Efforts to Balance the Potential Vorticity Budget in MPAS

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Background

- Ertel's potential vorticity [PV] is an important quantity in atmospheric dynamics that succinctly encompasses the principles of mass, momentum, and energy conservation
  - *Materially conserved for adiabatic, frictionless motions*
  - *Applicable to all scales of motion*

Ertel's Potential Vorticity [q]

$$q = \frac{(\vec{\omega} + f\hat{k}) \cdot \nabla\theta}{\rho} = \frac{1}{\rho}\left[\xi\frac{\partial\theta}{\partial x} + \eta\frac{\partial\theta}{\partial y} + (\zeta + f)\frac{\partial\theta}{\partial z}\right] \quad \text{[Eq. 1]}$$

Horizontal vorticity & horizontal potential temperature gradient; Vertical vorticity & vertical potential temperature gradient

- Modifications to the PV distribution by nonconservative processes can be used to diagnose model errors and investigate the dynamical pathways for upscale error growth—particularly those stemming from the representation of moist processes and convection
  - *In numerical models, these nonconservative processes predominantly arise from the parameterization of subgrid-scale physical processes [e.g., microphysics]*
  - *However, PV nonconservation can also arise from the model's dynamical core [e.g., due to numerical diffusion]*

Potential Vorticity Tendency

$$\frac{\partial q}{\partial t} = -\vec{u} \cdot \nabla q + \frac{1}{\rho}\left[(\vec{\omega} + f\hat{k}) \cdot \nabla\dot{\theta}\right] + \frac{1}{\rho}\left[\nabla \times \vec{F} \cdot \nabla\theta\right] \quad \text{[Eq. 2]}$$

PV Advection; Diabatic Forcing [related to potential temperature tendency]; Frictional Forcing [related to wind tendency]

PV Diagnostics in MPAS

- A PV diagnostics package was first implemented into MPAS-Atmosphere v5.0 and was updated in v7.2 with a number of bug fixes
  - *MPAS v7.3 was used for the global simulations described here which were conducted on a 15-km mesh*
- This diagnostics package contains calculations for PV and PV tendencies from physical and dynamical processes, including:
  - Diabatic tendencies: *longwave radiation, shortwave radiation, planetary boundary layer [PBL], cumulus, and microphysics parameterizations; explicit horizontal mixing*
  - Frictional tendencies: *PBL, gravity wave drag, and cumulus parameterizations; explicit horizontal mixing*
- Additionally, several quantities, including the diabatic and frictional PV tendencies, are interpolated onto the dynamic tropopause, which is defined as the 2-PVU surface

Some Issues…

- The PV diagnostics are called at each output interval rather than at each time step
- Tendencies are only instantaneous [i.e., valid over a single time step] rather than accumulated over successive time steps
- This diagnostics package does not include any calculations of PV advection—a major contributor to the PV tendency in the budget equation
  - *Requires that advection is computed offline, likely using simple centered differences on the regridded PV field—highly error prone even when fields are output at every time step*

