The Implementation of a PV-Based Leading Control Variable in Variational Data Assimilation. Part I: Transforms

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A set of new, potential vorticity (PV)-based control variables used within an atmospheric variational data assimilation (Var.) scheme has advantages over sets that are currently used operationally by some leading meteorological centres. A choice of new variables, formulated by Mike Cullen, of which a PV-related field is the leading variable, is described together with the strategy for its implementation within the Met Office's Var. scheme. Detailed is the transformation from the PV-based set to model variables, its adjoint, its inverse and the boundary conditions that must be considered when solving the transformation equations.

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The process of variational data assimilation can be described as the task of adjusting a model state vector in view of gaining optimal consistency simultaneously with (i) a background state and (ii) a set of observations, relevant to some time window. Other constraints are sometimes also imposed that encourage the state vector, e.g., to obey balance conditions or to discourage model error. The whole process is achieved by minimizing a cost function that penalizes misfit between the state vector variable and the background, and the state vector's 'prediction' of the observations and the observations themselves (plus costs that penalize departure from the other conditions imposed). The state vector that achieves this best fit within the characterised errors of the background and observations is called the *analysis*. The cost function is minimized at the anlysis.

Atmospheric assimilation schemes make extensive use of numerical weather prediction (NWP) models to provide a background state (a forecast from a previous analysis) and, in four-dimensional variational data assimilation (4d-var.), the time evolution part of the forward model and its adjoint. The state vectors used by these models describe the atmosphere typically by the fields u, v, θ, q, etc. These are represented on a set of model levels in the vertical and either a real- or spectral-space representation in the horizontal. It is helpful to refer to this representation of the state vector as in *model space*.

All information that goes into the Var. scheme has uncertainties, and it is very important to take uncertainties into account. The background error covariance matrix characterizes the uncertainties within the background state by describing variances of and covariances between the model variables (in a Gaussian context). The model state space is of high rank (10^6-10^7) and so we cannot represent the background error covariance matrix explicitly.

Most leading assimilation schemes do not perform the minimization process in model space, but instead use a *transformed* or *control* space. This new space is chosen to have a special and desirable property - when the background field is represented in this space, its errors are uncorellated and variances are of unit size (the problem is said to be *preconditioned*). It is very convenient to express state vectors in this form in the minimization process as the background error covariance matrix becomes the identity matrix. The remaining problem is determine the transformation that (at least approximately) achieves this.

The transformation between model and control variables is practically a multi-step process. The first stage involves a change of parameters (the *parameter* transform). This is designed to shift from the model variables - whose background errors are strongly correlated (multivariate) - to an alternative set of parameters - whose background errors are uncorrelated (univariate) (or at least weakly correlated). There however remains non-local correlations within each of the parameter's fields. The role of the remaining (vertical and horizontal) parts of the transformation is to project the parameters onto sets of vertical and horizontal modes that have no background error correlations.

This paper is about the first step in the transformation. It describes a change from model variables to a proposed set of pseudo-uncorrelated parameters which are partitioned according to whether they are *balanced* or *unbalanced*. The choice of parameters is discussed, together with the mathematical details of the transformations that need to be solved.

The key advantages of using a set of pseudo-uncorrelated parameters as part of the transformation include the following (in no particular order).

1. The parameter transform is an essential stage in the preconditioning process. This procedure block-diagonalizes the background error covariance matrix thus limiting the amount of information needed to describe it. This simplifies the process of determining the approximate eigenmodes (EOFs) of the background error covariance matrix whose variances (eigenvalues) are required for the preconditioning to work. A preconditioned cost function helps to control better the iterations of the minimization procedure, resulting in a well behaved algorithm that should converge quickly. With parameters that have a minimum of correlation between them, the full variances of the real problem is preserved during the transformation.

2. The atmospheric state can be partitioned into *balanced* (*slow manifold*) and *unbalanced* components, which often have separate spatio-time scales, and evolve in a quasi-independent manner. This is a useful property in data assimilation, not only for item 1, but also so that each component can treated according to its own error characteristics. Balanced modes of variability often have greater variance than that of unbalanced modes. This has two consequences in data assimilation. Firstly, Var. will implicitly weight its analysis increment to the variances of each mode, resulting in a largely balanced increment. Secondly, unbalanced modes will be tightly constrained automatically in Var., which will lessen the need for initialization of the analysis.

components. Thus most of the flow should be represented by one (*leading*) control parameter). The other parameters represent the residual flow.

4. A set of PV-based balanced/unbalanced partitioned parameters is expected to satisfy better the assumption of non-correlation between parameters than for existing control parameters. Thus the true background errors are expected to be better approximated with the proposed method. The new parameters are thus expected to lie close to the true principal axes of the background error covariance matrix, and so we expect to capture more of the variance of the background errors. As a consequence, the problem posed in terms of the PV-based parameters will be worse conditioned than for the existing parameters, but this will be compensated for in the vertical and horizontal transforms.

5. PV is a non-linear parameter. In formulating the transforms, it is linearized about a non-zero and synoptic dependent reference state. This introduces some flow-dependence to the errors.

6. Many of the transforms that arise from the proposed PV-based scheme involve solving three-dimensional elliptic equations. Sets of only two-dimensional equations are involved in the current scheme. The vertical coupling may improve vertical consistency.

This is the philosophy behind many leading atmospheric data assimilation schemes, such as those used by the United Kingdom Meteorological Office (Met Office) and the European Centre for Medium Range Weather Forecasts (E.C.M.W.F.). Their choice of control variables are, for practical reasons, not properly partioned into balanced and imbalanced components and so their schemes cannot exploit to the full the advantages outlined above. The focus of this report is to describe a new set of parameters that is alternative to the existing set used in the Met Office's operational 3d-var scheme. The new set is designed around potential vorticity (PV), and is hoped to be advantagous in the scope of the points outlined above.

In the present scheme used by the Met Office, the control parameters are (i) streamfunction, (ii) velocity potential, (iii) geostrophically unbalanced pressure and (iv) relative humidity. Streamfunction is the leading parameter that is meant to represent the balanced component of the flow (but only approximately over some flow regimes). Our new set will involve parameters that will be related to (i) PV, (ii) departure from linear balance, (iii) divergence and (iv) relative humidity. Our leading control variable related to PV is better suited to describe the balanced part of the flow than is the streamfunction.

Although the proposed scheme is expected to improve the representation of the background error covariance matrix, we also point out what it will not do. According to Kalman filter theory, the background error covariance matrix is a projection, forward in time, of the previous cycle's analysis error covariance matrix (the inverse hessian). This covariance matrix is influenced by the observations that are used in the previous analysis. A projection onto dynamically pseudo-decoupled parameters will not take into account the covariances introduced by the observing system.

Fields will be described as deviations from a reference state. The deviations (or increments) will be denoted by primes. Let the state $\vec{X}'$ be the vector of model variable increments of zonal velocity, meridional velocity and pressure,

$$\vec{X}' = \begin{pmatrix} u' \\ v' \\ p' \end{pmatrix}. \tag{1}$$

It is important to note that the elements of $\vec{X}'$ are themselves fields, spanning the model space. $\vec{X}'$ has a vector property because it represents a number of fields. A temperature parameter is missing from Eq. (1). This can be derived diagnostically from the parameters present (see Eq. (107) of appendix C). The control parameters will be described by the vector $\vec{Y}'$,

$$\vec{Y}' = \begin{pmatrix} s' \\ {}^{u}p' \\ \chi' \end{pmatrix}, \tag{2}$$

where the field s' describes principally the balanced part of the flow (related to PV), ${}^{u}p'$ the remaining non-divergent flow (our unbalanced pressure field that we shall associate with a quantity called anti-PV, or $\bar{PV}'$), and χ' the velocity potential pertaining to the divergent component of the flow. The derivation of these quantities will be performed later in this report. Note that here we are interested in the change between the (u', v', p') and (s', ${}^{u}p'$, χ') parameters and not in the transformation of the space into modes.

