Response to Reviewer 2

We thank the reviewer for carefully evaluating our manuscript and for providing thoughtful and constructive comments. We have considered all of the points raised and have revised the manuscript accordingly. Below, we have listed the reviewer's major and minor comments (in italic font), followed by our responses (in regular font).

Major comments

1. Organization: A brief recap of constant pressure boundary condition is given in Sec. 2 "Diurnal heating test case", including Eqs. (3) and (4). This is confusing. A separate short section recapping the BC preceding the Diurnal heating test case would be easier to follow.

We agree that the description of this global diurnal heating test case was not well organized. We have restructured this section accordingly and believe that these modifications have significantly improved the clarity of the presentation for this test case. The description of the coordinate transformation and the calculation of the height of the constant pressure upper boundary are now contained in a labeled subsection. Reviewer 1 also provided suggestions for improving the organization of this section, so we have included the revised text for the first part of this section below:

---

2. Diurnal heating test case

2.1 Analytic temperature field and internal diabatic heating rate

The 2-D diurnal heating test case described in KS22 is based on a linear analytic solution for a steady periodic wave driven by a propagating internal heating function. To modify this test case for a global domain, we specify an initial temperature field and a time dependent diurnal heating rate that are essentially the same as that in KS22 at the equator, but that tapers the initial temperature perturbation and the heating rate to zero at the north and south poles. The analytic temperature field is specified in a form that permits the hydrostatic equation to be integrated vertically to yield a closed form analytic expression for pressure. For this implementation on the globe, the analytic temperature T_a maintains the same form as in the 2-D case:

$$T_a = T_t \left[\frac{T_t}{T_b}(1 - \tanh \tilde{z}) + \tanh \tilde{z} \right]^{-1}. \tag{1}$$

Here, T_b is the constant temperature at the fixed height z_b of the lower boundary of the simulation domain, z_d is the scale height for the lower level vertical temperature gradients, with $\tilde{z} = (z - z_b)/z_d$, and T_t is the temperature

at $z \to \infty$, given by

$$T_t = \overline{T} + \Delta T_d \cdot \sin(\lambda + 2\pi\omega t)\cos\gamma, \tag{2}$$

where $\overline{T}$ is the initial mean temperature at the top boundary, and ΔT_d defines the amplitude of the initial sinusoidal diurnal variation along the upper boundary. In specifying the horizontal variation of T_t, γ and λ denote the latitude and longitude, respectively, and $\omega = \text{day}^{-1}$. For this test case, T_t also accurately represents the temperature along the constant pressure upper boundary of the simulation domain. Here, equations (1) and (2) are the same as KS22 (14) and (16) except for the addition of the $\cos\gamma$ dependence in (2). Since the linear analytic solution derived in KS2 does not include the influences of the horizontal winds, the global analytic solution is the same as in the 2D case except for the latitudinal dependence included in (2).

The diurnal heating rate Q_d governs the evolution of the flow as a forcing term in the thermodynamic equation. Taking the time derivative of (1), Q_d becomes

$$Q_d = \frac{\partial T_a}{\partial t} = \frac{\partial T_t}{\partial t}\tanh\tilde{z}\left[\frac{T_t}{T_b} + \left(1 - \frac{T_t}{T_b}\right)\tanh\tilde{z}\right]^{-2}. \tag{3}$$

where

$$\frac{\partial T_t}{\partial t} = 2\pi\omega\Delta T_d \cdot \cos(\lambda + 2\pi\omega t)\cos\gamma. \tag{4}$$

This expression for Q_d is the same as in KS22 except that the second term in the numerator of KS22 (15) has been dropped as it is negligible for this case.

2.2 Height of the constant pressure upper boundary

To achieve a constant pressure upper boundary condition in MPAS, KS22 implemented a coordinate transformation in the upper portion of the model domain to allow the hybrid coordinate surfaces to transition adaptively from a constant height surface at a specified height z_p to one at height H that follows a specified constant pressure surface at the model top:

$$z = \left(\frac{\zeta - z_p}{H_0 - z_p}\right)^2 (H - H_0) + \zeta, \quad \text{for} \quad z > z_p \tag{5}$$