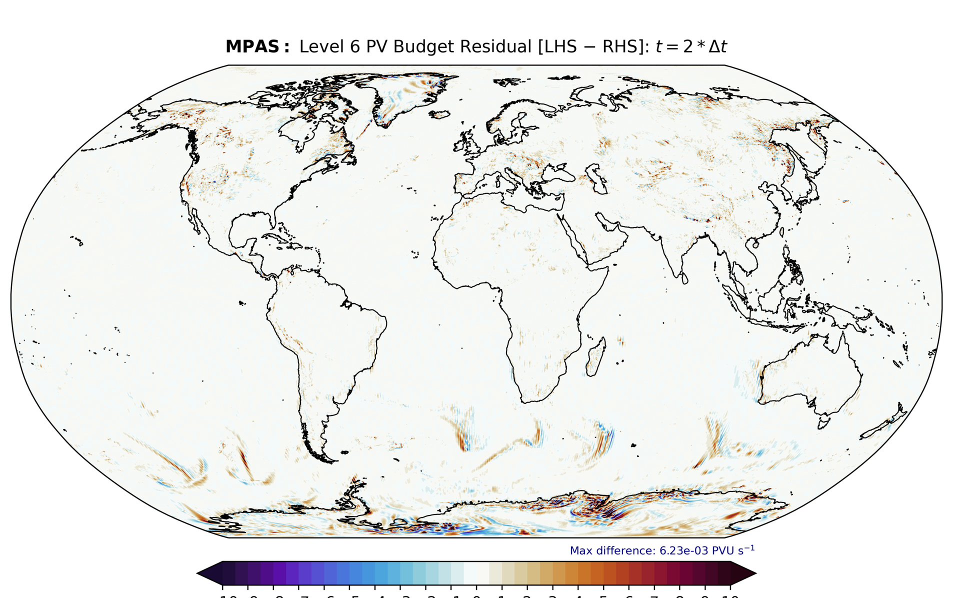

Fig. 1. *Residual of the PV budget, calculated as lhs of the PV tendency equation – rhs of the PV tendency equation, where the residual comprises any PV tendency contributions that are not accounted for in the calculations of PV advection, diabatic forcing, and frictional forcing, as well as any other sources of error [e.g., from discretization or interpolation]. In this case, advection was calculated offline using centered differences after fields were regridded to a constant 0.15° latitude-longitude mesh.*

Ultimately, the PV budget does not close, which prompted our thorough effort to [1] uncover the sources of the large residuals and [2] reduce these residuals such that they are effectively insignificant relative to the PV tendencies and resulting PV values

Efforts to Close the PV Budget: *Major Changes*

New Formulation for Calculating Horizontal Spatial Gradients

- The original formulation was difficult to follow and seemed to be based upon a loose application of the divergence theorem, whereby the volume integral of the gradient of a scalar is equal to the area integral of the scalar over all the cell faces
  - *The volume of the cell was crudely computed as* `areaCell*avgHt`*, where* `avgHt` *was prescribed as 100 m*
  - *Separate calculations were also performed for the vertical gradients*

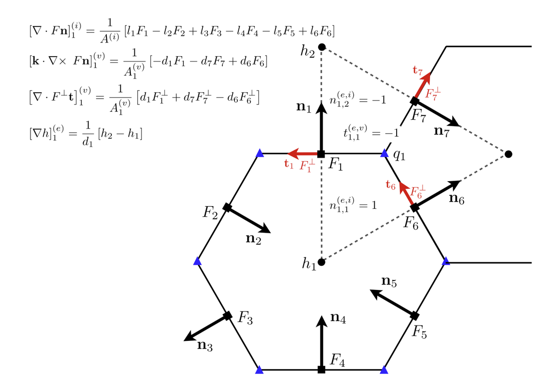

Fig. 2. *Depiction of the primal and dual mesh MPAS cells and discrete divergence, curl, and gradient operators from Ringler et al. [2010]. The last equation for the gradient operator was applied in revised calculations of PV and PV tendencies.*

- New formulation **calculates horizontal gradients on the cell edges** following Ringler et al. [2010] and **reconstructs the edge gradients to the cell center** in a manner consistent with the reconstruction of horizontal winds in MPAS
  - *This provides zonal and meridional gradients at the cell center for all quantities needed in the calculations of PV and PV tendencies*
  - *Code is generalizable for all purposes of calculating horizontal gradients on the native MPAS mesh*