2.1 The U_p transform formalism

We denote the parameter transform operator that produces the model state $\vec{X}'$ given the parameter state $\vec{Y}'$, as U_p:

$$\vec{X}' = U_p \vec{Y}'. \tag{3}$$

It is helpful to write the U_p operator in terms of its components,

$$U_p = \begin{pmatrix} \vec{e}_1 & \vec{e}_2 & \vec{e}_3 \end{pmatrix} = \begin{pmatrix} e_{11} & e_{12} & e_{13} \\ e_{21} & e_{22} & e_{23} \\ e_{31} & e_{32} & e_{33} \end{pmatrix}, \tag{4}$$

where the columns of the matrix are the components of the $\vec{e}_n$-vectors. It is important to note that each of the $\vec{e}_n$-vectors (and the e_{mn} components) are themselves operators acting on the control variable fields. We shall assume for now that we know what these operators are (see section 3). Acting with Eq. (4) on the state $\vec{Y}'$ to give $\vec{X}'$ yields, component-by-component,

$$\vec{X}' = \begin{pmatrix} u' \\ v' \\ p' \end{pmatrix} = U_p \vec{Y}' = U_p \begin{pmatrix} s' \\ {}^{u}p' \\ \chi' \end{pmatrix} = \vec{e}_1 s' + \vec{e}_2 {}^{u}p' + \vec{e}_3 \chi', \tag{5}$$

which can be further written,

$$\begin{array}{rcccccc} \vec{X}' & = & \vec{X}'_1 & + & \vec{X}'_2 & + & \vec{X}'_3 \\ & = & \vec{e}_1 s' & + & \vec{e}_2 {}^{u}p' & + & \vec{e}_3 \chi' \\ & = & \begin{pmatrix} e_{11} \\ e_{21} \\ e_{31} \end{pmatrix} s' & + & \begin{pmatrix} e_{12} \\ e_{22} \\ e_{32} \end{pmatrix} {}^{u}p' & + & \begin{pmatrix} e_{13} \\ e_{23} \\ e_{33} \end{pmatrix} \chi'. \end{array} \tag{6}$$

U_p has been designed such that these contributions have a special meaning. The first term in Eq. (6), $\vec{X}'_1$, is the *balanced* contribution to the flow, the second term, $\vec{X}'_2$, is the *residual non-divergent* part, and the third term, $\vec{X}'_3$, is the *divergent* part. Hence we can associate each column of U_p with each respective parameter in a mathematical and a physical way. The last row of Eq. (6) breaks the operators up into those parts that give the individual components of the model state, so e.g., $e_{31} s'$ will give the 'balanced' pressure increment. We will show in section 3 how these operators are formed.

The T_p transform performs the inverse of the U_p operator. Unlike for the U_p operator, we find that it is generally not possible to write down an explicit form for T_p. It will be helpful to define a *dual basis* operator, A, as a first step to achieving the inverse operation. Let,

$$A = \begin{pmatrix} \vec{f}_1^* \\ \vec{f}_2^* \\ \vec{f}_3^* \end{pmatrix} = \begin{pmatrix} f_{11}^* & f_{12}^* & f_{13}^* \\ f_{21}^* & f_{22}^* & f_{23}^* \\ f_{31}^* & f_{32}^* & f_{33}^* \end{pmatrix}, \tag{7}$$

where the components of the dual basis $\vec{f}^*$-row vector operators have been expanded out into their components. A acts on a state of model variables, namely,

$$A\vec{X}' = \begin{pmatrix} \vec{f}_1^*\vec{X}' \\ \vec{f}_2^*\vec{X}' \\ \vec{f}_3^*\vec{X}' \end{pmatrix} = \begin{pmatrix} f_{11}^*u' + f_{12}^*v' + f_{13}^*p' \\ f_{21}^*u' + f_{22}^*v' + f_{23}^*p' \\ f_{31}^*u' + f_{32}^*v' + f_{33}^*p' \end{pmatrix} \propto \begin{pmatrix} PV' \\ \bar{PV}' \\ \nabla_z \cdot \mathbf{u_h}' \end{pmatrix}. \tag{8}$$

We are reminded that terms like $\vec{f}_n^*\vec{X}'$ are inner products and therefore each give a single field. We design the $\vec{f}_1^*$, $\vec{f}_2^*$ and $\vec{f}_3^*$ operators to be for quantities proportional to PV, $\bar{PV}'$ and horizontal divergence respectively, as inidcated in Eq. (8).

Both sides of Eq. (3) is a state of model variables and so we can operate on each side with A. Doing this yields,

$$A\vec{X}' = AU_p\vec{Y}', \tag{9}$$

which provides us with a set of equations we can use as a basis for doing the inverse operation. Expanding Eq. (9) gives,

$$\begin{pmatrix} PV' \\ \bar{PV}' \\ \nabla_z \cdot \mathbf{u_h}' \end{pmatrix} \propto \begin{pmatrix} \vec{f}_1^*U_p \\ \vec{f}_2^*U_p \\ \vec{f}_3^*U_p \end{pmatrix} \vec{Y}' = \begin{pmatrix} \vec{f}_1^*\vec{e}_1 & \vec{f}_1^*\vec{e}_2 & \vec{f}_1^*\vec{e}_3 \\ \vec{f}_2^*\vec{e}_1 & \vec{f}_2^*\vec{e}_2 & \vec{f}_2^*\vec{e}_3 \\ \vec{f}_3^*\vec{e}_1 & \vec{f}_3^*\vec{e}_2 & \vec{f}_3^*\vec{e}_3 \end{pmatrix} \begin{pmatrix} s' \\ {}^up' \\ \chi' \end{pmatrix}, \tag{10}$$

where the inner products $\vec{f}_m^*\vec{e}_n$ are scalar operators.

With $\vec{e}_1$, $\vec{e}_2$ and $\vec{e}_3$ predetermined (to be shown in section 3), we have some flexibility in our choice of the dual operators $\vec{f}_1^*$, $\vec{f}_2^*$ and $\vec{f}_3^*$. We choose these such that the combined operator, AU_p, on right hand side of Eq. (10) is at least lower triagonal, *ie*,

$$\begin{aligned} \vec{f}_1^*\vec{e}_2{}^up' &= 0, \\ \vec{f}_1^*\vec{e}_3\chi' &= 0, \\ \vec{f}_2^*\vec{e}_3\chi' &= 0, \end{aligned} \tag{11}$$

but our combination of dual and control parameter space has the additional property that other elements are zero also such that AU_p is diagonal (see section 4),

$$\begin{aligned} \vec{f}_2^*\vec{e}_1 s' &= 0, \\ \vec{f}_3^*\vec{e}_1 s' &= 0, \\ \vec{f}_3^*\vec{e}_2{}^up' &= 0. \end{aligned} \tag{12}$$

What does this mean? Take the first line of Eq. (10). Since the operators $\vec{f}_2^*$ and $\vec{f}_3^*$ are designed such that $\vec{f}_1^*\vec{e}_2{}^up'$ and $\vec{f}_1^*\vec{e}_3\chi' = 0$ (we say that $\vec{f}_1^*$ is in the kernal of both $\vec{e}_2$ and $\vec{e}_3$), this means that the parts of the flow described by ${}^up'$ and χ' have no PV contribution. Similarly for the remaining rows, s' and χ' have no anti-PV, and s' and ${}^up'$ have no divergence. We develop the $\vec{f}_1^*$, $\vec{f}_2^*$ and $\vec{f}_3^*$ operators in section 4. The diagonal property of AU_p means that the inverse of the U_p operator (T_p) can be performed easily.

3.1 The first equation, PV'

3.1.1 Bulk potential vorticity

We start with the definition of Ertel PV in height co-ordinates (first term of Eq. (70) of appendix A),

$$PV = \frac{\zeta_0 + f}{\rho_0}\frac{\partial \theta_0}{\partial z} \tag{13}$$

where ζ_0 is the vertical component of relative vorticity evaluated on a constant height surface, f is the Coriolis parameter, ρ_0 is the fluid density, and θ_0 is potential temperature. The '0' subscripts denote reference state quantities. In the first version of this work, we shall average the reference state quantities zonally, and so they are a function of latitude and height only.

