A potential vorticity diagnostics package for MPAS-Atmosphere

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Abstract

Ertel’s potential vorticity (PV) is an important quantity in atmospheric dynamics that succinctly encompasses the principles of mass, momentum, and energy conservation and is applicable to all scales of motion. In this paper, we describe the implementation of a PV diagnostics package into the atmospheric component of the Model for Prediction Across Scales (MPAS), a fully compressible nonhydrostatic global model that enables regional mesh refinement to convection-permitting resolutions and is highly suited for studies on multiscale process interactions and forecast error-growth dynamics.

The version of the PV diagnostics package emphasized herein will be included in an upcoming MPAS release and significantly improves upon an original version that was introduced in MPAS v5.0. Specifically, this revised version enables the calculation of the full Eulerian PV budget at each time step $\Delta t$ (i.e., the instantaneous budget) and the accumulation of PV tendencies throughout the model integration (i.e., the accumulated budget). Through the formulation of the discretized PV budget equation and global simulations conducted on a 15–3-km variable-resolution mesh, we demonstrate that the instantaneous PV budget closes down to machine roundoff in both single- and double-precisions. Further, we find that the PV budget computed using accumulated PV tendencies leads to a small source of residual that arises due to the inherent nonlinearity of PV, which leads to mathematical inconsistencies between the discretized equation for calculating the PV budget over any arbitrary period longer than $\Delta t$ and that which results from accumulating the PV tendencies themselves over successive time steps.
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Key Points:

• We implemented a potential vorticity (PV) diagnostics package into MPAS-Atmosphere for use in global simulations
• The Eulerian PV budget computed over a single time step is closed to machine roundoff, and the accumulated PV budget is approximately closed
• This package provides the community with a powerful tool for studying multiscale process interactions and forecast error-growth dynamics

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Plain Language Summary

Ertel’s potential vorticity (PV) is an important quantity that contains information about the temperature, density, and wind distributions in the atmosphere. This quantity has key properties that make it extremely useful for understanding weather patterns and how they evolve in model forecasts, which is highly dependent on the simulated representation of processes that we do not fully understand, such as clouds and precipitation. In this paper, we implement calculations of PV and its changes over time from various atmospheric processes into a state-of-the-art global model that enables high-resolution simulations of weather and climate. Further, we show that all modeled processes responsible for modifying PV are accounted for in our calculations. This diagnostics package thus makes it easier for the weather and climate communities to conduct research on atmospheric processes and enables the sources of forecast errors to be reliably identified and better understood.

1 Introduction

Ertel’s potential vorticity (PV; Ertel, 1942) is an important quantity in atmospheric dynamics that succinctly contains information about both the mass and momentum fields and is fully applicable to all scales of motion and flow regimes. Given its key properties of invertibility and material conservation under adiabatic, frictionless conditions (e.g., Haynes & McIntyre, 1990; Hoskins et al., 1985) and its inherent generalizability, studies have applied “PV thinking” to a vast array of atmospheric phenomena, including moist convection (e.g., Davis & Weisman, 1994; Oertel et al., 2020; Weijenborg et al., 2017; D.-L. Zhang & Kieu, 2006), extratropical cyclones (e.g., Attinger et al., 2021; Davis & Emanuel, 1991; Stoeckinga, 1996), jet–front systems (e.g., Bukenberger et al., 2023; Shapiro & Keyser, 1990), and Rossby waves (e.g., Pähl et al., 2015; Rossby, 1940; Wirth et al., 2018). Moreover, PV has proven to be an incredibly useful framework for studying multiscale process interactions—particularly those resulting from nonconservative processes such as latent heat release (e.g., Chasteen & Koch, 2022; Grams & Archambault, 2016; Harvey et al., 2020)—and their implications for forecast model error growth (e.g., Baumgart et al., 2018; Grams et al., 2018; Rodwell et al., 2013).
The considerable expansion of computing power over the past two decades has made global nonhydrostatic numerical weather prediction (NWP) feasible (e.g., J.-H. Chen et al., 2019; Magnusson et al., 2022) and has enabled global simulations to be conducted in experimental settings with convection-permitting grid spacings situated over part or all of the globe (e.g., Stevens et al., 2019; L. Zhou et al., 2019). Such high-resolution global models improve the representation of mesoscale processes compared to traditional coarser models, and—in the case of models with convection-permitting grid spacings—reduce the reliance on cumulus parameterizations for simulating tropical and midlatitude weather systems (e.g., Satoh et al., 2019). One such model is the atmospheric component of the Model for Prediction Across Scales (MPAS-Atmosphere, or just MPAS; Skamarock et al., 2012, 2014), a fully compressible nonhydrostatic global model that has seen increasing adoption by members of the weather and climate community in recent years. MPAS employs an unstructured centroidal Voronoi mesh with nominally hexagonal cells covering the globe. These global meshes can be either quasi-uniform (e.g., cell spacing of \(\sim 15 \text{ km}\) or \(\sim 3 \text{ km}\)) or variable-resolution (e.g., cell spacing ranging from \(\sim 15 – 3 \text{ km}\)), the latter of which permits seamless refinement over a region of interest without the need for lateral boundary conditions (e.g., Heinzeller et al., 2016; Schwartz, 2019). Consequently, global MPAS is highly suited for studies on multiscale process interactions and forecast error-growth dynamics, especially those related to moist processes and convective clouds (Judt, 2018, 2020).

In this paper, we describe the implementation of a PV diagnostics package into MPAS that enables the online calculation of terms in the Eulerian PV budget during model integration and thus provides the community with an invaluable tool for investigating the dynamics of atmospheric processes ranging from the mesoscale to the planetary scale in global simulations.\(^1\) Numerous past modeling studies have utilized a PV budget framework to quantify the respective changes to the PV distribution from resolved and subgrid-scale (i.e., parameterized) processes, the latter of which are predominantly responsible for PV nonconservation and are thus a notable source of model error (e.g., Wernli & Gray, 2023). These studies typically take one of two approaches: (1) calculating terms in the PV budget at each model grid point in an Eulerian framework (e.g., Cavallo & Hakim, 2009; Russell et al., 2020; Sheng et al., 2021); or (2) treating PV as a tracer and calculating terms in the PV budget along tracer paths or trajectories in a Lagrangian framework (e.g., Chagnon et al., 2013; Davis et al., 1993; Gray, 2006; Saffin et al., 2016; Spreitzer et al., 2019; Stoelinga, 1996). Because outputting process tendencies at each model time step is infeasible for most purposes, PV tendencies are often accumulated throughout the model integration and output at regular—but relatively infrequent—intervals (e.g., multihourly) in these studies. Common to both approaches is the difficulty in achieving a balanced PV budget, which results from several factors, including: PV being a diagnostic—rather than a prognostic—quantity; the inherent nonlinearity in its calculation as the product of multiple state variables and/or spatial derivatives thereof; numerical discrepancies resulting from discretization and/or interpolation procedures; and failing to properly account for all model tendencies that alter PV throughout the course of a simulation.

The discussion herein will focus primarily on a revised version of the PV diagnostics package that was first implemented into the MPAS-Atmosphere v5.0 release in early 2017. This revised version—planned for inclusion in an upcoming release later in 2024—comprises several important code modifications and additions that provide accurate calculations of all terms in the Eulerian PV budget and extend its utility to the greater weather and climate community. As we will show using MPAS simulations configured with different levels of numerical precision, the PV budget in the revised version is closed to machine roundoff (e.g., Stoer et al., 1980) when calculating the PV tendency terms over a

\(^1\) We note that—at the time of writing this paper—the PV diagnostics package is unsupported for regional (i.e., limited-area) MPAS simulations.
single time step of model integration (hereafter the “instantaneous PV budget”). Mathematically, a small—but not necessarily significant—residual is expected when accumulating the calculated PV tendencies over successive time steps (hereafter the “accumulated PV budget”). We demonstrate that this residual arises from the nonlinearity in the calculation of PV and propose a potential solution to mitigate the issue by instead accumulating and outputting the parent process tendency terms and calculating the budget offline. The remainder of this paper is organized as follows. We begin by reviewing the properties of PV both conceptually and mathematically in section 2. Section 3 describes MPAS and the implementation and functionality of the PV diagnostics package, with a summary of important differences between the original and revised versions. In section 4, global nonhydrostatic simulations employing a variable-resolution mesh are used to illustrate key differences between the two versions and demonstrate the features and performance of the revised PV diagnostics. Finally, a summary is presented in section 5.

2 Potential Vorticity

2.1 Properties and Utility of PV

Ertel’s PV \( q \) is defined mathematically as

\[
q = \frac{1}{\rho} \bar{\eta} \cdot \nabla \theta ,
\]

(1)

where \( \nabla = \left( \frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \right) \) is the three-dimensional (3D) gradient vector in Cartesian coordinates, \( \bar{\eta} = \left( \nabla \times \bar{u} \right) + f \hat{k} \) is the 3D absolute vorticity vector, \( \bar{u} \) is the 3D wind vector, \( f \) is the Coriolis parameter, \( \hat{k} \) is the vertical unit vector, \( \rho \) is the air density, and \( \theta \) is the potential temperature.\(^2\) The two primary properties of PV are its (1) Lagrangian conservation under adiabatic, frictionless conditions, and its (2) invertibility, whereby the global PV distribution can be used to diagnose all other 3D dynamic variables (e.g., temperature, pressure, wind) that satisfy a prescribed balance condition relating the mass and momentum fields (e.g., Davis, 1992; Haynes & McIntyre, 1990; Hoskins et al., 1985). The former property—namely that Lagrangian nonconservation of PV must be attributable to diabatic and/or frictional processes—is the centerpiece of the PV diagnostics package described herein, although the online calculation of the 3D PV field also enables users to more readily exploit the invertibility property.

The continuous form of the PV tendency equation is derived by taking the material time derivative of Equation 1,

\[
\frac{Dq}{Dt} = \frac{1}{\rho} \left( \bar{\eta} \cdot \nabla \frac{D\theta}{Dt} \right) + \frac{1}{\rho} \left( \nabla \theta \cdot \frac{D\bar{\eta}}{Dt} \right) - q \frac{D\rho}{Dt} ,
\]

(2)

where \( \frac{D}{Dt} = \frac{D}{Dt} + (\bar{u} \cdot \nabla) \) represents the sum of the Eulerian time derivative and advection. Expanding this equation by substituting in the tendency equations for density, absolute vorticity, and potential temperature (see Tory et al., 2012) yields cancellation of the density tendency term\(^3\) on the RHS of Equation 2 and the familiar equation for Ertel’s PV tendency,

\[
\frac{Dq}{Dt} = \frac{1}{\rho} \left( \bar{\eta} \cdot \nabla \dot{\theta} \right) + \frac{1}{\rho} \left( \ddot{\bar{\eta}} \cdot \nabla \theta \right) ,
\]

(3)

diabatic forcing frictional forcing

\(^2\)In this classical formulation, the atmosphere is assumed to be dry such that any effects from moisture and hydrometeors are neglected (e.g., Hausman et al., 2006; Schubert et al., 2001).