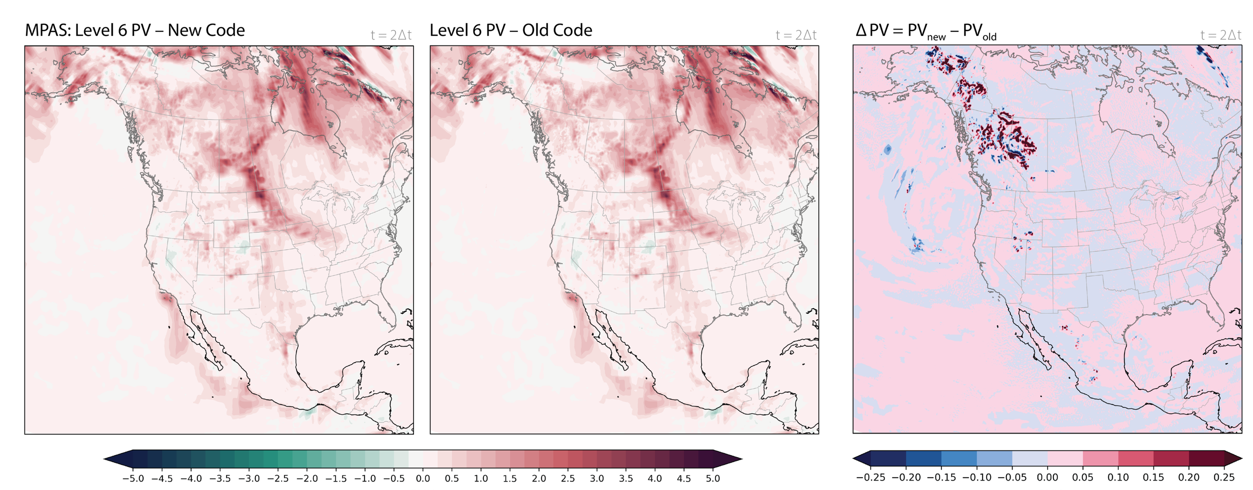

Fig. 3. *Ertel's PV on model level 6 calculated using the [left] new gradient formulation and [middle] old gradient formulation, and [right] the difference in the resulting PV fields.*

Inclusion of PV Advection Tendencies

- Previous studies that sought to close budgets of PV and other dynamical quantities in numerical models have emphasized the importance of calculating PV advection in a manner consistent with the model's dynamical core [e.g., Saffin et al. 2015]
- Three approaches were used to compute the PV advection tendencies online:
  - Gradient approach: *calculating and reconstructing the spatial gradients of PV using the procedure described above*
  - Scalar approach: *introducing a PV scalar variable to be advected by the scalar transport routine, which is reset to equal the updated PV field at the end of each time step*
  - Recalculation approach: *recomputing PV using variables that were stored immediately after the dynamics procedure and contain the tendencies resulting from advection*