Eq. (13) is a non-linear function of model variables. For the transformations, we require that equations are linear. Linearising Eq. (13) about a chosen state, $\vec{X}_0 = (u_0, v_0, p_0)^T$ can be done systematically by the following expansion,

$$PV' = \left.\frac{\partial PV}{\partial \zeta}\right|_0 \zeta', + \left.\frac{\partial PV}{\partial \rho}\right|_0 \rho', + \left.\frac{\partial PV}{\partial \theta_z}\right|_0 \theta'_z, \tag{14}$$

where primed quantities denote deviation from the reference state (e.g. $\zeta' = \zeta_0 + \zeta'$). Note that the basic state for vorticity, ζ_0 follows from u_0 and v_0 as $\zeta_0 = \mathbf{k}\cdot(\nabla_z \times \mathbf{u_{0h}}) = (\partial v_0/\partial x)_z - (\partial u_0/\partial y)_z$. The partial derivatives in Eq. (14) are,

$$\begin{aligned} \frac{\partial PV}{\partial \zeta} &= \frac{1}{\rho_0}\frac{\partial \theta_0}{\partial z}, & (15)\\ \frac{\partial PV}{\partial \rho}, &= -\frac{\zeta_{0z} + f}{\rho_0^2}\frac{\partial \theta_0}{\partial z} & (16)\\ \frac{\partial PV}{\partial \theta_z} &= \frac{\zeta_{0z} + f}{\rho_0}. & (17)\end{aligned}$$

We prefer not to work with density increments, so for the equation that we shall give for incremental PV, we use Eq. (108) (introduced in appendix C) to write density increments in terms of pressure increments. Also we use Eq. (109) to write θ'_z increments in terms of pressure increments. Putting all of this into Eq. (14) and assuming small Rossby number ($f \gg \zeta_0$) we obtain,

$$\begin{aligned} PV' &= \frac{\theta_{0z}}{\rho_0}\zeta' - \\ &\quad \frac{f\theta_{0z}}{\rho_0^2}\left\{\frac{1-\kappa}{R\Pi_0\hat{\theta}_0}p' + \frac{\rho_0}{\hat{\theta}_0}\overbrace{\frac{1}{\Pi_{0z}}\left[\theta_0\frac{\partial}{\partial z}\left(\kappa\frac{\Pi_0}{p_0}p'\right)\right]}\right\} + \\ &\quad \frac{f}{\rho_0}\frac{g}{c_p}\left\{\frac{1}{\hat{\Pi}_{0z}^2}\frac{\partial^2}{\partial z^2}\left(\kappa\frac{\Pi_0}{p_0}p'\right) - \frac{2\Pi_{0zz}}{\hat{\Pi}_{0z}^3}\overbrace{\frac{\partial}{\partial z}\left(\kappa\frac{\Pi_0}{p_0}p'\right)}\right\}, & (18)\\ &= \frac{\theta_{0z}}{\rho_0}\zeta' - \frac{f\theta_{0z}}{\rho_0^2}\left\{\frac{1-\kappa}{R\Pi_0\hat{\theta}_0}p' + \frac{\rho_0}{\hat{\theta}_0}\hat{Q}\right\} + \frac{f}{\rho_0}\frac{g}{c_p}\left\{\frac{1}{\hat{\Pi}_{0z}^2}R - \frac{2\Pi_{0zz}}{\hat{\Pi}_{0z}^3}\hat{S}\right\}, & (19)\end{aligned}$$

where the following substitions have been made in Eq. (19),

$$\begin{aligned} Q &= \frac{1}{\Pi_{0z}}\left[\theta_0\frac{\partial}{\partial z}\left(\kappa\frac{\Pi_0}{p_0}p'\right)\right], & (20)\\ R &= \frac{\partial^2}{\partial z^2}\left(\kappa\frac{\Pi_0}{p_0}p'\right), & (21)\\ S &= \frac{\partial}{\partial z}\left(\kappa\frac{\Pi_0}{p_0}p'\right). & (22)\end{aligned}$$

The notation Π_{0z} means the first vertical derivative of exner pressure reference and Π_{0zz} means the second derivative (similarly for other variables). Each term in Eq. (14) falls naturally on p-levels in the on θ-levels, e.g. vertical derivative of Π. Such terms need to be vertically interpolated to p-levels. In Eq. (18), this is denoted by the hat, $\hat{}$, for single variables or by the overbrace for expressions (generally this notation indicates that vertical interpolation is performed to levels not natural to the quantity in question; this could be θ- to p-levels, as above, or the other way around). It is important to respect the vertical grid staggering in this way to minimize numerical problems. We do not consider the horizontal grid staggering at this stage as this is less important. It is considered when we discretize the equations fully - as done in appendix D.

3.1.2 Boundary potential vorticity

Equation (18) cannot be evaluated at the top- and bottom-most levels due to the presence of the vertical second derivatives of pressure. The missing PV information must come from elsewhere. To this end, we use two alternative two dimensional fields of PV-like quantities which are non-locally related to model increments. The alternative quantities involve vertical integrals and are justified in appendix B. The first field, PV_1' (Eq. (80) in the appendix) is,

$$PV_1' = \int_{z=0}^{z_{top}} \mathrm{d}z \left\{ \rho_0 \zeta' - f \left(\frac{1-\kappa}{R\Pi_0 \hat{\theta}_0} p' + \frac{\rho_0}{\hat{\theta}_0} \overbrace{\frac{1}{\Pi_{0z}} \left\{ \theta_0 \frac{\partial}{\partial z} \left(\kappa \frac{\Pi_0}{p_0} p' \right) \right\}} \right) \right\}, \tag{23}$$

$$= \int_{z=0}^{z_{top}} \mathrm{d}z \left\{ \rho_0 \zeta' - f \left(\frac{1-\kappa}{R\Pi_0 \hat{\theta}_0} p' + \frac{\rho_0}{\hat{\theta}_0} \hat{Q} \right) \right\}. \tag{24}$$

and the second, PV_2' (Eq. (95) in the appendix) is,

$$\begin{aligned} PV_2' = {} & f \int_{z=0}^{z_{top}} \mathrm{d}z \overbrace{\frac{1}{\Pi_{0z}} \left\{ \theta_0 \frac{\partial}{\partial z} \left(\kappa \frac{\Pi_0}{p_0} p' \right) \right\}} - \\ & f \int_{z=0}^{z_{top}} \mathrm{d}z \frac{\theta_{0z}}{\rho_0} \int_{z'=0}^{z} \mathrm{d}z' \left\{ \frac{1-\kappa}{R\Pi_0 \hat{\theta}_0} p' + \frac{\rho_0}{\hat{\theta}_0} \overbrace{\frac{1}{\Pi_{0z}} \left\{ \theta_0 \frac{\partial}{\partial z} \left(\kappa \frac{\Pi_0}{p_0} p' \right) \right\}} \right\} + \\ & \int_{z=0}^{z_{top}} \mathrm{d}z \frac{\theta_{0z}}{\rho_0} \left\{ \int_{z'=0}^{z} \mathrm{d}z' \rho_0 \zeta' - \frac{PV_1' \int_{z'=0}^{z} \mathrm{d}z' \rho_0}{\int_{z'=0}^{z_{top}} \mathrm{d}z' \rho_0} \right\}, \end{aligned} \tag{25}$$

$$\begin{aligned} = {} & f \int_{z=0}^{z_{top}} \mathrm{d}z \hat{Q} - \\ & f \int_{z=0}^{z_{top}} \mathrm{d}z \frac{\theta_{0z}}{\rho_0} \int_{z'=0}^{z} \mathrm{d}z' \left\{ \frac{1-\kappa}{R\Pi_0 \hat{\theta}_0} p' + \frac{\rho_0}{\hat{\theta}_0} \hat{Q} \right\} + \\ & \int_{z=0}^{z_{top}} \mathrm{d}z \frac{\theta_{0z}}{\rho_0} \left\{ \int_{z'=0}^{z} \mathrm{d}z' \rho_0 \zeta' - \frac{PV_1' \int_{z'=0}^{z} \mathrm{d}z' \rho_0}{\int_{z'=0}^{z_{top}} \mathrm{d}z' \rho_0} \right\}, \end{aligned} \tag{26}$$

These definitions of PV, PV_1' and PV_2' will be used later when dealing with the second U_p trasnform (section 3.2), and also with the T_p-transform (section 4).