\(^3\)As we will show in the following subsection, this term persists in the Eulerian forward-in-time discretized PV tendency equation.
where $\dot{\theta}$ is the potential temperature tendency due to diabatic processes, and $\dot{\eta}$ is the absolute vorticity tendency due to frictional processes, which is often written as $\dot{\eta} = (\nabla \times \vec{F}) = \left( \nabla \times \vec{\dot{u}} \right)$, with $\vec{F}$ as the frictional force per unit mass that promotes a momentum tendency, $\vec{u}$. This equation states that—for an air parcel moving with the flow—PV can only be altered by (1) gradients in diabatic heating/cooling oriented along the absolute vorticity vector, and (2) frictionally induced vector changes in absolute vorticity oriented along the potential temperature gradient. In an Eulerian framework, such as at a fixed model grid point, the PV tendency equation also contains an adiabatic advection term as follows:

$$\frac{\partial q}{\partial t} = -\vec{u} \cdot \nabla q \left( \frac{1}{\rho} (\dot{\eta} \cdot \nabla \dot{\theta}) \right) + \frac{1}{\rho} (\dot{\eta} \cdot \nabla \dot{\theta}) \ . \tag{4}$$

This formulation will be the basis for the discretized PV tendency equation that is now described.

### 2.2 Discretized PV Tendency Equations

The discretized PV budget equation is formulated by computing the forward-in-time change in PV over a time step $\Delta t$ from time-level $t$:

$$\frac{q^{t+\Delta t} - q^t}{\Delta t} = \frac{1}{\Delta t} \left[ \frac{1}{\rho} (\dot{\eta} \cdot \nabla \dot{\theta})^{t+\Delta t} - \frac{1}{\rho} (\dot{\eta} \cdot \nabla \dot{\theta})^t \right]. \tag{5}$$

By expanding the terms on the RHS and rearranging (see derivation in Appendix A), we obtain

$$\frac{q^{t+\Delta t} - q^t}{\Delta t} = \frac{\dot{\eta}^t}{\rho^{t+\Delta t}} \cdot \left( \nabla \dot{\theta}^{t+\Delta t} - \nabla \dot{\theta}^t \right) + \frac{\nabla \dot{\theta}^{t+\Delta t}}{\rho^{t+\Delta t}} \cdot \left( \frac{\dot{\eta}^{t+\Delta t} - \dot{\eta}^t}{\Delta t} \right)$$

$$- \frac{q^t}{\rho^{t+\Delta t}} \left( \frac{\rho^{t+\Delta t} - \rho^t}{\Delta t} \right). \tag{6}$$

Alternatively, we could expand and rearrange the RHS of Equation 5 to obtain

$$\frac{q^{t+\Delta t} - q^t}{\Delta t} = \frac{\dot{\eta}^{t+\Delta t}}{\rho^t} \cdot \left( \nabla \dot{\theta}^{t+\Delta t} - \nabla \dot{\theta}^t \right) + \frac{\nabla \dot{\theta}^t}{\rho^t} \cdot \left( \frac{\dot{\eta}^{t+\Delta t} - \dot{\eta}^t}{\Delta t} \right)$$

$$- \frac{q^{t+\Delta t}}{\rho^t} \left( \frac{\rho^{t+\Delta t} - \rho^t}{\Delta t} \right). \tag{7}$$

Both equations are time-discretized forms of Equation 2 and are mathematically equivalent even though the time-levels at which each term is evaluated differ between the two formulations. Moreover, the differences between the time levels used in the coefficient of the discretized density tendency term on the RHS of each equation are precisely why this term persists in the discretized forms of the PV tendency equation despite its cancellation in the continuous form to yield Equation 3.

Equation 6 is the basis for the PV budget incorporated into MPAS and thus will be the sole focus of the remaining discussion. In this equation, the absolute vorticity in the first term on the RHS is evaluated at time-level $t$, whereas the potential temperature gradient in the second term on the RHS is evaluated at time-level $t + \Delta t$. The density used in the coefficients of all terms is valid at time-level $t + \Delta t$, and the third term on the RHS (i.e., the density tendency term) includes the PV valid at time-level $t$.

For simplicity, the following notation will be adopted to represent the respective tendencies in the absolute vorticity, potential temperature gradient, and density:
dependence on the values of these variables at the intermediate time step.

By inspecting this equation, we can see that this requires knowledge of the absolute vorticity, potential temperature gradient, and density at both bounding time levels, with no explicit process tendencies in MPAS is described further in section 3.

2.3 Calculation of Instantaneous Versus Accumulated Tendencies

Before delving into the MPAS-specific implementation of the PV budget, we first provide a general discussion of some potentially important nuances pertaining to the calculation of the accumulated PV budget using the discretized equation. Under the assumption that PV is a model diagnostic variable, Equations 5–7 represent the exact change (down to machine roundoff) in the model-diagnosed PV over a single time step $\Delta t$.

Equation 5 can be generalized as follows to represent the exact PV change over any period of model integration defined by $t = (t_1, t_2)$:

$$
\frac{q^{t_2} - q^{t_1}}{t_2 - t_1} = \frac{1}{t_2 - t_1} \left[ \frac{1}{\rho^{t_2}} \vec{\eta}^{t_2} \cdot \nabla \theta^{t_2} - \frac{1}{\rho^{t_1}} \vec{\eta}^{t_1} \cdot \nabla \theta^{t_1} \right],
$$

which better elucidates how the PV budget can be calculated using stored time tendencies from various processes within the numerical model. The application of this equation to the process tendencies in MPAS is described further in section 3.

Equation 6 can then be written as

$$
\frac{q^{t+\Delta t} - q^t}{\Delta t} = \frac{1}{\rho^{t+\Delta t}} (\vec{\eta}^t \cdot \nabla \theta^t) + \frac{1}{\rho^{t+\Delta t}} (\vec{\eta}^{t+\Delta t} \cdot \nabla \theta^{t+\Delta t}) - \frac{1}{\rho^{t+\Delta t}} \left( q^{t+\Delta t} \rho^t - q^t \rho^{t+\Delta t} \right),
$$

where $q^t$ and $q^{t+\Delta t}$ represent the diagnosed PV fields at each respective time. The generalized form of Equation 6 therefore follows as

$$
\frac{q^{t_2} - q^{t_1}}{t_2 - t_1} = \frac{\vec{\eta}^{t_1}}{\rho^{t_1}} \cdot \left( \frac{\nabla \theta^{t_2} - \nabla \theta^{t_1}}{t_2 - t_1} \right) + \frac{\vec{\eta}^{t_2}}{\rho^{t_2}} \cdot \left( \frac{\nabla \theta^{t_2} - \nabla \theta^{t_1}}{t_2 - t_1} \right) = \frac{\vec{\eta}^{t_1}}{\rho^{t_1}} \left( \frac{\rho^{t_2} - \rho^{t_1}}{t_2 - t_1} \right).
$$

If, for instance, we want to calculate the change in PV over two consecutive time steps (i.e., from $t = (t_1, t_1 + 2\Delta t)$, we can do so exactly by substituting those time levels into Equation 13 as

$$
\frac{q^{t_1+2\Delta t} - q^{t_1}}{2\Delta t} = \frac{\vec{\eta}^{t_1}}{\rho^{t_1+2\Delta t}} \cdot \left( \frac{\nabla \theta^{t_1+2\Delta t} - \nabla \theta^{t_1}}{2\Delta t} \right) + \frac{\vec{\eta}^{t_1+2\Delta t}}{\rho^{t_1+2\Delta t}} \cdot \left( \frac{\nabla \theta^{t_1+2\Delta t} - \nabla \theta^{t_1}}{2\Delta t} \right) - \frac{\vec{\eta}^{t_1}}{\rho^{t_1+2\Delta t}} \left( \frac{\rho^{t_1+2\Delta t} - \rho^{t_1}}{2\Delta t} \right).
$$

By inspecting this equation, we can see that this requires knowledge of the absolute vorticity, potential temperature gradient, and density at both bounding time levels, with no explicit dependence on the values of these variables at the intermediate time step $t = t_1 + \Delta t$. 

-6-
We now contrast this equation to what results from calculating the PV tendency terms at each time step and accumulating these tendencies over successive time steps of model integration—an approach that is often used in studies\textsuperscript{4} employing PV budgets (e.g., Cavallo & Hakim, 2009; Gray, 2006; Saffin et al., 2016). We can demonstrate these differences by focusing on the PV change from just the first term on the RHS of Equations 13–14 (i.e., the potential temperature gradient term) when integrating from $t = (t_1, t_1 + \Delta t)$ and $t = (t_1 + \Delta t, t_1 + 2\Delta t)$ in turn and accumulating the tendencies over these two time steps:

\begin{align}
q^{t_1+\Delta t} &= q^{t_1} + \frac{\vec{\eta}^{t_1}}{\rho^{t_1+\Delta t}} \cdot \left( \frac{\nabla \theta^{t_1+\Delta t} - \nabla \theta^{t_1}}{\Delta t} \right) \Delta t, \\
q^{t_1+2\Delta t} &= q^{t_1+\Delta t} + \frac{\vec{\eta}^{t_1+\Delta t}}{\rho^{t_1+2\Delta t}} \cdot \left( \frac{\nabla \theta^{t_1+2\Delta t} - \nabla \theta^{t_1+\Delta t}}{\Delta t} \right) \Delta t.
\end{align}

Substituting Equation 15 into 16 and rearranging yields

\begin{equation}
\frac{q^{t_1+2\Delta t} - q^{t_1}}{\Delta t} = \frac{\vec{\eta}^{t_1}}{\rho^{t_1+\Delta t}} \cdot \left( \frac{\nabla \theta^{t_1+\Delta t} - \nabla \theta^{t_1}}{\Delta t} \right) + \frac{\vec{\eta}^{t_1+\Delta t}}{\rho^{t_1+2\Delta t}} \cdot \left( \frac{\nabla \theta^{t_1+2\Delta t} - \nabla \theta^{t_1+\Delta t}}{\Delta t} \right),
\end{equation}

which differs from the expression in the first term on the RHS of Equation 14 owing to the inherent nonlinearity of PV (see Appendix B for the full equation). The consequence of this mathematical discrepancy is a source of residual in the accumulated PV budget when the PV tendencies themselves are accumulated over successive time steps. Nevertheless, this was the approach taken in the MPAS PV diagnostics package for several reasons, including the relative simplicity and broad applicability of the online calculations, reduced reliance on offline post-processing, straightforward attribution of modeled PV changes to specific processes, and lower data storage requirements given the need to output fewer variables. In principle, one could overcome this budget residual by either (1) saving $\rho$, $\nabla \theta$, $\vec{\eta}$, and $q$ to the relevant output files and computing the RHS of Equation 13 offline—an approach that would make process attribution much more difficult, if not impossible—or (2) saving those variables alongside the accumulated tendencies for each constituent variable (i.e., $\dot{\rho}$, $\nabla \dot{\theta}$, and $\vec{\dot{\eta}}$, collectively referenced hereafter as the “parent tendencies”) from all modifying model processes and then computing the budget equation offline—an approach that would require storing many more variables with greater dimensionality. We will compare the accumulated PV budget residuals arising from these different approaches using a global MPAS simulation in section 4.