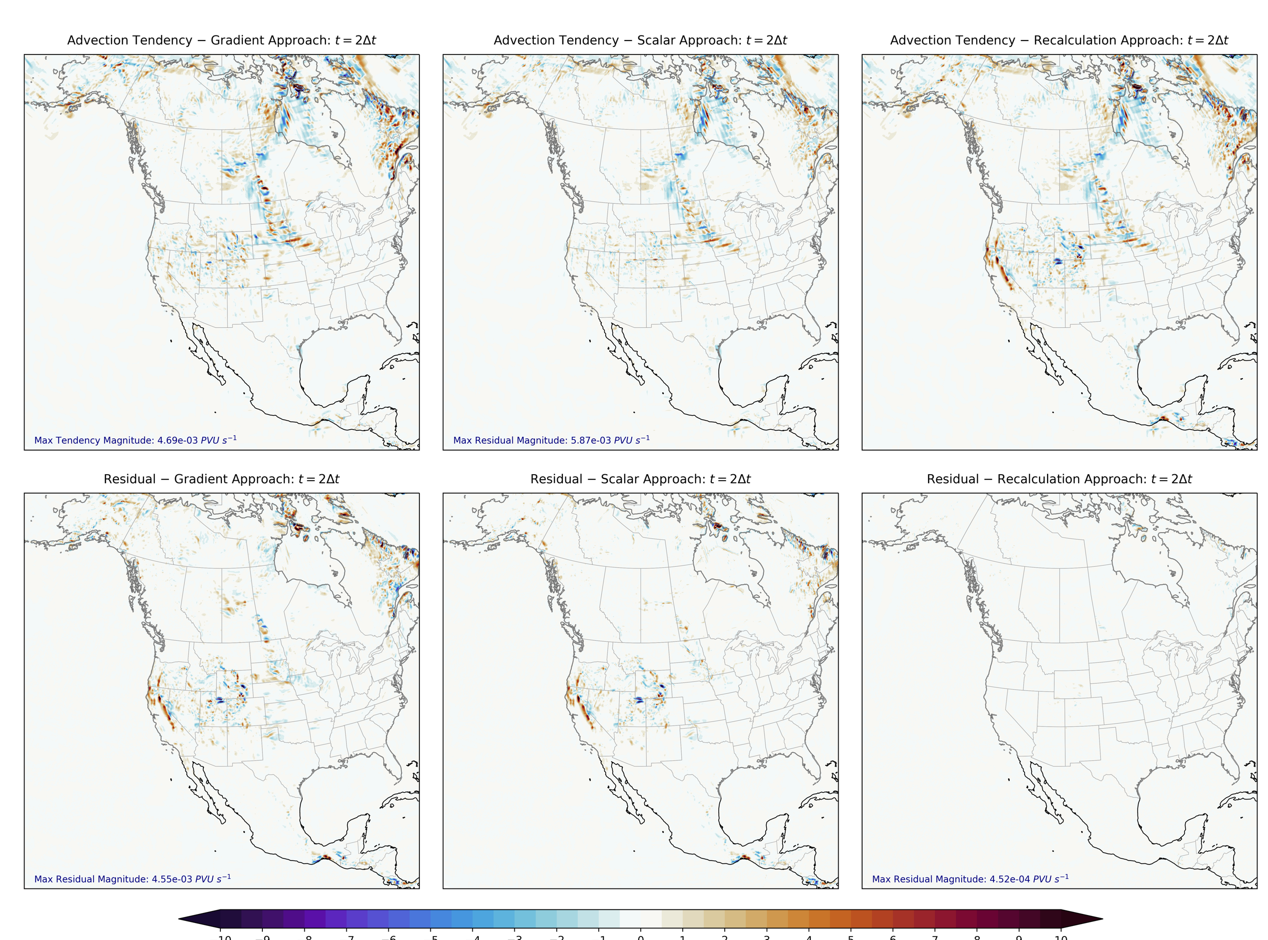

Fig. 4. *PV tendencies from advection [left] computed using the gradient, scalar, and recalculation approaches, and [right] the residual of the PV budget resulting from these different advection formulations with model physics turned off. The budgets were calculated using the described tendency term corrections and initial time level modifications.*

Efforts to Close the PV Budget: *Other Changes & Additions*

Corrections to Diabatic Mixing & Frictional Tendency Terms

- Errors were discovered in the calculations of the diabatic and frictional tendencies from horizontal mixing
  - Diabatic tendency: *term was calculated by converting* `tend_theta_euler` *to a tendency for dry potential temperature, but this term erroneously remained coupled to mass*
  - Frictional tendency: *term was calculated using* `tend_u_euler` *and* `tend_w_euler`*, which contain additional tendency contributions from processes other than diffusion [e.g., PGF] and also remained coupled to mass*
- Additionally, a bug was found in the frictional tendency calculation that stemmed from not initializing and resetting `tend_u_phys = 0` before its calculation at each time step, which resulted in the tendencies accumulating over time

Time Level Modifications in Tendency Calculations

- The original calculations for the **diabatic PV tendencies** comprised the gradient of the potential temperature tendency multiplied by the vorticity calculated with the updated wind fields, and those for the **frictional PV tendencies** comprised the curl of the wind tendencies by the gradient of the updated potential temperature field
- These calculations were modified to multiply the tendency components by either the vorticity or potential temperature gradient from the *beginning of the time step*, which required storing these "previous" fields as additional model variables
  - *This is in the process of being revised following the discrete product rule for forward differences*

Additions

- **Accumulated PV tendencies** were added for each instantaneous PV tendency variable to enable evaluation of the budget and net PV modifications without outputting fields every time step
- **Microphysical process tendencies** were incorporated into the Thompson scheme to allow the net PV modifications from microphysics to be attributed to contributions from [1] net condensation/evaporation of cloud water, [2] evaporation of rain water, [3] net sublimation/deposition of ice, [4] melting, and [5] freezing

Some Considerations, Next Steps, & Future Efforts

Discretized PV Tendency Equation

- PV can be discretized in time by using a combination of the product and quotient rules, which leads to several possible equations that theoretically yield equal solutions, including:

$$\frac{q^{t+\Delta t} - q^t}{\Delta t} = \frac{\vec{\eta}^{\,t+\Delta t}}{\rho^{t+\Delta t}} \cdot \left(\frac{\nabla\theta^{t+\Delta t} - \nabla\theta^t}{\Delta t}\right) + \frac{\nabla\theta^t}{\rho^{t+\Delta t}} \cdot \left(\frac{\vec{\eta}^{\,t+\Delta t} - \vec{\eta}^{\,t}}{\Delta t}\right) - \frac{q^t}{\rho^{t+\Delta t}}\left(\frac{\rho^{t+\Delta t} - \rho^t}{\Delta t}\right) \quad \text{[Eq. 3]}$$

  - *Compared to Eq. 2, this equation contains an extra term for the density tendency that is cancelled in the derivation using continuous derivatives*
  - *Note that the time levels used in the terms outside the parentheses vary*

Ongoing Work & Next Steps

- Evaluate budgets for the individual components of PV [e.g., potential temperature and its gradient] to better isolate the sources of the residual
- Evaluate tendencies and other quantities interpolated to dynamic tropopause
- Test code changes on a finer grid scale mesh [e.g., 15–3-km]

Ultimately…

- Upload a stand-alone version with our improvements to GitHub for community use
- Incorporate changes into a future MPAS release

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References

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