3.1.3 The first U_p transform

In Eq. (18) we have assumed that we are in the domain of small Rossby number, i.e. that $f \gg \zeta_0$. Also valid in this domain is the linear balance relationship which we impose between the mass and wind fields when dealing with PV',

$$\nabla_z \cdot (f \rho_0 \nabla_z s') - \nabla_z^2 p_1' = 0. \tag{27}$$

In writing Eq. (27) we have assumed that horizontal variations in the density are negligible. The standard relationship between the balanced streamfunction and its horizontal velocity increments is also required,

$$\mathbf{v_1}' = \mathbf{k} \times \nabla_z s'. \tag{28}$$

The last two equations can be used to define the part of the U_p-operator $\vec{e}_1$, that, when acting on s' (which we know as it is a control variable) gives the balanced increments, $\vec{X}_1' = (u_1', v_1', p_1)^T$,

$$\vec{X}_1' = \vec{e}_1 s' = \begin{pmatrix} -\partial/\partial y \\ \partial/\partial x \\ \nabla_z^{-2} \nabla_z \cdot (f \rho_0 \nabla_z) \end{pmatrix} s'. \tag{29}$$

straightforward to evaluate the velocity components (first two rows of Eq.(29)). These have been specified in local cartesian coordinates in Eq. (29), but on the sphere, spherical coordinates will obviously have to be used. The pressure (last component) is found by solving one elliptic equation per height surface.

3.2 The second equation, $\bar{PV}'$

In the last section we showed how we can compute the balanced component of the analysis increment, $\vec{X}'$ via the $\vec{e}_1$ operator acting on s'. Under general conditions, the actual flow is not balanced and so s' does not provide a complete description. The first of the two residuals that we shall consider is via our unbalanced pressure parameter, ${}^u p'$, the second variable representing the analysis increment in parameter space (Eq. (2)).

3.2.1 Anti-potential vorticity

We wish for ${}^u p'$ to be associated with the departure from linear balance of the rotational flow. This is to be based on the quantity, $\bar{PV}'$ (anti-PV), defined as f multiplied by the residual of the linear balance equation,

$$\bar{PV}' = f(\nabla_z \cdot (f\rho_0 \nabla_z \psi') - \nabla_z^2 p'), \tag{30}$$

where the linear balance equation has been used before in Eq. (27). The $\bar{PV}$ describes the vortical flow fields not accounted for by the PV and will be used next in section 4 in connection with the T_p-transform. We will show later that the balanced and divergent components of the flow (from the first and third transforms) have zero $\bar{PV}$.

3.2.2 The second U_p transformation in the bulk

The model increments, $\vec{X}_2' = (u_2', v_2', p_2')^T$ that are the 'rotational departure from linear balance' are designed to have no PV. This is the strategy for developing the second U_p transform. Since PV in the bulk is defined differently to PV at the top and bottom boundaries, the second (unbalanced) set of U_p transforms are treated separately for the bulk and for the boundary.

For the bulk transform, follow this prescription:

1. Setting $PV' = 0$ (using Eq. (18)) yields a relationship between pressure and vorticity. This is the equation that we will use to gain a set of wind increments (via vorticity) from the second control variable, ${}^u p'$, which is a pressure. Given this pressure increment the vorticity increment is ${}^u\zeta'$, and is found from Eq. (18) set to zero and rearranged,

$$\begin{aligned} {}^u\zeta' &= \frac{f}{\rho_0}\left\{\frac{1-\kappa}{R\Pi_0\hat{\theta}_0}{}^u p' + \frac{\rho_0}{\hat{\theta}_0}\overbrace{\frac{1}{\Pi_{0z}}\left[\theta_0\frac{\partial}{\partial z}\left(\kappa\frac{\Pi_0}{p_0}{}^u p'\right)\right]}\right\} - \\ &\quad \frac{f}{\theta_{0z}}\frac{g}{c_p}\left\{\frac{1}{\hat{\Pi}_{0z}^2}\frac{\partial^2}{\partial z^2}\left(\kappa\frac{\Pi_0}{p_0}{}^u p'\right) - \frac{2\Pi_{0zz}}{\hat{\Pi}_{0z}^3}\overbrace{\frac{\partial}{\partial z}\left(\kappa\frac{\Pi_0}{p_0}{}^u p'\right)}\right\}. \end{aligned} \tag{31}$$

   Note: Vorticity on the left hand side is normally stored on a ψ- point (Fig. I), but the right hand side of the above is suited to p-points. For the second U_p transform, we perform the calculation of Eq. (31) on p-points; interpolation will be done later.

2. This vorticity increment must be decomposed into velocity increments. Streamfunction is derived from vorticity by solving Poisson's equation,

$${}^u\zeta_z' = \nabla_z^2 {}^u\psi', \tag{32}$$

   with both quantities (${}^u\zeta_z'$ and ψ') held on p-points. After streamfunction is determined on p-points, it is interpolated to its desired position on ψ-points where velocity follows,

$$\begin{aligned} {}^u\mathbf{u}' &= \mathbf{k} \times \nabla_z {}^u\psi' \\ \begin{pmatrix} {}^u u' \\ {}^u v' \end{pmatrix} &= \begin{pmatrix} -\partial^u\psi'/\partial y \\ \partial^u\psi'/\partial x \end{pmatrix}. \end{aligned} \tag{33}$$

and Eq. (33) allows the second set of model increments (in the bulk), $\vec{X}_2' = (u_2', v_2', p_2')^T$ to be written,

$$
\begin{aligned}
\vec{X}_2' &= \vec{e}_2 {}^u p' \\
&= \begin{pmatrix}
-\frac{\partial}{\partial y}\nabla^{-2}\frac{f}{\rho_0}\left\{\frac{1-\kappa}{R\Pi_0\hat{\theta}_0}\star + \frac{\rho_0}{\hat{\theta}_0}\overbrace{\frac{1}{\Pi_{0z}}\left[\theta_0\frac{\partial}{\partial z}\left(\kappa\frac{\Pi_0}{p_0}\star\right)\right]}\right\} - \frac{f}{\theta_{0z}}\frac{g}{c_p}\left\{\frac{1}{\Pi_{0z}^{\hat{2}}}\frac{\partial^2}{\partial z^2}\left(\kappa\frac{\Pi_0}{p_0}\star\right) - \frac{2\Pi_{0zz}}{\Pi_{0z}^{\hat{3}}}\overbrace{\frac{\partial}{\partial z}\left(\kappa\frac{\Pi_0}{p_0}\star\right)}\right\} \\
\frac{\partial}{\partial x}\nabla^{-2}\frac{f}{\rho_0}\left\{\frac{1-\kappa}{R\Pi_0\hat{\theta}_0}\star + \frac{\rho_0}{\hat{\theta}_0}\overbrace{\frac{1}{\Pi_{0z}}\left[\theta_0\frac{\partial}{\partial z}\left(\kappa\frac{\Pi_0}{p_0}\star\right)\right]}\right\} - \frac{f}{\theta_{0z}}\frac{g}{c_p}\left\{\frac{1}{\Pi_{0z}^{\hat{2}}}\frac{\partial^2}{\partial z^2}\left(\kappa\frac{\Pi_0}{p_0}\star\right) - \frac{2\Pi_{0zz}}{\Pi_{0z}^{\hat{3}}}\overbrace{\frac{\partial}{\partial z}\left(\kappa\frac{\Pi_0}{p_0}\star\right)}\right\} \\
1
\end{pmatrix} \\
&\quad \times {}^u p',
\end{aligned}
\tag{34}
$$

where ${}^u p'$, which is acted upon by the $\vec{e}_2$ operator (large braces) appears where there is a star, $\star$ (this is done for clarity). As in previous equations, cartesian components have been used for illustration. Spherical coordinates would be used in practice (see appendix E which is concerned with discretization).

3.2.3 The second U_p transformation at the vertical boundaries

The second contribution to the model's winds involves a special treatment at the vertical boundaries (the contribution to the pressure at the vertical boundaries is identical to that shown in Eq. (34), and is thus covered above). Instead of having zero PV' (PV' defined in Eq. (18)), we enforce zero PV_1' and PV_2'. The procedure itself involves complicated-looking vertical summations, but the principle is simple. Two simultaneous linear equations per vertical column emerge in terms of the unknowns ${}^u\zeta'(1)$ and ${}^u\zeta'(N)$ which can be solved for these quantities. The bulk transforms (as above), giving ${}^u\zeta'(k)$, $1 < k < N$ and $p'(k)$, $1 \leq k \leq N$ must be done first as the solution here requires these quantities.