3 Implementation of PV Diagnostics into MPAS

3.1 MPAS Description

We begin this discussion by providing a description of the MPAS-Atmosphere model and its relevant characteristics for calculating terms in the PV budget. As previously mentioned, the atmospheric component of MPAS employs an unstructured centroidal Voronoi mesh to discretize the fully compressible nonhydrostatic equations on the globe (Skamarock et al., 2012). MPAS uses a finite-volume numerical solver with 3D C-grid staggering of the prognostic variables and a hybrid terrain-following vertical height coordinate (Klemp, 2011). The equations are discretized in time using either a second- or third-order Runge-Kutta (RK) scheme with split-explicit time integration for the treatment of acoustic and gravity wave modes (Klemp et al., 2007; Wicker & Skamarock, 2002). In this approach, each full model time step is subdivided into multiple RK time steps wherein the forward time integration occurs, and terms related to acoustic and

\textsuperscript{4}Many of these studies explicitly recalculate the PV after every modifying model process is called and then obtain PV tendencies for each process by subtracting the prior PV field from the newly updated PV field, which would seemingly mitigate this issue (e.g., Gray, 2006).
Figure 1. Schematic showing (a) horizontal plan view of three cells with the normal ($\hat{u}$; purple vectors) and tangential horizontal wind components ($\tilde{v}$; teal vectors) on the cell edges. Cell centers are depicted by black circles, edge points are depicted by purple squares, and vertices are depicted by blue triangles. Following Ringler et al. (2010), the expression for the horizontal gradient operator applied to a variable located at the centers of $C_1$ and $C_2$ is shown in the top left, where $d_1$ is the distance between the two cell centers, and the subscript $e_1$ denotes that the gradient is valid at the point along the edge separating the two cells (highlighted in red) — i.e., a positive gradient is collocated and aligned with $\tilde{u}_1$ and the gray normal vector, $\hat{n}$. In (b), vertical depiction of two adjacent cells and their vertical cell faces with the corresponding locations of relevant variables with C-grid staggering. Here, green circles and orange squares represent the centers and lateral edge points of the vertical faces, respectively. The orange vector $-\hat{k} \times \vec{\eta}_h$ represents the shear components used in the calculation of horizontal vorticity when using $\tilde{u}$ and $w$ at their native locations.
gravity wave propagation are integrated over smaller acoustic substeps for computational efficiency. Dynamic time-step splitting is also an option to carry out scalar transport over a larger time step and reduce computational cost.

The MPAS prognostic variables include the flux-form 3D wind components comprising two orthogonal horizontal velocities and a vertical velocity oriented radially outward from the center of the earth, mixing ratios of individual water species, and moist potential temperature, which is defined as $\Theta_m = \rho_d \theta_m = \rho_d \theta [1 + (R_v/R_d) q_v]$, where $\rho_d$ is the density of dry air, $R_d$ and $R_v$ are the gas constants for dry air and water vapor, respectively, and $q_v$ is the water vapor mixing ratio. The nonhydrostatic dynamical core exactly conserves dry air mass, scalar mass, and $\Theta_m$ but does not fully conserve energy or PV, unlike in its intended formulation\(^5\) (see Skamarock et al., 2012, for more details). We note that this does not preclude the implemented Eulerian PV budget from closing so long as all model processes responsible for modifying the diagnostic PV field are properly taken into account.

Vector-invariant, flux-forms of the horizontal momentum equations are used, and the horizontal momentum component normal to each cell edge, $\tilde{u}$, is prognosed at the respective cell edge, consistent with C-grid staggering (Ringler et al., 2010; Skamarock et al., 2012). In contrast, the tangential component of the horizontal momentum, $\tilde{v}$, is a diagnostic quantity. Mass variables, including $\rho_d$ and $\Theta_m$, are prognosed at the centers of each cell,\(^6\) and the vertical momentum component $w$ is prognosed on the vertical cell faces above and below each cell center. This is depicted schematically in Fig. 1 MPAS uses a normal-vector convention to establish the directionality of vectors and fluxes on each cell edge. Using Fig. 1a as an example, the normal vector $\hat{n}$ on edge $e_1$ is defined to be directed from $C_1$ to $C_2$ such that a positive value of the edge-normal velocity $\tilde{u}_1$ accordingly represents flow from $C_1$ to $C_2$. The zonal and meridional horizontal momentum components at each cell center ($u$ and $v$, respectively) are reconstructed from $\tilde{u}$ on all its cell edges using a radial basis function. This reconstruction method can be extended to any vector quantity located on and oriented normal to the cell edges—such as the horizontal gradient of a variable situated at $C_1$ and $C_2$ (Fig. 1)—to retrieve the corresponding horizontal vector components at the cell centers and will thus be exploited herein for the PV diagnostics calculations.

### 3.2 Application of the Discretized PV Equations to MPAS

Within MPAS, the model processes that contribute to changes in the absolute vorticity, potential temperature gradient, and dry-air density are partitioned as:

\[
\tilde{\eta} = \tilde{\eta}_{\text{dyn}} + \tilde{\eta}_{\text{diff}} + \tilde{\eta}_{\text{phys}}
\]

\[
\nabla \tilde{\theta} = \nabla \tilde{\theta}_{\text{dyn}} + \nabla \tilde{\theta}_{\text{diff}} + \nabla \tilde{\theta}_{\text{phys}}
\]

\[
\dot{\rho}_d = \dot{\rho}_{\text{dyn}},
\]

where subscripts ‘dyn’, ‘diff’, and ‘phys’ represent the tendencies from the dynamics component (including advection and Rayleigh damping), explicit horizontal diffusion\(^7\), and physics parameterizations, respectively.

Substituting Equations 18–20 into Equation 11 and rearranging gives the following:

\(^5\)As described by Skamarock et al. (2012), numerical instabilities developed when the kinetic energy term was computed in a conservative manner following Ringler et al. (2010). Thus, this term was modified to mitigate this issue, rendering it nonconservative.

\(^6\)In MPAS, $\theta$ is a diagnostic that is obtained from $\rho_d$, $\Theta_m$, and $q_v$.

\(^7\)If enabled, tendencies from explicit vertical diffusion would be included in this term.
\[
\frac{q^{t+\Delta t} - q^t}{\Delta t} = \frac{1}{\rho^{t+\Delta t}} \nabla \theta^{t+\Delta t} \cdot \tilde{\eta}_{\text{dyn}} + \frac{1}{\rho^{t+\Delta t}} \tilde{q}^{t} \cdot \nabla \dot{\theta}_{\text{dyn}} - \frac{1}{\rho^{t+\Delta t}} (q^{t} \dot{\rho}_{\text{dyn}}) \\
+ \frac{1}{\rho^{t+\Delta t}} \nabla \theta^{t+\Delta t} \cdot \left( \tilde{\eta}_{\text{diff}} + \tilde{\eta}_{\text{phys}} \right) \\
+ \frac{1}{\rho^{t+\Delta t}} \tilde{q}^{t} \cdot \left( \nabla \dot{\theta}_{\text{diff}} + \nabla \dot{\theta}_{\text{phys}} \right) .
\]

Here, \( \rho \) represents the dry air density variable in MPAS but with the subscript omitted for simplicity. The dynamics PV tendency term \( \dot{q}_{\text{dynamics}} \) comprises contributions to \( \tilde{u}, \tilde{w}, \rho_d, \) and \( \theta \) (converted from \( \Theta_m \)) from advection and any Rayleigh damping that is applied near the model top to absorb reflective waves off of rigid model lids. Next, the frictional PV tendency term \( \dot{q}_{\text{friction}} \) includes horizontal and vertical momentum tendencies from explicit diffusion and horizontal momentum tendencies from physics parameterization schemes. Finally, the diabatic PV tendency term \( \dot{q}_{\text{diabatic}} \) contains the potential temperature tendency contributions from explicit diffusion and physics parameterizations schemes. With a typical model physics configuration for weather applications, the parameterizations that contribute to the horizontal momentum tendency include the planetary boundary layer (PBL), orographic gravity-wave drag, and scale-aware cumulus schemes, whereas the parameterizations that contribute to the potential temperature tendency include the PBL, shortwave and longwave radiation, scale-aware cumulus, and microphysics schemes. These are summarized in Table 1.

<table>
<thead>
<tr>
<th>Tendency Term</th>
<th>Model Processes</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \dot{q}_{\text{dynamics}} )</td>
<td>Horizontal and vertical momentum tendencies from dynamics updates, excluding explicit diffusion</td>
</tr>
<tr>
<td>( \tilde{\eta}_{\text{dyn}} )</td>
<td>Potential temperature tendency from dynamics updates, excluding explicit diffusion</td>
</tr>
<tr>
<td>( \nabla \dot{\theta}_{\text{dyn}} )</td>
<td>Density tendency from dynamics updates</td>
</tr>
<tr>
<td>( \dot{\rho}_{\text{dyn}} )</td>
<td></td>
</tr>
<tr>
<td>( \dot{q}_{\text{diabatic}} )</td>
<td>Potential temperature tendency from explicit diffusion</td>
</tr>
<tr>
<td>( \nabla \dot{\theta}_{\text{diff}} )</td>
<td>Potential temperature tendency from PBL, shortwave and longwave radiation, cumulus, and microphysics schemes</td>
</tr>
<tr>
<td>( \nabla \dot{\theta}_{\text{phys}} )</td>
<td></td>
</tr>
<tr>
<td>( \dot{q}_{\text{friction}} )</td>
<td>Horizontal momentum tendency from explicit horizontal diffusion</td>
</tr>
<tr>
<td>( \tilde{\eta}_{\text{diff}} )</td>
<td>Horizontal momentum tendency from PBL, orographic gravity-wave drag, and cumulus schemes</td>
</tr>
<tr>
<td>( \tilde{\eta}_{\text{phys}} )</td>
<td></td>
</tr>
</tbody>
</table>
Although the prognostic variable for temperature in MPAS is the mass-coupled moist potential temperature $\Theta_m$, the heating tendencies directly output from the model physics parameterizations are uncoupled dry potential temperature tendencies, which are then converted to coupled moist potential temperature tendencies for the dynamics integration. While the heating tendencies output from the model physics therefore could be used as-is in the calculation of the diabatic PV tendency terms (which—as described in section 4.2.1—was done in the original version of the PV diagnostics package), these tendencies were found to be insufficient for closing the potential temperature budget owing to the inherent coupling between $\theta$ and $q_v$ via the moist potential temperature prognostic variable. To remedy this issue, mass-decoupled $\theta_m$ tendencies are stored alongside $q_v$ tendencies from each modifying physics scheme. The corresponding $\theta$ tendencies are then derived by applying the product rule to the discretized equation for $\theta_m$, which is similar to the procedure used to derive the discretized PV tendency equation in Appendix A.