such that the transformed coordinate $\zeta = H_0$ at $z = H$. For this test case, we follow KS22 and set $z_p = 200$ km. We specify the desired constant pressure along the top boundary to be $p_{top} = 2.18\text{x}10^{-8}$ Pa, which is the value obtained by vertically integrating the hydrostatic equation for the sounding with $T_t = \overline{T}$ in (1) and $z_d = 50$ km from z_b to H_0. We then adjust the height H of the top boundary at the end of each time step based on the deviations of the top pressure from the target value p_{top} using the hydrostatic vertical extrapolation based on $\phi^* = \ln(p^*/p_0)$ as defined in KS22 eq. (5):

$$H = H^* + \alpha\frac{R_d T^*}{g}(\phi^* - \phi_{top}), \tag{6}$$

where the asterisk superscript denotes values along the upper surface at the current time step or iteration and $\phi_{top} = \ln(p_{top}/p_0)$. The dimensionless height adjustment coefficient α is unity for a full hydrostatic extrapolation, but can be adjusted to smaller values to remove any oscillations in the upper boundary height, if necessary.

We initialize the thermodynamic fields and the height of the constant pressure upper boundary by utilizing the iterative technique described in KS22. With this approach, we first compute the hydrostatically balanced thermodynamic fields using (1) and (2) based on a rigid-lid upper boundary at the nominal height of the top boundary H_0. A new height H for the top boundary is computed from (6) with the adjustment coefficient α set at its full value $\alpha = 1.0$ for this test case. With this new height, we adjust the height of the coordinate surfaces using (5), reinitialize the thermodynamic fields on the modified coordinate surfaces, and then continue the iterative process. This approach yields a well converged initialization with a constant pressure along the model upper boundary in three iterations. The initial temperature field is displayed in the vertical cross section along the equator in Fig. 1, which is similar to Fig. 2 in KS22.

[Figure 1]

2.3 Test case parameters and model configuration

Following KS22, we place the lower boundary at $z_b = 100$ km, where we specify a constant temperature $T_b = 200$ K and pressure $p_b = 0.03$ Pa. At the top boundary of the simulation domain, we specify an initial mean height $H_0 = 600$ km, and define the initial top temperature $T_t(t = 0)$ from (2) using $\overline{T} = 850$ K and $\Delta T_d = 150$ K for this test case. Although the thermodynamic coefficients and gravity vary throughout the thermosphere, for consistency with the analytic solution, we specify constant values for the gas constant ($R = 500$ m^{2}s^{-2}K^{-1}), the heat capacity ($c_p = 1300$ m^{2}s^{-2}K^{-1}), and the gravitational acceleration ($g = 9.81$ ms^{-2}), as in KS22.

As mentioned above, we seek qualitative guidance in evaluating the results from this idealized test case through comparisons with a simulation from the WACCM-X model (Liu et al. 2018). For this purpose, we have chosen a WACCM-X simulation valid at 00Z on 21 March 2000 for comparison because at the spring equinox the global flow fields are most symmetrical about the equator, based on climatology. The parameters for our idealized diurnal heating test case are the same as those used in KS22 except that $\overline{T}$ has a lower value for better consistency with this WACCM-X simulation

In simulating this test case on the globe, we employ the same configuration of MPAS-A as in the 2-D simulations described in KS22 except that the 2-D mesh configuration is replaced by the 10242 cell global mesh (∼240 km horizontal grid size). We employ the transformed vertical coordinate described

in KS22 that follows the height of the time dependent constant pressure upper boundary as described in KS22 with a constant $\Delta\zeta = 5$ km nominal vertical grid spacing on the transformed grid.

After initializing the model fields as described above, the dynamical equations are stepped forward in time using the split-explicit integration numerics in MPAS-A, as described in Skamarock et al. 2012, with an overall time step of $\Delta t = 600$ s and a smaller acoustic time step $\Delta\tau = 100$ s. A diurnal heating function based on (3) and (4) is included in the prognostic equation for the potential temperature to provide the periodic thermodynamic forcing. As explained in KS22, the linear analytic solution produces unrealistically large horizontal velocities (even exceeding the speed of sound). Consequently, in lieu of realistic model physics, a dissipation mechanism is required to limit the unrealistic growth of the horizontal velocity and to produce a proper phase relationship between the temperature and the zonal wind. Thus, we include a Rayleigh damping term in the horizontal velocity equation with a coefficient of $K = 0.001$ s^{-1}.