The actual equations that have to be solved involve the discretized form of PV_1' and PV_2' (Eqs. (123) and (128) in appendix E), rather than the original form (Eqs. (23) and (25) above). Hence we work with the discretized form. Note that for compactness, we drop the horizontal position index (i, j) in the analysis below when writing the discretized equations. Also, all increments refer to the unbalanced component (second contribution, $\vec{X}_2'$) implicitly.

Setting $PV_1' = 0$ Setting PV_1' (Eq. (123), but on p-points) to zero with the unbalanced increments yields the first line of the following. In the remaining lines, the vorticity contributions from the top and bottom layers of the integral $I_A(N)$ Eq. (124) from appendix E) are separated from the bulk integral.

$$
\begin{aligned}
PV_1' &= \tilde{I}_A(N) - f_u I_B(N) = 0, \\
&= {}^u\zeta'(1)\rho_0(1)(r_0^\theta(1) - r_0^\theta(0)) + \sum_{k=2}^{N-1} {}^u\zeta'(k)\rho_0(k)(r_0^\theta(k) - r_0^\theta(k-1)) + \\
&\quad {}^u\zeta'(N)\rho_0(N)(r_0^\theta(N) - r_0^\theta(N-1)) - f_u I_B(N) = 0, \\
&= F_1 {}^u\zeta'(1) + I_1 + F_2 {}^u\zeta'(N) - f_u I_B(N) = 0,
\end{aligned}
\tag{35}
$$

where $\tilde{I}_A(N)$ is here defined as Eq. (124), but without the interpolation to ψ-points (i.e. remove the overbar in that equation). Recall that, for the moment, ${}^u\zeta'$ is on p-points until we derive winds from it (see the comment just after Eq. (31). In Eq. (35), the following have been defined,

$$
F_1 = \rho_0(1)(r_0^\theta(1) - r_0^\theta(0)), \tag{36}
$$

$$
I_1 = \sum_{k=2}^{N-1} {}^u\zeta'(k)\rho_0(k)(r_0^\theta(k) - r_0^\theta(k-1)), \tag{37}
$$

$$
F_2 = \rho_0(N)(r_0^\theta(N) - r_0^\theta(N-1)), \tag{38}
$$

and $I_B(N)$ is given in appendix E as Eq. (125). The vorticity integral, $\tilde{I}_A(N)$, has been split into bottom, bulk and top contributions because only the top- and bottom-most levels are unknown. The pressure integral, $I_B(N)$, has not been split in this way because it is known at all levels. Equation (35) constitutes the first simultaneous equation that will be used to find ${}^u\zeta'(1)$ and ${}^u\zeta'(N)$.

of the double integrals. Setting Eq. (128) - but on p-points - to zero yields,

$$\begin{aligned}
PV_2' &= I_2 - (I_{3A} + I_{3B}) + \\
&\frac{1}{2}\left\{\sum_{k=1}^{N-1} \overbrace{\frac{\theta_{0z}(k)}{\rho_0(k)}}(r_0^\theta(k+1) - r_0^\theta(k))\tilde{I}_A(k) + \right. \\
&\left.\sum_{k=1}^{N} \overbrace{\frac{\theta_{0z}(k)}{\rho_0(k)}}(r_0^\theta(k) - r_0^\theta(k-1))\tilde{I}_A(k)\right\} - \\
&\frac{\tilde{PV}_1'}{2I_\rho(N)}\left\{\sum_{k=1}^{N} \overbrace{\frac{\theta_{0z}(k)}{\rho_0(k)}}\, I_\rho(k)(r_0^\theta(k) - r_0^\theta(k-1)) + \right. \\
&\left.\sum_{k=1}^{N-1} \overbrace{\frac{\theta_{0z}(k)}{\rho_0(k)}}\, I_\rho(k)(r_0^\theta(k+1) - r_0^\theta(k))\right\} = 0, \\
&= I_2 - (I_{3A} + I_{3B}) + \\
&\frac{1}{2}\left\{\sum_{k=1}^{N-1} \overbrace{\frac{\theta_{0z}(k)}{\rho_0(k)}}(r_0^\theta(k+1) - r_0^\theta(k))\tilde{I}_A(k) + \right. \\
&\left.\sum_{k=1}^{N-1} \overbrace{\frac{\theta_{0z}(k)}{\rho_0(k)}}(r_0^\theta(k) - r_0^\theta(k-1))\tilde{I}_A(k) + \overbrace{\frac{\theta_{0z}(N)}{\rho_0(N)}}(r_0^\theta(N) - r_0^\theta(N-1))\tilde{I}_A(N)\right\} - \\
&\frac{\tilde{PV}_1'}{2I_\rho(N)}\left\{\sum_{k=1}^{N} \overbrace{\frac{\theta_{0z}(k)}{\rho_0(k)}}\, I_\rho(k)(r_0^\theta(k) - r_0^\theta(k-1)) + \right. \\
&\left.\sum_{k=1}^{N-1} \overbrace{\frac{\theta_{0z}(k)}{\rho_0(k)}}\, I_\rho(k)(r_0^\theta(k+1) - r_0^\theta(k))\right\} = 0, \qquad (39)
\end{aligned}$$

where the following have been defined,

$$I_2 = f_u \sum_{k=1}^{N} \hat{Q}(k)(r_0^\theta(k) - r_0^\theta(k-1)), \qquad (40)$$

$$I_{3A} = \frac{f_u}{2}\sum_{k=1}^{N-1} \overbrace{\frac{\theta_{0z}(k)}{\rho_0(k)}}\, I_B(k)(r_0^\theta(k+1) - r_0^\theta(k)), \qquad (41)$$

$$I_{3B} = \frac{f_u}{2}\sum_{k=1}^{N} \overbrace{\frac{\theta_{0z}(k)}{\rho_0(k)}}\, I_B(k)(r_0^\theta(k) - r_0^\theta(k-1)), \qquad (42)$$

and $\tilde{I}_A$, I_B, and I_ρ are given in appendix E as Eqs. (129), (130) and (127) respectively. Note that, as before, the tilde in $\tilde{I}_A$ has the special meaning that we ignore the overbar in Eq. (129), so that it is evaluated on p-points. The integral $I_A(k)$ is a vertical summation involving ζ', and so it needs to be split into parts that are known (bulk) and parts that are unknown (boundary). In developing Eq. (39), we have separated those terms that do not involve $\zeta'(N)$ and those that do (the $\zeta'(1)$ contriutions are dealt with below). Developing I_A for (i) when $k < N$ and (ii) when $k = N$ gives,

$$k < N: \; \tilde{I}_A(k) = {}^u\zeta'(1)\rho_0(1)(r_0^\theta(1) - r_0^\theta(0)) + (1 - \delta_{k1})\sum_{k'=2}^{k} {}^u\zeta'(k')\rho_0(k')(r_0^\theta(k') - r_0^\theta(k'-1)), \qquad (43)$$

$$\begin{aligned}
k = N: \; \tilde{I}_A(N) &= {}^u\zeta'(1)\rho_0(1)(r_0^\theta(1) - r_0^\theta(0)) + \sum_{k'=2}^{N-1} {}^u\zeta'(k')\rho_0(k')(r_0^\theta(k') - r_0^\theta(k'-1)) + \\
&{}^u\zeta'(N)\rho_0(N)(r_0^\theta(N) - r_0^\theta(N-1)). \qquad (44)
\end{aligned}$$

Since the situation when $k = 0$ never arises (by arranging the k summation limits in Eq. (39) to start at 1 instead of 0), this factor is always 1 and so is omitted. We have introduced other δ-functions that multiply the summations in Eqs. (43) and (44). These will also become redundent when Eqs. (43) and (44) are substituted into Eq. Eq. (39) and the k summation limits are adjusted.