Analogously, in order to retrieve the potential temperature tendencies from the dynamical core in solving the equations of motion and calculating the explicit horizontal diffusion, the prognostic $\Theta_m$ tendencies first need to be decoupled from mass and then converted to $\theta$ tendencies by decoupling from $q_v$. During each time step of model integration, the explicit horizontal diffusion tendency is evaluated at time-level $t$ (i.e., at the beginning of the time step), so the $\Theta_m$ tendency is accordingly decoupled from mass using the density at time-level $t$. Explicit diffusion is not currently applied to the scalar fields, so no $q_v$ tendency from mixing is included during the moisture decoupling procedure. The resulting $\theta$ tendency from diffusion is then used in the calculation of $\dot{q}_{\text{diabatic}}$. To obtain the $\theta$ tendency from the dynamics integration that is used to compute $\dot{q}_{\text{dynamics}}$, we track the $q_v$ tendency from scalar advection and the decoupled $\theta_m$ tendency over one full model time step. A separate tendency component arising from the mass decoupling procedure is also calculated and included in the $\theta_m$ tendency (see Equation 2 in Wong et al. (2020) for more details). The $\theta$ tendency from dynamics is then derived from the tendencies for $\theta_m$ and $q_v$. The resulting budget for $\theta$ was evaluated and confirmed to successfully close (not shown).

For the horizontal and vertical momentum components, the prognosed variables in MPAS are the mass-coupled forms of $\tilde{u}$ and $w$, respectively. Both components—the horizontal momentum on the cell edges and the vertical velocity on the vertical cell faces—are updated by the dynamics integration and explicit horizontal diffusion calculations, and two tendency variables for each momentum component are introduced that comprise the respective tendencies from explicit horizontal diffusion and the sums of all other tendency contributions that arise during the dynamics integration (i.e., excluding diffusion). The tendencies for both momentum variables are similarly decoupled from mass and transformed from the native terrain-following vertical height coordinate into a conventional geometric height coordinate. Separate tendency components arising from the mass-decoupling procedures are likewise calculated and included in the dynamics tendencies for both $\tilde{u}$ and $w$ that are then used to compute $\dot{q}_{\text{dynamics}}$. In contrast, the tendencies from explicit horizontal diffusion are treated as contributions to $\dot{q}_{\text{friction}}$. For the physics contributions to $\dot{q}_{\text{friction}}$, two variables are introduced that contain the uncoupled $\tilde{u}$ tendencies from the cumulus scheme and the summed contributions from the PBL and orographic gravity-wave drag schemes; there are no direct updates to $w$ by the physics schemes. The budgets for $\tilde{u}$ and $w$ were each evaluated and confirmed to close (not shown), ensuring that all model processes modifying PV are properly taken into account in the PV budget calculation.

### 3.3 Calculation of Terms in the PV Budget

Calculating the PV budget entails computing PV and its tendencies, which—as Equations 1 and 18–21 indicate—requires computing 3D spatial gradients on the native unstructured mesh. We begin by describing the general procedure to calculate PV, which
can then be extended to the calculation of various tendency terms using the appropriate quantities and time levels. We note that the PV diagnostics are called at the end of each model time step (i.e., at $t + \Delta t$), and the PV variable is therefore calculated using the updated model fields.\(^8\)

The PV equation comprises the 3D absolute vorticity vector and the 3D gradient in potential temperature. In our updated version of the PV diagnostics package, the horizontal $\theta$ gradient $\nabla_h \theta$ is calculated for all adjacent cells following Equation 22 in Ringler et al. (2010), also shown in Fig. 1a, which yields gradient components that are located on and oriented normal to each cell edge. Following the radial basis function reconstruction procedure used to obtain the zonal and meridional wind components at each cell center, the edge-normal gradients are then reconstructed to the cell centers to provide zonal and meridional components of $\nabla_h \theta$ for each cell. The same procedure could be extended to $w$ on its native levels as part of the calculation for horizontal vorticity, which would then yield zonal and meridional gradients of $w$ located half a grid level above and below each cell center (orange vectors in Fig. 1b) that could then be vertically interpolated to each mass level. Instead, $w$ is first vertically interpolated to each cell center, and the horizontal gradient of $w_{\text{cell}}$ is then computed and reconstructed to the cell centers following the procedure for $\nabla_h \theta$. Vertical gradients of $\theta$, $u$, and $v$ are calculated at each level $k$ by taking one-sided differences between $k$ and its adjacent levels. These differences are then averaged to approximate the central difference at each level $k$ for all but the bottom- and top-most model levels, where the one-sided differences are used. Finally, the calculation of absolute vertical vorticity requires taking the curl of the horizontal wind field and then adding the Coriolis parameter to give $\zeta + f$, where $\zeta$ is the relative vertical vorticity. The absolute vertical vorticity at each cell vertex is precomputed within MPAS during the dynamics integration following Equation 23 in Ringler et al. (2010) and is therefore simply interpolated to each cell center. The components of $\vec{\eta}$ and $\nabla \theta$ are combined into the respective 3D vectors, and taking the dot product between these two vectors and dividing by $\rho$ completes the calculation of PV at each cell center.

Calculation of the $\dot{q}_{\text{diabatic}}$ term in Equation 21 is done using the separate potential temperature tendencies from explicit horizontal diffusion and the following physics schemes: PBL, shortwave radiation, longwave radiation, cumulus, and microphysics (Table 1). Thus, there are six diabatic PV tendency terms that are individually computed and summed together to yield a combined diabatic PV tendency term, all of which may be output by the model. The procedure to calculate these individual terms follows that for PV, except that the 3D gradient of $\theta$ over the current model time step $\Delta t$ is taken in lieu of $\theta$. Additionally, $\vec{\eta}$ is constructed using the 3D wind field from the beginning of the model time step (i.e., at $t$) following Equation 21, which requires storing these prior variables for use in the PV tendency calculations. The dot product between these two vectors is taken and then divided by the updated density (i.e., at $t + \Delta t$) to produce the six individual diabatic PV tendency terms at each cell center.

Likewise, calculation of the $\dot{q}_{\text{friction}}$ term is done in its partitioned form using the $\vec{u}$ and $w$ tendencies from explicit horizontal diffusion and the $\vec{u}$ tendency contributions from the cumulus scheme and combined PBL and orographic gravity-wave drag schemes.\(^9\) The three resulting frictional PV tendency terms are then summed together to provide the full frictional PV tendency term. The procedure to calculate the 3D absolute vorticity tendency vector generally follows that for PV, except that the momentum tendencies over $\Delta t$ are used instead of the momentum components themselves. Additionally, the vertical vorticity tendency from each process must be calculated at the cell vertices by taking the vertical curl of the $\vec{u}$ tendency and then interpolating to the cell center. This calculation follows

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\(^8\) The PV diagnostics are also called during model initialization, at which point the PV field is calculated using values from the initial conditions.

\(^9\) For the physics contributions to $\dot{q}_{\text{friction}}$, the $w$ tendency is taken as zero.
that used in MPAS for $\zeta$. Following Equation 21, the dot product between the 3D absolute vorticity tendency vector and the 3D gradient in the updated potential temperature are taken and then divided by the updated density to produce the three individual frictional PV tendency terms at each cell center.

Finally, a similar approach to those above is used to calculate the $\dot{q}_{\text{dynamics}}$ terms, which are typically the largest contributors to the PV budget and also the most challenging to properly represent when PV is a model diagnostic (Saffin et al., 2016; Whitehead et al., 2015). The momentum tendencies from dynamics were used to calculate the first $\dot{q}_{\text{dynamics}}$ term in Equation 21 following the approach for the $\dot{q}_{\text{friction}}$ calculations, while the $\theta$ tendency from dynamics was used to calculate the second term following the procedure for computing the $\dot{q}_{\text{diabatic}}$ terms. Because $\rho_d$ is only modified during the dynamics integration, the density tendency over $\Delta t$ was calculated following Equation 20, which was then multiplied by the PV field at the beginning of the time step and divided by the updated density to produce the third term. These terms were then aggregated to produce a single dynamics PV tendency variable.

### 3.4 Features and Implementation of the PV Diagnostics Package

The original version of the PV diagnostics package premiered in the MPAS-Atmosphere v5.0 release in early 2017, which was followed by an update containing several bug fixes in v7.2 in 2022. These versions—collectively referred to as the original version of the PV diagnostics package—contained calculations for the 3D PV field and instantaneous tendencies from diabatic and frictional processes. Additionally, an iterative flood-fill procedure (Foley et al., 1990; Szapiro, 2019) was implemented to identify the level of the dynamic tropopause (DT; defined as the 2-PVU isosurface, where 1 PVU = $10^{-6}$ m$^2$ K s$^{-1}$ kg$^{-1}$) from the diagnosed PV field, and several model variables—including $\theta$ and the diabatic and frictional PV tendencies—were interpolated onto the identified DT.

The emphasis of this paper is on the revised version of the PV diagnostics package that will be included in an upcoming MPAS release in 2024. This revised version builds upon the original version and contains several important modifications and extensions that are summarized below.

- **Changes to the formulation of horizontal gradients.** The original version approximated the horizontal derivatives by applying the divergence theorem to each axis, which required approximating the volume of each cell and the surface area of its faces, and in practice used a prescribed constant value for the height of each lateral cell face. The revised version follows the equations presented by Ringler et al. (2010), requires no assumptions or approximations, and can be applied to any cell-centered quantity. While these revisions required substantial changes to the structure of the PV diagnostics code, the differences in calculated fields are relatively minor overall, as we will show in section 3.2.

- **Increased frequency of calls to the PV diagnostics package.** The original version of the PV diagnostics package was configured such that the diagnostic quantities were only calculated during the time steps immediately prior to writing an output file. Changes are made in the revised version to ensure that the diagnostic calculations are called at the end of each time step, which is essential for correctly calculating the tendency terms in the discretized budget equation and accumulating the PV tendencies throughout the model integration.

- **Changes to time levels used in tendency calculations.** The time levels used in the calculation of the diabatic and frictional PV tendencies are altered in the revised version to be consistent with Equation 21. Ultimately, this only produces changes to the diabatic tendency terms as the updated variables (i.e., $\rho_d$, $\overline{\eta}$, and $\nabla \theta$ at $t + \Delta t$) were previously used in both the diabatic and frictional PV tendency calculations.
• **Modifications to potential temperature tendencies used in diabatic PV tendency calculations.** In the original version, the potential temperature tendencies output directly from the physics parameterization schemes were applied verbatim in the diabatic PV calculations. Because these tendencies are inadequate for closing the potential temperature budget due to the coupling between $\theta$ and $q_v$ via the moist potential temperature prognostic variable, the revised version uses $\theta$ tendencies that are derived by applying the product rule to the discretized equation for $\theta_m$.

• **Corrections to calculation of PV tendencies from explicit horizontal diffusion.** Important corrections are made to both the diabatic and frictional PV tendencies arising from explicit horizontal diffusion. For the diabatic tendency, the original potential temperature tendency from mixing used in the calculation was not properly decoupled from mass. The original version also used $\tilde{u}$ and $w$ tendencies in the friction term that comprised more than just the tendencies resulting from diffusion—specifically, tendencies from the pressure gradient force and buoyancy. These have been fixed in the revised version.

