, C. (2014). Atmospheric kinetic energy spectra from global high-resolution nonhydrostatic simulations. *Journal of the Atmospheric Sciences, 71*, 4369–4381. https://doi.org/10.1175/JAS-D-14-0114.1

Thuburn, J., Ringler, T., Skamarock, W. C., & Klemp, J. B. (2009). Numerical representation of geostrophic modes on arbitrarily structured C-grids. *Journal of Computational Physics, 228*, 8321–8335. https://doi.org/10.1016/j.jcp.2009.08.006

Vadas, S. L., & Fritts, D. C. (2005). Thermospheric responses to gravity waves: Influences of increasing viscosity and thermal diffusivity. *Journal of Geophysical Research, 110*, D15103. https://doi.org/10.1029/2004JD005574

Weller, H., & Shahrokhi, A. (2014). Curl-free pressure gradients over orography in a solution of the fully compressible Euler equations with implicit treatment of acoustic and gravity waves. *Monthly Weather Review, 142*(12), 4439–4457. https://doi.org/10.1175/mwr-d-14-00054.1

White, A. A., Hoskins, B. J., Roulstone, I., & Staniforth, A. (2005). Consistent approximate models of the global atmosphere: Shallow, deep, hydrostatic, quasi-hydrostatic and non-hydrostatic. *Quarterly Journal of the Royal Meteorological Society, 131*(609), 2081–2107. https://doi.org/10.1256/qj.04.49