Putting Eqs. (43) and (44) into Eq. (39) yields the following,

$$\begin{aligned}
PV_2' &= I_2 - (I_{3A} + I_{3B}) + \\
&\frac{1}{2}\Bigg\{ \sum_{k=1}^{N-1} \frac{\widetilde{\theta_{0z}(k)}}{\rho_0(k)} (r_0^\theta(k+1) - r_0^\theta(k))\rho_0(1)(r_0^\theta(1) - r_0^\theta(0))^u \zeta'(1) + \\
&\sum_{k=2}^{N-1} \frac{\widetilde{\theta_{0z}(k)}}{\rho_0(k)} (r_0^\theta(k+1) - r_0^\theta(k)) \sum_{k'=2}^{k} \rho_0(k')(r_0^\theta(k') - r_0^\theta(k'-1))^u \zeta'(k') + \\
&\sum_{k=1}^{N-1} \frac{\widetilde{\theta_{0z}(k)}}{\rho_0(k)} (r_0^\theta(k) - r_0^\theta(k-1))\rho_0(1)(r_0^\theta(1) - r_0^\theta(0))^u \zeta'(1) + \\
&\sum_{k=2}^{N-1} \frac{\widetilde{\theta_{0z}(k)}}{\rho_0(k)} (r_0^\theta(k) - r_0^\theta(k-1)) \sum_{k'=2}^{k} \rho_0(k')(r_0^\theta(k') - r_0^\theta(k'-1))^u \zeta'(k') + \\
&\frac{\widetilde{\theta_{0z}(N)}}{\rho_0(N)} (r_0^\theta(N) - r_0^\theta(N-1))\rho_0(1)(r_0^\theta(1) - r_0^\theta(0))^u \zeta'(1) + \\
&\frac{\widetilde{\theta_{0z}(N)}}{\rho_0(N)} (r_0^\theta(N) - r_0^\theta(N-1)) \sum_{k'=2}^{N-1} \rho_0(k')(r_0^\theta(k') - r_0^\theta(k'-1))^u \zeta'(k') + \\
&\frac{\widetilde{\theta_{0z}(N)}}{\rho_0(N)} (r_0^\theta(N) - r_0^\theta(N-1))\rho_0(N)(r_0^\theta(N) - r_0^\theta(N-1))^u \zeta'(N) - \\
&\frac{\tilde{PV_1'}}{I_\rho(N)} \Bigg[\sum_{k=1}^{N} \frac{\widetilde{\theta_{0z}(k)}}{\rho_0(k)} I_\rho(k)(r_0^\theta(k) - r_0^\theta(k-1)) + \\
&\sum_{k=1}^{N-1} \frac{\widetilde{\theta_{0z}(k)}}{\rho_0(k)} I_\rho(k)(r_0^\theta(k+1) - r_0^\theta(k)) \Bigg] \Bigg\} = 0, \qquad (45) \\
&= I_2 - (I_{3A} + I_{3B}) + F_3{}^u \zeta'(1) + I_4 + F_4{}^u \zeta'(1) + I_5 + F_5{}^u \zeta'(1) + I_6 + F_6{}^u \zeta'(N) - I_7 = 0 \qquad (46)
\end{aligned}$$

The idea behind Eq. (45), as with Eq. (35), has been to write the equation is such a way that all occuences of $\zeta'(k')$ never refer to $\zeta'(1)$ or $\zeta'(N)$; these terms have been written separately and explicitly. In Eq. (46) we have written complicated terms, which are known, as single symbols which are defined

$$F_3 = \frac{1}{2} \sum_{k=1}^{N-1} \overbrace{\frac{\theta_{0z}(k)}{\rho_0(k)}} (r_0^\theta(k+1) - r_0^\theta(k)) \rho_0(1)(r_0^\theta(1) - r_0^\theta(0)), \quad (47)$$

$$I_4 = \frac{1}{2} \sum_{k=2}^{N-1} \overbrace{\frac{\theta_{0z}(k)}{\rho_0(k)}} (r_0^\theta(k+1) - r_0^\theta(k)) \sum_{k'=2}^{k} \rho_0(k')(r_0^\theta(k') - r_0^\theta(k'-1))^u\zeta'(k'), \quad (48)$$

$$F_4 = \frac{1}{2} \sum_{k=1}^{N-1} \overbrace{\frac{\theta_{0z}(k)}{\rho_0(k)}} (r_0^\theta(k) - r_0^\theta(k-1)) \rho_0(1)(r_0^\theta(1) - r_0^\theta(0)), \quad (49)$$

$$I_5 = \frac{1}{2} \sum_{k=2}^{N-1} \overbrace{\frac{\theta_{0z}(k)}{\rho_0(k)}} (r_0^\theta(k) - r_0^\theta(k-1)) \sum_{k'=2}^{k} \rho_0(k')(r_0^\theta(k') - r_0^\theta(k'-1))^u\zeta'(k'), \quad (50)$$

$$F_5 = \frac{1}{2} \overbrace{\frac{\theta_{0z}(N)}{\rho_0(N)}} (r_0^\theta(N) - r_0^\theta(N-1)) \rho_0(1)(r_0^\theta(1) - r_0^\theta(0)), \quad (51)$$

$$I_6 = \frac{1}{2} \overbrace{\frac{\theta_{0z}(N)}{\rho_0(N)}} (r_0^\theta(N) - r_0^\theta(N-1)) \sum_{k'=2}^{N-1} \rho_0(k')(r_0^\theta(k') - r_0^\theta(k'-1))^u\zeta'(k'), \quad (52)$$

$$F_6 = \frac{1}{2} \overbrace{\frac{\theta_{0z}(N)}{\rho_0(N)}} (r_0^\theta(N) - r_0^\theta(N-1)) \rho_0(N)(r_0^\theta(N) - r_0^\theta(N-1)), \quad (53)$$

$$I_7 = \frac{\tilde{PV}_1'}{2I_\rho(N)} \left[\sum_{k=1}^{N} \overbrace{\frac{\theta_{0z}(k)}{\rho_0(k)}} I_\rho(k)(r_0^\theta(k) - r_0^\theta(k-1)) + \sum_{k=1}^{N-1} \overbrace{\frac{\theta_{0z}(k)}{\rho_0(k)}} I_\rho(k)(r_0^\theta(k+1) - r_0^\theta(k)) \right]. \quad (54)$$

Equation (46) is the second simultaneous equation. In Eqs. (35) and (46) the terms, I_n and F_n are known as they involve either integrals of ${}^u p'$, ${}^u\zeta'$ over the bulk, or linearization state quantities. Hence Eqs. (35) and (46) form a couple of simultaneous equations that can be solved for ${}^u\zeta'(1)$ and ${}^u\zeta'(N)$. This yields,

$${}^u\zeta'(1) = \frac{(I_1 - f_u I_B(N))F_6 - F_2(I_2 - I_{3A} - I_{3B} + I_4 + I_5 + I_6 - I_7)}{F_2(F_3 + F_4 + F_5) - F_1 F_6}, \quad (55)$$

$${}^u\zeta'(N) = \frac{F_1(I_2 - I_{3A} - I_{3B} + I_4 + I_5 + I_6 - I_7) - (I_1 - f_u I_B(N))(F_3 + F_4 + F_5)}{F_2(F_3 + F_4 + F_5) - F_1 F_6}, \quad (56)$$

which can be converted into winds by Eq. (32). Important note: $I_7 = 0$ by definition. Since I_7 depends upon PV_1' (Eq. (54)), which is zero, so will $I_7 = 0$.

3.3 The third equation, χ'

The third control variable is velocity potential increment, χ'. This describes the irrotational component to the flow. For the U_p transform, the $\vec{e}_3$ operator has the simplest structure of the three variables. For the divergent flow, $\vec{X}_3' = (u_3', v_3', p_3')^T$ is given simply by the divergence operator with zero pressure increment,

$$\vec{X}_3' = \vec{e}_3 \chi' = \begin{pmatrix} \partial/\partial x \\ \partial/\partial y \\ 0 \end{pmatrix} \chi', \quad (57)$$

which is, once more, in local cartesian coordinates.

Knowing Eqs. (29), (34), (55), (56) and (57), we can in principle compute the full field increments from the parameter increments output from the optimization part of the assimilation scheme. The $\vec{e}_n$ operators (except for $\vec{e}_3$) are implicit, requiring the solution of an elliptical equation.

This section is under revision.

The objective of the T_p transform is to determine the fields of the control variables, s', ${}^{u}p'$ and χ' given increments in the model fields. For assimilation, this step is needed when calibrating the background error statistics, and for each outer loop in the assimilation, if implemented. We discuss below, in turn, the equations needed to determine each field.