• **Partitioning of frictional PV tendency.** The original version of the PV diagnostics package summed the momentum tendencies from physics and diffusion to compute a single frictional PV tendency variable. In the revised version, the frictional PV tendency is partitioned like the diabatic PV tendency such that the individual contributions from the following processes are explicitly calculated and available for output: explicit horizontal diffusion, cumulus scheme, and combined PBL and orographic gravity-wave drag schemes. These are then summed to yield a net frictional PV tendency.

• **Addition of PV tendencies from dynamics.** The most significant improvement to the PV diagnostics package is the inclusion of PV tendencies from dynamics in the revised version, which were entirely absent in the original version. Consequently, any evaluation of the PV budget using the original version required calculating the PV advection tendencies offline, which is highly error-prone and destined to result in a large PV budget residual, particularly when relying on temporally coarse model output. Thus, the revised version enables a highly accurate assessment of the PV budget and reliable attribution of PV changes to specific processes operating within the model.

• **Addition of accumulated PV tendencies.** Another major upgrade to the PV diagnostics package is the incorporation of accumulated PV tendency variables that continually sum all the individual instantaneous PV tendencies throughout the model integration. The inclusion of accumulated tendencies enables users to compute the PV budget over longer time intervals much more accurately than with just the instantaneous PV tendencies output at relatively coarse time intervals. This has practical consequences given that the vast majority of prospective users will not be storing model output at each time step, thus extending the utility of the PV diagnostics package to the broader community.

• **Addition of PV tendencies from individual microphysics processes.** The revised version includes the option to partition the diabatic PV tendency from the Thompson microphysics scheme (Thompson et al., 2008)—currently the default option in the convection-permitting physics suite—and obtain the PV tendency contributions from five microphysical processes: (1) net condensation and evaporation of cloud water; (2) evaporation of rain water; (3) net deposition and sublimation of all ice hydrometeors; (4) melting of all ice hydrometeors; and (5) freezing of all ice hydrometeors. This addition can be especially valuable for investigations into how model error and upscale error growth relate to uncertainties in the parameterized representation of moist processes.
• **Improvements to DT identification and interpolation routines.** The revised diagnostics package features improved DT identification and interpolation routines that extend the original flood-fill procedure to better ensure that the identified DT demarcates regions with $|\text{sign}(f) \ast q| < 2$ PVU (characteristic of the troposphere) from regions of $|\text{sign}(f) \ast q| \geq 2$ PVU (characteristic of the stratosphere). These changes are primarily sought to mitigate the misidentification of the DT in the presence of stratospheric PV minima, which often form downstream of major mountain ranges (e.g., Menchaca & Durran, 2018) and may include values of “negative PV”—i.e., where $|\text{sign}(f) \ast q| < 0$ PVU.

• **Addition of a PV scalar variable.** Several studies utilizing a Lagrangian PV framework have employed a passive PV tracer that is advected by the model’s transport scheme and thus provides an estimate of the adiabatic contributions to the PV field in the Lagrangian PV budget calculation. While this approach has known shortcomings (e.g., Saffin et al., 2016), we have incorporated an optional PV scalar variable into the model that is initialized as the 3D PV field at $t = 0$ and transported passively throughout the model integration. Unlike for other MPAS scalars, neither the positive-definite nor monotonic constraints (Skamarock & Gassmann, 2011; Skamarock et al., 2012) are applied during the PV scalar transport. We emphasize that this is not an adequate substitution for the $\dot{q}$ dynamics terms computed in the revised package but facilitates comparisons of the two approaches.

Ultimately, the greatest improvement in the revised PV diagnostics package is the closure of the Eulerian PV budget down to machine roundoff. We demonstrate this improvement in the following section via a case-study global MPAS simulation.

4 MPAS Simulation: 20 May 2019 Case Study

4.1 Model Configuration

The simulations presented herein were conducted using both the out-of-the-box and modified versions of MPAS v7.3 to demonstrate (1) the changes in PV diagnostic fields resulting from the changes described in section 3.4 and (2) the utility and robustness of the revised diagnostics package. All simulations were initialized using initial conditions from NCEP’s Global Forecast System (GFS) 0.5° analysis valid at 0000 UTC 20 May 2019, which was in the midst of an exceptionally active period of severe convective weather over the central United States. These forecasts employed a variable-resolution 15–3-km global mesh with regional refinement over North America such that the conterminous United States (CONUS) was simulated at convection-permitting cell spacings (Fig. 2). Moreover, we used a stretched vertical grid comprising 55 levels up to a model top of 30 km, and Rayleigh damping on $w$ was applied above 22 km. The chosen physics parameterization schemes were largely consistent with the default settings of MPAS’s “convection-permitting suite” and are listed in Table 2. The lone exception was the use of the scale-aware New Tiedtke cumulus scheme (X. Zhou et al., 2017; Wang, 2022), which is designed to seamlessly allow the transition from primarily parameterized to primarily resolved deep convection as cell spacings decrease below 15 km on the variable-resolution mesh.

In general, accurately calculating the PV budget is complicated by the small magnitude of PV and its tendencies relative to the level of numerical precision typically used in numerical weather and climate models,\textsuperscript{10} the need to perform several finite-difference and arithmetic operations when computing each term, and the propensity

\textsuperscript{10}Although double floating-point precision (64 bit) has long been the standard in weather and climate models, single precision (32 bit) has seen increasing adoption in both the dynamics and physics components of numerical models in recent years (e.g., Váňa et al., 2017). However, either precision level may be problematic.
Figure 2. Approximate cell spacing (km) of the 15–3-km variable-resolution global mesh.
Table 2. Summary of the model configuration and physics parameterization schemes used in the three MPAS simulations.

<table>
<thead>
<tr>
<th>Configuration</th>
<th>Setting</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial Conditions</td>
<td>0.5° GFS Analysis</td>
<td>0000 UTC 20 May 2019</td>
</tr>
<tr>
<td>Mesh Type &amp; Cell Spacing</td>
<td>Variable resolution 15-3-km global mesh</td>
<td>—</td>
</tr>
<tr>
<td>Time Step</td>
<td>18 s</td>
<td>—</td>
</tr>
<tr>
<td>Number of Vertical Levels</td>
<td>55</td>
<td>—</td>
</tr>
<tr>
<td>Model Top</td>
<td>30 km</td>
<td>—</td>
</tr>
<tr>
<td>Base of Rayleigh Damping Layer</td>
<td>22 km</td>
<td>—</td>
</tr>
<tr>
<td>Rayleigh Damping Coefficient</td>
<td>0.2</td>
<td>—</td>
</tr>
<tr>
<td>Explicit Horizontal Diffusion</td>
<td>2D Smagorinsky</td>
<td>Smagorinsky (1963)</td>
</tr>
<tr>
<td>Cumulus</td>
<td>Scale-aware New Tiedtke</td>
<td>C. Zhang and Wang (2017); Wang (2022)</td>
</tr>
<tr>
<td>Microphysics</td>
<td>Thompson (non-aerosol aware)</td>
<td>Thompson et al. (2008)</td>
</tr>
<tr>
<td>Orographic Gravity Wave Drag</td>
<td>Yeonsei University (YSU)</td>
<td>Choi and Hong (2015)</td>
</tr>
<tr>
<td>Cloud Fraction for Radiation</td>
<td>Xu-Randall</td>
<td>Xu and Randall (1996)</td>
</tr>
<tr>
<td>Shortwave and Longwave Radiation</td>
<td>Rapid Radiative Transfer Model for global climate models (RRTMG)</td>
<td>Iacono et al. (2008)</td>
</tr>
<tr>
<td>Land Surface</td>
<td>Unified Noah</td>
<td>F. Chen and Dudhia (2001)</td>
</tr>
</tbody>
</table>
for individual tendency terms to oppose one another, which may lead to significant errors from cancellation and/or truncation (e.g., Tory et al., 2012). To address the issue of numerical precision, we compare output from three MPAS simulations: (1) the original PV diagnostics package compiled in single precision; (2) the revised PV diagnostics package compiled in single precision; and (3) the revised PV diagnostics package compiled in double precision.

All three variable-resolution simulations were integrated forward to 03:00:00 UTC 20 May to allow time for clouds and precipitation to spin up. The simulations were then restarted from 03:00:00 UTC and integrated forward for 36 s (i.e., $2\Delta t$) with output files written after each time step. The simulations were again restarted from 03:00:00 UTC and integrated forward for 2 h with output files written every 1 h. For the analyses presented herein, the instantaneous PV budget was evaluated over the single 18-s time step beginning at 03:00:18 UTC, while the accumulated PV budget was evaluated over the 1-h period beginning at 04:00:00 UTC. All plotted spatial fields were first interpolated onto a regular $0.15^\circ$ latitude-longitude grid.

4.2 Demonstration of the PV Diagnostics Package

4.2.1 Comparison: Original and Revised Versions

We begin our demonstration of the MPAS PV diagnostics package by first comparing fields calculated with the original and revised versions. The global distribution of PV multiplied by the sign of the Coriolis parameter $[\text{sign}(f)q]$ on model level 32 ($\sim9.5$ km AGL) is shown in Fig. 3. The two versions produce similar PV fields, although small differences are discernible in areas of enhanced PV values (e.g., within the PV streamer over the North Pacific Ocean) and over North America within the region of mesh refinement and finer cell spacing (Fig. 3c). These differences solely result from changes to the formulation of horizontal spatial gradients in the revised version following Ringler et al. (2010), which produces a much smoother PV field at finer cell spacing compared to the original version.

The summed diabatic and frictional PV tendencies calculated in both versions are shown in Figs. 4 and 5, respectively, for model levels 10 ($\sim1.0$ km AGL) and 32. The differences between the original and revised versions are much more substantial than for PV owing to the considerable changes made to the tendency calculations. Specifically, the potential temperature tendencies from physics applied in the original version are output directly by the parameterization schemes, which—when used to calculate the $\theta$ budget—produces a large residual owing to the coupling between $\theta$ and $q_v$ (not shown). This residual is greatest in regions where the overall $q_v$ tendency is large, and contributions to the residual are larger for the physics schemes that directly modify $q_v$ (i.e., microphysics, cumulus, and PBL). The apparent differences in the diabatic PV tendency fields (Figs. 4e-f) are largely attributable to this correction in the revised version. Moreover, the $\theta$ tendency from explicit horizontal mixing used in the original diabatic PV tendency calculation remains coupled to mass, which also leads to residuals in the $\theta$ and PV budgets. Finally, modifications to the time levels used in the tendency calculations to ensure their consistency with the discretized PV equation also contribute to the differences seen in both the diabatic and frictional PV tendencies (Figs. 4e-f and 5e-f), although this effect is likely comparatively minor given the small (18 s) time step used in the simulations evaluated herein. In contrast, the most significant differences in the frictional PV tendencies (Figs. 5e-f) arise from the explicit horizontal diffusion portion because the parent momentum tendencies applied in the original version also inadvertently comprise tendencies from other processes.