In conducting simulations over several diurnal periods with the above described configuration, we found that the longitudinal and meridional winds developed an essentially steady periodic structure, but the temperature field at upper levels continued to increase over time. This temperature rise appears to be associated with a net positive change in the internal energy as the simulation evolves, and may occur because appropriate cooling mechanisms, such as molecular thermal conduction, are not considered in the model. The heating function (3) we derived in KS22 for the 2-D diurnal heating case was based on the linear equations in which the horizontal winds are neglected as they are higher order. Thus, to restrict the continuing increase in temperature due to nonlinear effects, we have modified the heating function by adding a Newtonian cooling term that acts on the deviation of the temperature from what it would be if the solution was linear and the horizontal winds were ignored. The modified heating rate Q'_d then can be written as:

$$Q'_d = \frac{\partial T_a}{\partial t} - \beta(T - T_a) \tag{7}$$

where $\partial T_a/\partial t$ is as defined in (3) and T_a is the analytic temperature based on (1). The Rayleigh damping coefficient is set at $\beta = 2 \times 10^{-5}$ s^{-1} as this was about the smallest value that still allowed the simulated temperature field to converge to a nearly steady periodic structure.

2.4 Simulation results

[Remainder of section 2]

---

2. The diabatic heating/cooling for a 70 km nominal height forecast is insignificant compared to the heating/cooling in the thermospheric, where temperature swings of 400 K are possible. Hence the forecast in Sec. 3 does not represent the problem discussed in the Introduction. Indeed, the authors note that the constant pressure height BC and the rigid lid BC yield comparable results. Are there any numerical advantages to using the new BC with a 70 km nominal lid?

We agree that the diabatic heating/cooling in the lower mesosphere is much less than that in the thermosphere and that either a constant pressure upper boundary or a rigid lid may be suitable for these applications. We have discussed this in the Introduction. Our motivation for simulating the forecast in section 3 is to document that our technique for implementing a constant pressure upper boundary in a height based vertical coordinate also works well for real data NWP applications. For this we were constrained in specifying the top height of the model domain by the availability of real data analyses. Our simulation of this real data case for both a constant pressure upper boundary and a rigid lid provides an apples-to-apples comparison of the two upper boundary conditions in the same model that has not previously been possible.

Minor comments

1. Author List: Second Author's first name is not spelled correctly.

Fixed

2. Introduction, page 1: A more recent high altitude NEPTUNE/NUMA paper has been published:

Kelly, James F., Felipe AV De Bragan¸ca Alves, Stephen D. Eckermann, Francis X. Giraldo, P. Alex Reinecke, and John T. Emmert. "A nonhydrostatic mass-conserving dynamical core for deep atmospheres of variable composition." Journal of Computa- tional Physics (2026): 114683.

Unlike Kelly et al. (2023), this more recent paper describes the dynamical core and a broader range of idealized tests, similar to Klemp and Skamarock (2021).

We have included a citation to this more recent paper in the Introduction.

3. Page 2, Line 31: The authors claim that proposed BC "maintains exact conservation of scalar mass", but no numerical evidence is shown, either in this paper or KS22. A plot or table to back up this claim would strengthen this claim.

Because we solve the prognostic equations in flux form, scalar mass is conserved to machine accuracy within the model domain. Since the upper

boundary is treated as a material surface, overall mass conservation is assured. we have verified this conservation by summing the mass in each grid volume over the domain.

4. Page 3, Line 66: "taper" should be "tapers".

Fixed

5. Page 4, Eq. (4): You have assumed a constant specific gas constant and constant gravitational acceleration in this expression. Neither of these assumptions are valid in the thermosphere: the specific gas constant increases as the atmospheric composition transitions to lighter elements, and gravity decreases according to the usual inverse square law. I'm guessing you could relax these assumptions with minimal effort. At any rate, please warn the reader of these limitations.

Although these parameters clearly vary over the depth of the thermosphere, the analytic solution for this test case requires these parameters to be constants. To maintain a similarity between the numerical simulations and the analytic solution, we also treat these parameters as constant We have added an explanation for this in the revised text in the subsection 2.3 above.

6. Page 8 line 156: "can't" should be "cannot".

Fixed

7. Page 8, lines 164-165: The instability of a global diurnal test with a rigid lid was also observed in Sec. 4.4 of Kelly et al. (2023).

Thanks for pointing this out. In discussing the problems with a rigid lid upper boundary, we added the sentence:

'The instability of a similar global diurnal heating test case with a rigid lid at 205 km was also observed by Kelly et al. (2023).'

8. Page 14, Figure 7: In panels a and c, why does the colorbar extend to 76 km when the largest height is about 72 km?

We've rescaled the color bar to the range 63-72 km