4.1 The first equation, PV'

Referring to the expanded form of the equation that will allow us to perform the T_p transform (Eq. (10)), recall that we wish to design the dual operator $\vec{f}_1^* \vec{X}'$ to yield a PV increment (where PV' is linearized as in Eq. (18) in the bulk and Eqs. (23) and (25) for the vertical boundaries). At the same time, we insist that both $\vec{f}_1^* \vec{e}_2 {}^{u}p'$ and $\vec{f}_1^* \vec{e}_3 \chi'$ are zero valued, which will be imposed as a result of the choice of U transforms (imposing that the balanced component has no $\bar{PV}'$ and that the leading unbalanced component has no PV', etc.).

To form the equations that we wish to solve, first substitute the balanced components (from Eq. (29)) into PV' (Eq. (18), PV'_1 (Eq. (23) and PV'_2 (Eq. (25), noting that $\zeta' = \nabla_z^2 s'$,

$$
\begin{aligned}
PV' \;=\;& \frac{\theta_{0z}}{\rho_0} \nabla_z^2 s' - \\
& \frac{f\theta_{0z}}{\rho_0^2} \left\{ \frac{1-\kappa}{R\Pi_0 \hat{\theta}_0} \nabla_z^{-2} \rho_0 \nabla_z \cdot (f \nabla_z s') + \right. \\
& \left. \frac{\rho_0}{\hat{\theta}_0} \overbrace{\frac{1}{\Pi_{0z}} \left[\theta_0 \frac{\partial}{\partial z} \left(\kappa \frac{\Pi_0}{p_0} \nabla_z^{-2} \rho_0 \nabla_z \cdot (f \nabla_z s') \right) \right]} \right\} + \\
& \frac{f}{\rho_0} \frac{g}{c_p} \left\{ \frac{1}{\Pi_{0z}^2} \frac{\partial^2}{\partial z^2} \left(\kappa \frac{\Pi_0}{p_0} \nabla_z^{-2} \rho_0 \nabla_z \cdot (f \nabla_z s') \right) - \right. \\
& \left. \frac{2\Pi_{0zz}}{\Pi_{0z}^3} \overbrace{\frac{\partial}{\partial z} \left(\kappa \frac{\Pi_0}{p_0} \nabla_z^{-2} \rho_0 \nabla_z \cdot (f \nabla_z s') \right)} \right\}.
\end{aligned}
\tag{58}
$$

$$
\begin{aligned}
PV'_1 \;=\;& \int_{z=0}^{z_{top}} \mathrm{d}z \left\{ \rho_0 \nabla_z^2 s' - \right. \\
& f \left(\frac{1-\kappa}{R\Pi_0 \hat{\theta}_0} \nabla_z^{-2} \rho_0 \nabla_z \cdot (f \nabla_z s') + \right. \\
& \left. \left. \frac{\rho_0}{\hat{\theta}_0} \overbrace{\frac{1}{\Pi_{0z}} \left\{ \theta_0 \frac{\partial}{\partial z} \left(\kappa \frac{\Pi_0}{p_0} \nabla_z^{-2} \rho_0 \nabla_z \cdot (f \nabla_z s') \right) \right\}} \right) \right\},
\end{aligned}
\tag{59}
$$

$$
\begin{aligned}
PV'_2 \;=\;& \int_{z=0}^{z_{top}} \mathrm{d}z \overbrace{\frac{1}{\Pi_{0z}} \left\{ \theta_0 \frac{\partial}{\partial z} \left(\kappa \frac{\Pi_0}{p_0} \nabla_z^{-2} \rho_0 \nabla_z \cdot (f \nabla_z s') \right) \right\}} - \\
& \int_{z=0}^{z_{top}} \mathrm{d}z \frac{\theta_{0z}}{\rho_0} \int_{z'=0}^{z} \mathrm{d}z' \left\{ \frac{1-\kappa}{R\Pi_0 \hat{\theta}_0} \nabla_z^{-2} \rho_0 \nabla_z \cdot (f \nabla_z s') + \right. \\
& \left. \frac{\rho_0}{\hat{\theta}_0} \overbrace{\frac{1}{\Pi_{0z}} \left\{ \theta_0 \frac{\partial}{\partial z} \left(\kappa \frac{\Pi_0}{p_0} \nabla_z^{-2} \rho_0 \nabla_z \cdot (f \nabla_z s') \right) \right\}} \right\} + \\
& \frac{1}{f} \int_{z=0}^{z_{top}} \mathrm{d}z \frac{\theta_{0z}}{\rho_0} \int_{z'=0}^{z} \mathrm{d}z' \rho_0 \nabla_z^2 s'.
\end{aligned}
\tag{60}
$$

The bulk and boundary equations together form a set of simultaneous equations that we must solve for s' in the T_p transform. In order to do this, the left-hand-sides, PV', PV'_1 and PV'_2, must be known corresponding to the balanced component of the model state that we wish to transform. The premise however is that PV' can be calculated from the full increment, $\vec{X}'$. It follows that this is the case given that $\vec{f}_1^* \vec{e}_2 {}^{u}p'$ and $\vec{f}_1^* \vec{e}_3 \chi'$ are zero (see the first line of Eq. (10)) in this linearized framework. The unbalanced component of the flow has no PV by design of the transforms, and the divergent part respectively non-zero PV', PV_1' and PV_2'.

4.2 The second equation, $\bar{PV}'$

The second stage in the T_p transform will involve computing the $\bar{PV}'$. The procedure is along the same lines as above. The equation that we have to solve is the second row of Eq. (10). Given that the balanced, s' and divergence, χ' control variables contribute nothing to $\bar{PV}'$, $\bar{PV}'$ is due solely to ${}^u p'$. Thus substitute the model increments associated with ${}^u p'$ (Eqs. (34), (55) and (56)) into Eq. (30). The T_p procedure to calculate the ${}^u p'$ control variable then consists of solving the following equation, which is the second stage of the T_p transform,

$$
\begin{aligned}
\bar{PV}' &= -\rho_0 f \left(f + \frac{\mathrm{d}f}{\mathrm{d}y} \nabla^{-2} \frac{\partial}{\partial y} \right) \times \\
&\left\{ \left(\frac{p_0 p_{0zz}}{p_{0z}^2} - \frac{c_v}{c_p} \right)^{-1} f \left(\frac{p_0}{p_{0z}^2} {}^u p'_{zz} + \frac{c_v}{c_p} \left(\left(\frac{p_{0zz}}{p_{0z}^2} + \frac{\kappa}{p_0} \right) {}^u p' + \frac{1}{p_{0z}} {}^u p'_z \right) - 3 \frac{p_0 p_{0zz}}{p_{0z}^3} {}^u p'_z \right) \right\} - \\
&f \nabla_z^2 {}^u p',
\end{aligned}
\tag{61}
$$

when ${}^u p$ is in the bulk. For the vertical boundaries, the following completes the system of simultaneous equations,

$$
\begin{aligned}
\bar{PV}'(0) &= f \rho_0 \nabla_z \cdot (f \mathbf{k} \times \nabla^{-2} [\nabla \times {}^u \zeta'(0) \mathbf{k}]) - f \nabla_z^2 {}^u p'(0), && (62) \\
\bar{PV}'(z_{top}) &= f \rho_0 \nabla_z \cdot (f \mathbf{k} \times \nabla^{-2} [\nabla \times {}^u \zeta'(z_{top}) \mathbf{k}]) - f \nabla_z^2 {}^u p'(z_{top}). && (63)
\end{aligned}
$$

In Eqs. (62) and (63), $\zeta'(0)$ and $\zeta'(z_{top})$ must be substituted from Eqs. (55) and (56) respectively. This has not been done explicitly here for clarity. Note that in constructing the last equations, the following relations are useful,

$$
\begin{aligned}
\mathbf{u} &= -\nabla^{-2} (\nabla \times \zeta \mathbf{k}), && (64) \\
\nabla \psi &= \mathbf{k} \times \nabla^{-2} (\nabla \times \zeta \mathbf{k}), && (65)
\end{aligned}
$$

for $\mathbf{u}$ divergence-free.