for accurately calculating the PV budget depending on whether PV is scaled to PVU (i.e., multiplied by $10^6$) or expressed in terms of SI units.
Figure 3. Ertel’s PV calculated by the (a) original and (b) revised PV diagnostics packages on model level 32 (∼9.5 km AGL) and multiplied by sign($f$) (shaded; PVU), and (c) the difference in calculated PV between the revised and original packages (shaded; PVU) at 03:00:36 UTC 20 May 2019.
Figure 4. Instantaneous diabatic PV tendency (shaded; PVU s$^{-1}$) over the 18-s time step beginning at 03:00:18 UTC calculated by the (a,b) original and (c,d) revised PV diagnostics packages on model levels 10 (∼1.0 km AGL) and 32 (∼9.5 km AGL). Differences between the revised and original diabatic tendencies (shaded; PVU s$^{-1}$) are shown in (e,f) for the two respective model levels. Both simulations were compiled using single-precision floating-point numbers.
Figure 5. As in Fig. 4, but for the instantaneous frictional PV tendency over the 18-s time step beginning at 03:00:18 UTC.
Figure 6. The identified model level of the dynamic tropopause using the flood-fill procedure—intended to be the lowest level within the continuous region of stratospheric air where $|\text{sign}(f) \ast q| \geq 2$ PVU—in the (a) original and (b) revised versions of the PV diagnostics package (shaded), and potential temperature (shaded; K) linearly interpolated to the DT isosurface identified through the flood-fill procedure in the (c) original and (d) revised versions.
The procedure to identify and interpolate variables to the dynamic tropopause was improved in the revised version, and Fig. 6 illustrates the identified model level of the DT—precisely, this is the first model level above the identified DT and is thus located within the stratosphere—and the potential temperature linearly interpolated to the DT surface based on the assumption that the DT demarcates regions with \([\text{sign}(f) \times q] < 2 \text{ PVU}\) from those with \([\text{sign}(f) \times q] \geq 2 \text{ PVU}\). Overall, the DT model levels identified in the original and revised versions are largely consistent, although large differences are readily apparent over certain regions such as the southwestern United States and northern Mexico (Figs. 6a-b). These differences coincide with regions of highly complex terrain and thus likely arise from the presence of stratospheric PV minima. These minima are generally handled better in the revised DT identification algorithm, although further improvements to this procedure are still needed. The consequences of the misidentified DT levels are evident in the plots of \(\theta\) interpolated to the DT (Figs. 6c-d). In the original version, no check was in place to verify that the identified DT is bounded by the appropriate \([\text{sign}(f) \times q]\) values although the relative differences between the two bounding values and 2 PVU are used as weights in the linear interpolation procedure. Therefore, highly erroneous values may arise in the interpolated fields. The revised approach first incorporates this check into the DT identification algorithm, including other improvements to better account for the presence of “negative PV” in both the DT identification and interpolation procedures. The resulting interpolated fields in the revised version are much smoother with fewer and smaller regions of discontinuities stemming from DT misidentification, although these regions are not eliminated entirely.

### 4.2.2 PV Budget Evaluation

We now transition our discussion to the evaluation of the modeled PV budget. Because the original version of the PV diagnostics package lacked calculations of the PV tendency from advection, the full PV budget cannot be evaluated using terms computed online. Thus, we limit our comparison between the original and revised versions to the previous section, and all forthcoming discussion on the PV budget will pertain exclusively to the revised version. We begin by discussing the instantaneous and accumulated PV budgets calculated using the online PV tendencies (hereafter the “PV tendency method”) before comparing this method with the alternative methods introduced in section 2.3.

The terms in the instantaneous PV budget from the single- and double-precision simulations evaluated globally on model level 32 are shown in Fig. 7. Specifically, Figs. 7a-b depict the absolute PV change over \(\Delta t\) (i.e., the numerator on the LHS of Equation 21), Figs. 7c-d depict the summed PV change contributions from all modifying model process tendencies (i.e., the RHS of Equation 21 multiplied by \(\Delta t\)), and Figs. 7e-f depict the PV residual arising from the difference between these two quantities. The residual fields from both the single- and double-precision simulations are qualitatively similar and characterized by general randomness, with residual magnitudes scaling with the degree of model precision. Regions with slightly greater—but same order of magnitude—residual values are found where there are larger PV tendency values and/or in regions of mesh refinement (see Supplemental Figure S1 for the budget evaluation with simulations employing a quasi-uniform 15-km global mesh, which do not promote the region of enhanced residual magnitudes over North America associated with finer cell spacing). In either precision, the PV budget residual field on level 32 is consistent with calculation errors stemming from machine roundoff, with maximum (mean) residual magnitudes of \(9.10 \times 10^{-4}\) PVU (\(2.13 \times 10^{-5}\) PVU) and \(1.91 \times 10^{-12}\) PVU (\(4.31 \times 10^{-14}\) PVU) in the single- and double-precision simulations, respectively (Table 3).

To ensure that this finding is robust across all model levels, the maximum and mean absolute PV budget residual values evaluated globally as a function of height are shown in Fig. 8. Overall, the shapes of the maximum and mean residual profiles are consistent between the single- and double-precision simulations, while the residual magnitudes in each...
Figure 7. Evaluation of the instantaneous PV budget over the 18-s time step beginning at 03:00:18 UTC on model level 32 (~9.5 km AGL) with the revised diagnostics package for (left) single-precision and (right) double-precision compilations: (a,b) the total PV change over $\Delta t$ (shaded; PVU), (c,d) the summed instantaneous tendency contributions from all processes multiplied by $\Delta t$ (shaded; PVU), and (e,f) the budget residual (shaded; PVU) obtained by subtracting (c) and (d) from (a) and (b), respectively. Note that the PV budget residual values between the single- and double-precision configurations differ by ~8–9 orders of magnitude.
Table 3. Summary of the global maximum and mean absolute values of select terms in the revised PV budget calculated using fields at model level 32 on the native MPAS global mesh. For the PV budget residual terms, the “PV tendency” method uses the PV tendencies calculated from all modifying model process tendencies following Equation 21 for the instantaneous budget and the summed PV tendencies over all time steps during the 1-h period of interest for the accumulated budget. The “parent tendency” method applies the instantaneous and accumulated parent tendencies (e.g., the absolute vorticity tendency) to Equation 13, whereas the “exact” method considers only the fields (e.g., absolute vorticity) at each bounding time following Equation 13.

<table>
<thead>
<tr>
<th></th>
<th>Maximum Absolute Value [PVU]</th>
<th>Mean Absolute Value [PVU]</th>
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</thead>
<tbody>
<tr>
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<td></td>
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<td>∆t : 03:00:18–03:00:36Z</td>
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<tr>
<td>Single Precision</td>
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<tr>
<td>PV Change</td>
<td>$7.69 \times 10^0$</td>
<td>$3.06 \times 10^{-3}$</td>
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<tr>
<td>Budget Residual: PV Tendency</td>
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<td>$2.13 \times 10^{-5}$</td>
</tr>
<tr>
<td>Budget Residual: Parent Tendency</td>
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<td>$2.13 \times 10^{-5}$</td>
</tr>
<tr>
<td>Budget Residual: Exact</td>
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<td>PV Change</td>
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</tr>
<tr>
<td>Budget Residual: PV Tendency</td>
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<td>Budget Residual: Parent Tendency</td>
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</tr>
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<td><strong>Accumulated PV Budget</strong></td>
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<tr>
<td>Single Precision</td>
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<td></td>
</tr>
<tr>
<td>PV Change</td>
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<td>$2.56 \times 10^{-1}$</td>
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<tr>
<td>Budget Residual: PV Tendency</td>
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<td>$1.57 \times 10^{-4}$</td>
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<td>Budget Residual: Exact</td>
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<td>$1.75 \times 10^{-16}$</td>
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<tr>
<td>Residual Difference: PV – Parent</td>
<td>$8.29 \times 10^{-12}$</td>
<td>$5.55 \times 10^{-14}$</td>
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</table>
Figure 8. Vertical profiles of the (a,c) maximum and (b,d) mean absolute instantaneous PV budget residual values (PVU) evaluated over the full native MPAS global mesh for the 18-s time step beginning at 03:00:18 UTC. The single- and double-precision simulations are shown on the top and bottom, respectively.
profile scale according to the level of precision used. Slightly enhanced budget residuals are evident in the lowest 1–2 model levels and especially in the upper 5–6 model levels, where maximum and mean values near the model top are approximately an order of magnitude larger than those within the rest of the model column. However, even at the model top, the maximum absolute PV budget residuals remain on the order of $10^{-2}$ and $10^{-11}$ PVU for the single- and double-precision simulations, respectively, which is much less than the maximum absolute PV change at this level ($2.28 \times 10^2$ PVU; not shown). Therefore, we conclude that the instantaneous PV budget in the revised version is closed down to machine roundoff.

Figure 9. As in Fig. 7, but for the accumulated PV budget over the 1-h period from 04:00:00–05:00:00 UTC.

The accumulated PV budget was calculated by accumulating the PV tendencies over all 200 time steps during the 1-h period beginning at 04:00:00 UTC. The PV change over this 1-h period, summed PV change contributions from all modifying model process tendencies accumulated over 1 h, and PV residual arising from the inequality of these two quantities are shown in Fig. 9 for model level 32. Compared to the instantaneous PV change, the PV change over 1 h is approximately 2 orders of magnitude larger on average, which is consistent with the much longer period over which modifying model process tendencies were acting on the PV field (Table 3). Similar to the instantaneous PV budget residual, the accumulated budget residual fields were qualitatively similar between the single- and double-
precision simulations and had overall magnitudes that scaled with the level of precision (Figs. 9e-f). Moreover, the residual fields in both simulations exhibited a high degree of randomness, with relatively larger residual magnitudes located over the region of mesh refinement. Calculation of the global maximum and mean residual magnitudes on level 32 indicates that the accumulated budget yielded values of approximately 1 order of magnitude larger than the corresponding values from the instantaneous budget for both simulations (Table 3). Thus, the accumulated budget calculated by accumulating the PV tendencies over successive time steps appears to be highly reliable for the 1-h period evaluated.

![Figure 10](image-url). Instantaneous (left) and accumulated (right) PV budget residuals (shaded; PVU) on model level 32 calculated using the (a,b) PV tendency method, (c,d) parent tendency method, and (e,f) exact method from the double-precision simulation.

In section 2.3, we described how accumulating the PV tendencies over two consecutive time steps led to mathematical inconsistencies with the discretized equation used to calculate the exact PV change occurring over $2\Delta t$ (i.e., Equation 14). We explore this further by comparing both the instantaneous and 1-h accumulated PV budget residuals attained by (1) calculating the PV tendency terms for each process and summing those together following Equation 21 (and accumulating these over successive time steps for the accumulated budget); (2) calculating the parent tendency terms for each model process (and accumulating these over successive time steps for the accumulated budget) and then computing the PV tendencies offline using the appropriate time levels of the
coefficients in Equation 13 (hereafter the “parent tendency method”); and (3) calculating the exact PV change using $\mathbf{\eta}$, $\nabla \theta$, and $\rho$ at the bounding time levels following Equation 13 (hereafter the “exact method”). For the instantaneous PV budget, all three methods are mathematically equivalent and should accordingly produce equivalent results, notwithstanding differences arising from numerical errors and the propagation and accumulation thereof. For the accumulated PV budget, the parent tendency and exact methods are mathematically equivalent, but the PV tendency method differs from both. The resulting difference is expected to be greatest where the parent tendencies are large such that the coefficients in Equation B3 differ between successive time steps. Moreover, the difference is generally expected to be greater in simulations employing longer model time steps.

Table 4. Spearman’s rank correlation coefficient values for pairs of quantities related to the PV budget residuals on model level 32 from the three methods: \texttt{resid}_{PV}, \texttt{resid}_{parent}, \texttt{resid}_{exact}.

<table>
<thead>
<tr>
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<th>Single Precision</th>
<th>Double Precision</th>
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<td><strong>Instantaneous PV Budget</strong></td>
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<td></td>
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<tr>
<td>$\Delta t$: 03:00:18–03:00:36Z</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\texttt{resid}<em>{PV}$ &amp; $\texttt{resid}</em>{parent}$</td>
<td>&gt; 0.999</td>
<td>&gt; 0.999</td>
</tr>
<tr>
<td>$</td>
<td>\texttt{resid}_{PV}</td>
<td>$ &amp; $</td>
</tr>
<tr>
<td>$\texttt{resid}_{exact}$ &amp; $</td>
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<td>0.826</td>
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<tr>
<td><strong>Accumulated PV Budget</strong></td>
<td></td>
<td></td>
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<td>$\Delta t$: 04:00:00–05:00:00Z</td>
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<tr>
<td>$\texttt{resid}<em>{PV}$ &amp; $\texttt{resid}</em>{parent}$</td>
<td>0.963</td>
<td>0.963</td>
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<tr>
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<td>\texttt{PV}</td>
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<tr>
<td>$\texttt{resid}_{exact}$ &amp; $</td>
<td>\texttt{resid}<em>{PV} - \texttt{resid}</em>{parent}</td>
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</table>

The residuals arising from these three methods are summarized in Table 3 for level 32. Using the exact method, the global maximum and mean absolute budget residuals from each respective simulation are of comparable magnitudes for both the instantaneous and 1-h accumulated budgets, and their vertical profiles (not shown) have nearly the same shape as those in Fig. 8, with higher residual magnitudes occurring at the top few model levels. However, the residuals from the exact method—which result from machine roundoff—are approximately 2 orders of magnitude smaller than those from the PV and parent tendency methods for the instantaneous budget and approximately 3 orders of magnitude smaller for the accumulated budget. Further, the parent tendency method produces global maximum and mean absolute residual values that are comparable and of the same order of magnitude as the residuals from the PV tendency method for both the instantaneous and accumulated budgets, with the residuals in the accumulated budget being approximately 1 order of magnitude larger for both methods and model precisions. Despite these apparent similarities, the global maximum and mean absolute difference between the PV and parent tendency budget residuals indicates that their accumulated
budget residual fields are more dissimilar than those from the instantaneous budget (differences approximately 3 orders of magnitude larger), which is expected given the mathematical inconsistencies between the two methods for periods longer than $1\Delta t$. Therefore, using the PV tendency method to calculate the accumulated budget does seem to introduce a small source of error associated with the aforementioned mathematical inconsistencies, but—at least for relatively short accumulation periods (i.e., 1 h) and small model time steps (i.e., 18 s)—the residual stemming from this approach remains small compared to simulated PV change in regions where the PV change is nonzero. Further, both the residual magnitude and its difference from the residual produced by the parent tendency method scale according to the degree of precision used in the simulations, suggesting that it remains dominated by rounding errors.

The large differences in residuals from the exact method compared to the two tendency methods provoke questions given that the three are mathematically equivalent for the instantaneous budget and that the parent and exact methods remain mathematically equivalent for the accumulated budget. Spatial plots of the residual fields in Fig. 10 further illustrate the large differences produced by the exact and tendency methods in both the instantaneous and accumulated budgets, whereas a high degree of correspondence is evident between the residuals produced by the PV and parent tendency methods for both budgets. Spearman’s rank correlation coefficient $r$ was computed between the different residual fields and are summarized in Table 4. For the instantaneous PV budget, $r > 0.999$ for the PV and parent tendency residuals and their magnitudes, substantiating the high degree of spatial correspondence between the two fields. For the accumulated budget, $r$ drops to 0.963 and 0.940 for the residuals and residual magnitudes, respectively, further indicating that larger differences exist between the PV and parent tendency residual fields despite the overall correspondence. In contrast, a clear relationship is not apparent between the residuals from the exact and tendency methods for either the instantaneous or accumulated budgets, while a relatively high degree of spatial correspondence exists between the residual magnitudes calculated from the exact method and the magnitudes of PV used in the budget calculation (cf. Figs. 3f and 10e-f), which is substantiated by $r \approx 0.729 - 0.826$. This finding supports that the larger residual magnitudes stemming from rounding errors at least partially result from larger quantities being differenced within the calculations.

The most likely explanation for these peculiarities is the greater number of floating-point operations involved when calculating the PV budget using (typically small) individual process tendency variables compared to calculating the budget using the exact difference in quantities, which results in a greater reduction in precision owing to the increased propagation and accumulation of numerical errors throughout the budget calculations. This loss in precision is expected to be similar in both the parent and PV tendency budget calculations given that both contain several iterations of the gradient calculation and reconstruction routines, although the parent tendency method involves fewer iterations of the dot product. Thus, this loss in apparent precision from rounding errors seems to be an inevitable consequence of constructing the PV tendencies in such a manner that enables PV changes to be attributed to highly specific model processes and occurs regardless of whether the PV or parent tendencies are used to compute the PV budget. In light of this, the degree to which the PV tendency method produces a less accurate depiction of the accumulated PV budget than the parent tendency method remains unclear, as both methods appear to yield budgets with residuals of the same order of magnitude for the simulations analyzed herein. Given that the parent tendency method of evaluating the accumulated PV budget is mathematically correct, we conclude that the accumulated PV budget calculated with the parent tendency method is closed down to machine roundoff, while the accumulated budget calculated with the PV tendency method is approximately closed for simulations with short model time steps.
Microphysics Process Tendencies

We conclude this discussion by highlighting the added functionality of partitioning the diabatic PV tendency from the Thompson microphysics scheme to obtain the PV tendencies from individual microphysical processes. Figure 11 depicts vertical profiles of the instantaneous PV tendency from these microphysical components and the cumulus parameterization scheme at two different locations where precipitation processes were active.

In Fig. 11a, the vertical profiles were obtained from a point within the region of refined mesh spacing over the CONUS where convection was explicitly resolved. At this location, large positive PV tendencies are evident within the middle troposphere (∼2.5–5 km AGL) that primarily arise due to the net condensation/evaporation of cloud water. Smaller microphysics PV tendency contributions from rain evaporation, net deposition/sublimation of cloud ice, and freezing are also evident within this layer. Although the cell spacing at this location is ∼3 km, the scale-aware cumulus scheme is active in the middle troposphere and contributes to the net PV tendency from latent heating processes. In the lower troposphere, the PV tendency from latent heating is generally negative and is dominated by the net condensation/evaporation of cloud water above ∼1.5 km and the evaporation of rain water below ∼500 m.

In contrast, Fig. 11b depicts vertical profiles from a point in northeastern China where the cell spacing was ∼14 km and the representation of convection was thus primarily reliant on the cumulus parameterization. At this location, the diabatic PV tendencies from latent heating processes were confined to the ∼1.5–3 km layer and only comprised appreciable microphysical contributions from the net condensation/evaporation of cloud water and net deposition/sublimation of cloud ice. These PV tendencies were mostly positive above ∼2 km and offset by a large negative PV tendency contribution from the cumulus scheme. Below ∼2 km, the microphysics and cumulus PV tendencies both switched signs and continued to
largely offset each other, yielding only a small net positive PV tendency from latent heating
that resulted from the larger positive contribution from the cumulus scheme.

5 Summary

In this paper, we provided a formulation for the discretized Eulerian potential vorticity
budget and described the implementation of a diagnostics package into MPAS-Atmosphere
that comprises calculations for the terms in the PV budget and enables the attribution of
PV changes to various resolved and subgrid-scale model processes. Two versions of the
PV diagnostics package were compared: (1) the original version, which was introduced in
the v5.0 release in 2017, and (2) the revised version, which will be incorporated into an
upcoming release in 2024.

The revised version of the PV diagnostics package was the primary emphasis of this
paper and incorporates several important modifications and additions that considerably
enhance its utility to the broader weather and climate community. These include making
corrections and changes to the parent tendency variables used in the PV tendency
calculations, partitioning the frictional PV tendency into components from specific
processes (e.g., momentum tendencies from parameterized convection), calculating PV
tendencies from the dynamics integration, accumulating the instantaneous PV tendencies
throughout the model integration, and computing PV tendencies from specific
phase-changing processes in the Thompson microphysics scheme. These modifications
enable the full PV budget to be evaluated using PV tendency terms calculated online. The
overarching benefit of this effort is the closure of the instantaneous Eulerian PV budget
down to machine roundoff and the near closure of the accumulated PV budget using the
PV tendencies computed online during each time step and amassed throughout the model
integration. Thus, the revised PV diagnostics package can be an invaluable tool for
community use in process-based modeling investigations using MPAS.

To illustrate the differences between the two versions and demonstrate the features
of the revised package, global simulations were conducted on a variable-resolution 15–3-
km mesh using both the out-of-the-box and modified versions of the MPAS v7.3 code.
Comparing the diagnostic PV field from the original and revised versions showed only small
differences that were generally most pronounced in regions of refined mesh spacing over
the North America. In contrast, large differences were evident in both the diabatic and
frictional PV tendency fields owing to the substantial changes and corrections made to their
formulations in the revised version. Appreciable differences between the two versions were
also apparent in the identified dynamic tropopause level and DT potential temperature fields
near regions of mountainous terrain, and the improved procedure in the revised version—
while imperfect—will facilitate easier identification and tracking of dynamically important
perturbations on the DT. However, future efforts should be made to further refine this
procedure.

In our demonstration of the revised package, we compared simulations compiled with
single-precision and double-precision floating-point numbers. Using PV tendencies
computed online, both simulations successfully produced a closed PV budget (down to
machine roundoff) for a single time step, while—mathematically—a small source of
residual arises when accumulating the PV tendencies over multiple time steps. The
residual from the 1-h accumulated PV budget calculated using the accumulated PV
tendencies was compared to that which instead resulted from accumulating the parent
tendencies (e.g., 3D absolute vorticity tendency) and calculating the budget following the
discretized equation (Equation 13). Compared to the instantaneous budget wherein the
PV and parent tendency methods are mathematically equivalent, the residuals from the
two methods differed more substantially for the accumulated budget but overall still
exhibited a high degree of correspondence. Moreover, the accumulated budget residuals
produced by both methods scaled according to the level of numerical precision used. Given
that the accumulated PV budget calculated with the parent tendency method is exactly
closed down to machine roundoff, the residual similarities between the two methods
provides confidence that the PV tendency method produces an accumulated PV budget
that is approximately closed for simulations with short model time steps. Additional work
is needed to better understand how these differences manifest in simulations with different
meshes and model time steps and to quantify the impact they may have on accurately
evaluating the accumulated PV budget over various time intervals.

As expected, the relative significance of the PV budget residual arising from
rounding errors differed between the single- and double-precision simulations. Specifically,
the mean absolute instantaneous budget residual in the single-precision simulation was 2
orders of magnitude smaller than the mean absolute PV change over the 18-s time step
evaluated, whereas the residual in the double-precision simulation was 11 orders of
magnitude smaller. For both simulations, the absolute residual values for the 1-h
accumulated PV budget are approximately 1 order of magnitude larger than the
corresponding instantaneous budget residuals (regardless of whether the PV or parent
tendency method was used), although the mean absolute PV change over this period is 2
orders of magnitude larger. While the PV budget residual in either scenario would not
hinder efforts to accurately quantify the PV change contributions from physical processes
acting within the model, any potential uncertainty stemming from rounding errors is much
more likely to become an issue in the single-precision configuration due to the typically
small magnitudes of PV tendencies. Accordingly, using a double-precision compilation
may be preferred for investigators who wish to minimize this potential uncertainty.

The PV diagnostics package presented herein relates to the so-called “dry PV”, which
employs potential temperature as the relevant thermodynamic variable. However, other
atmospheric PV quantities have been described in the literature that use thermodynamic
variables that also encompass the effects of moisture, such as virtual potential temperature
θ_v, moist potential temperature θ_m, and equivalent potential temperature θ_e. As these
“moist PV” quantities come in different flavors, they accordingly all have different properties,
conservation laws, and inevitability principles (e.g., Cao & Cho, 1995; Kooloth et al., 2024;
Marquet, 2014; Peng et al., 2013; Schubert et al., 2001). While extending the PV diagnostics
package to some of these quantities is well beyond the scope of our efforts, the framework we
have provided could be useful to those who may wish to incorporate a moist PV diagnostics
package into MPAS-Atmosphere in the future, such as one utilizing the decoupled prognostic
thermodynamic variable, θ_m (Peng et al., 2013).

Appendix A Derivation of Discretized PV Budget Equation

Equation 5 can be expanded into Equations 6 and 7 by deriving the product and
quotient rules for the forward finite difference of a quantity with the form \( \frac{AB}{C} \), where \( A = A(t) \), \( B = B(t) \), and \( C = C(t) \) (e.g., Catone, 2019). This is shown by discretizing \( \frac{AB}{C} \) as

\[
\frac{\partial}{\partial t} \left( \frac{AB}{C} \right) \approx \frac{(\frac{AB}{C})^{t+\Delta t} - (\frac{AB}{C})^t}{\Delta t} = \frac{1}{\Delta t} \left( \frac{A^{t+\Delta t}B^{t+\Delta t}}{C^{t+\Delta t}} - \frac{A^tB^t}{C^t} \right). \tag{A1}
\]

We then rearrange the terms in parentheses by establishing a common denominator of
\( C^{t+\Delta t} \), adding and subtracting \( A^tB^{t+\Delta t}C^t \) from the numerator (alternatively,
\( A^{t+\Delta t}B^tC^{t+\Delta t} \), \( A^{t+\Delta t}B^tC^{t+\Delta t} \), or \( A^tB^{t+\Delta t}C^{t+\Delta t} \) could have been used), and grouping
like terms to give

\[
\left( \frac{A^{t+\Delta t}B^{t+\Delta t}}{C^{t+\Delta t}} - \frac{A^tB^t}{C^t} \right) = \frac{B^{t+\Delta t}C^{t}(A^{t+\Delta t} - A^t) + A^t(B^{t+\Delta t}C^t - B^tC^{t+\Delta t})}{C^tC^{t+\Delta t}}. \tag{A2}
\]
We now rearrange the second term in the numerator of Equation A2 in a similar manner as above by adding and subtracting $B^t C^t$ (alternatively, $B^{t+\Delta t} C^{t+\Delta t}$ could have been used). Putting it all together, the parentheses in Equation A1 becomes

$$
\left( \frac{A^{t+\Delta t} B^{t+\Delta t}}{C^{t+\Delta t}} - \frac{A^t B^t}{C^t} \right) = \frac{B^{t+\Delta t}}{C^{t+\Delta t}} \left( A^{t+\Delta t} - A^t \right) + \frac{A^t}{C^{t+\Delta t}} \left( B^{t+\Delta t} - B^t \right) - \frac{A^t B^t}{C^t C^{t+\Delta t}} \left( C^{t+\Delta t} - C^t \right).
$$

(A3)

Now we can apply this procedure to the equation for $q_t$, where $A = \eta(t)$, $B = \nabla \theta(t)$, $C = \rho(t)$, and the multiplication between vectors takes the form of a dot product. Substituting these relations into Equations A1 and A3 and rearranging, the discretized PV equation becomes

$$
\frac{\partial}{\partial t} \left( \frac{\vec{\eta} \cdot \nabla \theta}{\rho} \right) \approx \frac{\vec{\eta}^t}{\rho^{t+\Delta t}} \cdot \left( \frac{\nabla \theta^{t+\Delta t} - \nabla \theta^t}{\Delta t} \right) + \frac{\nabla \theta^{t+\Delta t}}{\rho^{t+\Delta t}} \cdot \left( \frac{\vec{\eta}^{t+\Delta t} - \vec{\eta}^t}{\Delta t} \right) - \frac{\vec{\eta}^t}{\rho^{t+\Delta t}} \left( \frac{\rho^{t+\Delta t} - \rho^t}{\Delta t} \right).
$$

(A4)

This same procedure could be used to obtain Equation 7 by adding and subtracting $A^{t+\Delta t} B^t C^{t+\Delta t}$ and $B^{t+\Delta t} C^{t+\Delta t}$ in turn. Although multiple arrangements of the discretized PV equation are possible, these equations are all mathematically equivalent and should therefore produce equivalent results.

**Appendix B  PV Budget Equation With Accumulated PV Tendencies**

Equation 17 was derived from the first term on the RHS of Equations 13–14 by integrating from $t = (t_1, t_1 + \Delta t)$ and $t = (t_1 + \Delta t, t_1 + 2\Delta t)$ in turn and accumulating the tendencies over these two successive time steps of model integration. Here we follow the same procedure to derive the corresponding equation using all three terms on the RHS of Equations 13–14:

$$
q_{t_1+\Delta t} = q_{t_1} + \left[ \frac{\vec{\eta}^t_{t_1}}{\rho_{t_1+\Delta t}} \cdot \left( \frac{\nabla \theta_{t_1+\Delta t} - \nabla \theta_{t_1}}{\Delta t} \right) \right] \Delta t
$$

(B1)

$$
q_{t_1+2\Delta t} = q_{t_1+\Delta t} + \left[ \frac{\vec{\eta}^t_{t_1+\Delta t}}{\rho_{t_1+2\Delta t}} \cdot \left( \frac{\nabla \theta_{t_1+2\Delta t} - \nabla \theta_{t_1+\Delta t}}{\Delta t} \right) \right] \Delta t.
$$

(B2)

Substituting Equation B2 into B1 and rearranging yields
\[
\frac{q^{t_1+2\Delta t} - q^{t_1}}{\Delta t} = \frac{\vec{\eta}^{t_1}}{\rho^{t_1+\Delta t}} \cdot \left( \frac{\nabla \theta^{t_1+\Delta t} - \nabla \theta^{t_1}}{\Delta t} \right) + \frac{\vec{\eta}^{t_1+\Delta t}}{\rho^{t_1+2\Delta t}} \cdot \left( \frac{\nabla \theta^{t_1+2\Delta t} - \nabla \theta^{t_1+\Delta t}}{\Delta t} \right) \\
+ \frac{\nabla \theta^{t_1+\Delta t}}{\rho^{t_1+\Delta t}} \cdot \left( \frac{\vec{\eta}^{t_1+\Delta t} - \vec{\eta}^{t_1}}{\Delta t} \right) + \frac{\nabla \theta^{t_1+2\Delta t}}{\rho^{t_1+2\Delta t}} \cdot \left( \frac{\vec{\eta}^{t_1+2\Delta t} - \vec{\eta}^{t_1+\Delta t}}{\Delta t} \right) \\
- \frac{q^{t_1}}{\rho^{t_1+\Delta t}} \left( \frac{\rho^{t_1+\Delta t} - \rho^{t_1}}{\Delta t} \right) - \frac{q^{t_1+\Delta t}}{\rho^{t_1+2\Delta t}} \left( \frac{\rho^{t_1+2\Delta t} - \rho^{t_1+\Delta t}}{\Delta t} \right), \quad (B3)
\]

which can be compared to Equation 14.

**Open Research Section**

The original and modified versions of the MPAS v7.3 code, the initial condition and namelist files used to produce the 15–3-km MPAS simulations, and the regridded output files can be accessed at https://gdex.ucar.edu/dataset/470.html (Chasteen et al., 2024). Python code used to produce the analyses herein is available at https://zenodo.org/doi/10.5281/zenodo.11206271 (Chasteen, 2024b). A GitHub repository containing the modified MPAS v7.3 code with the revised version of the PV diagnostics package is archived at https://zenodo.org/doi/10.5281/zenodo.11206291 (Chasteen, 2024a). All standard MPAS releases are openly accessible at https://github.com/MPAS-Dev/MPAS-Model/releases. The GFS analysis used to initialize the MPAS simulations was obtained from https://www.ncei.noaa.gov/products/weather-climate-models/global-forecast. Regridding was done using the convert_mpas utility (https://github.com/mgduda/convert_mpas).

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**References**


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Supporting Information for “A potential vorticity diagnostics package for MPAS-Atmosphere”

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Contents of this file

1. Figure S1

Introduction

Two additional simulations employing a quasi-uniform 15-km global mesh were conducted with the revised PV diagnostics package in single and double precision to enable the evaluation of the instantaneous PV budget for the sake of comparison with the budget from the 15–3-km variable-resolution simulations. All other configuration options are equivalent to those from the variable-resolution simulations, including the model time step. The 15-km global simulations were similarly integrated forward to 03:00:00 UTC 20 May to allow time for clouds and precipitation to spin up and then restarted from 03:00:00 UTC and integrated forward for 36 s (i.e., $2\Delta t$) with output files written after each time step. The instantaneous PV budget evaluated over the single 18-s time step beginning at 03:00:18 UTC from the single- and double-precision 15-km simulations is shown in Figure S1.
Figure S1. For a 15-km quasi-uniform global mesh, evaluation of the instantaneous PV budget over the 18-s time step beginning at 03:00:18 UTC on model level 32 (∼9.5 km AGL) with the revised diagnostics package for (left) single-precision and (right) double-precision compilations: (a,b) the total PV change over $\Delta t$ (shaded; PVU), (c,d) the summed instantaneous tendency contributions from all processes multiplied by $\Delta t$ (shaded; PVU), and (e,f) the budget residual (shaded; PVU) obtained by subtracting (c) and (d) from (a) and (b), respectively. Note that the PV budget residual values between the single- and double-precision configurations differ by ∼8–9 orders of magnitude.