The $\bar{PV}'$ due to s' increments is shown to be zero by substituting Eq. (29) for the corresponding model increments into Eq. (30) for $\bar{PV}'$. Similarly, χ' is shown to have zero $\bar{PV}'$ by substituting Eq. (57) into Eq. (30). These two zero results state equivalently that $\vec{f}_2^* \vec{e}_1 s' = 0$ and $\vec{f}_2^* \vec{e}_3 \chi' = 0$.

4.3 The third equation, $\nabla_z \cdot \mathbf{u_h}$

The third dual operator, $\vec{f}_3^*$, is designed to calculate the divergent part of the flow. The contribution from the χ' control variable is found by computing the divergence of u_3 and v_3 from Eq. (57),

$$
\nabla_z \cdot \mathbf{u_h}' = \vec{f}_3^* \vec{e}_3 \chi' = \nabla_z^2 \chi'. \tag{66}
$$

As before, we may show that $\vec{f}_3^* \vec{e}_1 s'$ and $\vec{f}_3^* \vec{e}_2 {}^u p'$ are zero, meaning that the total divergence of a model increment is the same as that of the contribution from the third term only. It is trivial to show that these results hold. This is achieved by computing the horizontal divergence of $(u_1', v_1')^T$ (from Eq. (29) and $(u_2', v_2')^T$ (from Eq. (34), and observing that they are zero.

Normally, Ertel PV is specified in isentropic co-ordinates,

$$Q = \frac{\zeta_\theta + f}{-\frac{1}{g}\frac{\partial p}{\partial \theta}}, \tag{67}$$

where the relative vorticity evaluated on an isentropic surface, ζ_θ, is,

$$\zeta_\theta = \mathbf{k} \cdot (\nabla_\theta \times \mathbf{u_h}). \tag{68}$$

In Eq. (68), $\mathbf{k}$ is the vectical unit vector, ∇_θ is the gradient operator evaluated along isentropic surfaces in the horizontal, and $\mathbf{v_h}$ is the horizontal vecocity. In order to transform to height (z) co-ordinates, we make use of the following relations in the vertical and in the horizontal,

$$\begin{aligned} \frac{\partial p}{\partial \theta} &= \frac{\partial z}{\partial \theta}\frac{\partial p}{\partial z} = -\frac{\partial z}{\partial \theta}\rho g \\ \left(\frac{\partial}{\partial x}\right)_z &= \left(\frac{\partial}{\partial x}\right)_\theta + \left(\frac{\partial \theta}{\partial x}\right)_z \frac{\partial}{\partial \theta} \\ \left(\frac{\partial}{\partial y}\right)_z &= \left(\frac{\partial}{\partial y}\right)_\theta + \left(\frac{\partial \theta}{\partial y}\right)_z \frac{\partial}{\partial \theta}. \end{aligned} \tag{69}$$

Inserting this information into Eq. (67), and the following emerges,

$$PV = \frac{1}{\rho}\left\{(\zeta_{zk} + f)\frac{\partial \theta}{\partial z} - \mathbf{k} \cdot \left(\nabla_z \theta \times \frac{\partial \mathbf{u_h}}{\partial z}\right)\right\}, \tag{70}$$

where ζ_{zk} means the vertical component of relative vorticity evaluated on a surface of constant height. In the text we will assume that the second term of Eq. (70) is much smaller in magnitude than the first.

7 Appendix B: The 'missing' PV modes

In order to develop two alternative PV-like quantities, to replace the linearized Ertel PV at the top and bottom we consider the following.

7.1 Missing mode 1

The continuity equation,

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0, \tag{71}$$

is linearized about a reference state of rest giving,

$$\frac{\partial \rho'}{\partial t} + \nabla \cdot (\rho_0 \mathbf{u}') = 0. \tag{72}$$

Separating-out the horizontal and vertical contributions to the inner products gives,

$$\frac{\partial \rho'}{\partial t} + \nabla_z \cdot (\rho_0 \mathbf{u_h'}) + \frac{\partial(\rho_0 w')}{\partial z} = 0. \tag{73}$$

Vertically integrate this equation over the depth of the model's atmosphere and multiply by f (assume no vertical motion at the top and bottom of the model's domain),

$$\int_{z=0}^{z_{top}} \mathrm{d}z f \frac{\partial \rho'}{\partial t} + \int_{z=0}^{z_{top}} \mathrm{d}z f \nabla_z \cdot (\rho_0 \mathbf{u_h'}) = 0. \tag{74}$$

The last term can be split into two using the product rule for differentiation. Writing in terms of the horizontal divergence, $\delta' = \nabla_z \cdot \mathbf{u_h'}$, where it appears gives the following,

$$\int_{z=0}^{z_{top}} \mathrm{d}z f \frac{\partial \rho'}{\partial t} + \int_{z=0}^{z_{top}} \mathrm{d}z f \rho_0 \delta' + \int_{z=0}^{z_{top}} \mathrm{d}z f \mathbf{u_h'} \cdot \nabla_z \rho_0 = 0. \tag{75}$$

$$\frac{\partial \zeta}{\partial t} + \mathbf{u} \cdot \nabla(\zeta + f) + \delta(\zeta + f) = 0 \tag{76}$$

is also linearized about a reference state of rest,

$$\frac{\partial \zeta'}{\partial t} + \mathbf{u}' \cdot \nabla f + \delta' f = 0. \tag{77}$$

Multiply this equation by ρ_0 and vertically integrate over the depth of the model's atmosphere,

$$\int_{z=0}^{z_{top}} \mathrm{d}z \rho_0 \frac{\partial \zeta'}{\partial t} + \int_{z=0}^{z_{top}} \mathrm{d}z \rho_0 \mathbf{u}' \cdot \nabla f + \int_{z=0}^{z_{top}} \mathrm{d}z \rho_0 \delta' f = 0. \tag{78}$$

Equations (75) and (78) both contain the term $\int \mathrm{d}z \rho_0 \delta' f$, which can be eliminated by taking Eq. (78) minus Eq. (75). Assuming furthermore that the time variation of ρ_0 is small gives,

$$\frac{\partial}{\partial t} \int_{z=0}^{z_{top}} \mathrm{d}z (\rho_0 \zeta' - f \rho') = - \int_{z=0}^{z_{top}} \mathrm{d}z \rho_0 \mathbf{u}' \cdot \nabla f + \int_{z=0}^{z_{top}} \mathrm{d}z f \mathbf{u}'_{\mathbf{h}} \cdot \nabla_z \rho_0. \tag{79}$$

The quantity that is differentiated with respect to time is the first 'missing' PV quantity ($\partial/\partial t \sim \mathrm{d}/\mathrm{d}t$ for this quantity). It is PV-like because it is approximately conserved (assuming that the right hand side is small, and perhaps more crucially, that its time evolution does not depend on divergence). It is more convenient to write the ρ' increment in terms of a pressure-like quantity. To achieve this, use Eq. (108) from appendix C. Making this substitution gives,

$$\begin{aligned} PV'_1 &= \int_{z=0}^{z_{top}} \mathrm{d}z (\rho_0 \zeta' - f \rho'), \\ &= \int_{z=0}^{z_{top}} \mathrm{d}z \rho_0 \zeta' - f \int_{z=0}^{z_{top}} \mathrm{d}z \left(\frac{1-\kappa}{R \Pi_0 \hat{\theta}_0} p' + \frac{\rho_0}{\hat{\theta}_0} \overbrace{\frac{1}{\Pi_{0z}} \left\{ \theta_0 \frac{\partial}{\partial z} \left(\kappa \frac{\Pi_0}{p_0} p' \right) \right\}} \right). \end{aligned} \tag{80}$$

7.2 Missing mode 2

The second missing PV-like mode is constructed in a similar way. The (adiabatic) thermodynamic equation is,

$$\frac{\partial \theta}{\partial t} + \mathbf{u} \cdot \nabla \theta = 0, \tag{81}$$

which is linearized about a reference state of rest and the inner products are separated into horizontal and vertical components,

$$\begin{aligned} \frac{\partial \theta'}{\partial t} + \mathbf{u}' \cdot \nabla \theta_0 &= 0, \\ \frac{\partial \theta'}{\partial t} + \mathbf{u}'_{\mathbf{h}} \cdot \nabla_z \theta_0 + w' \frac{\partial \theta_0}{\partial z} &= 0. \end{aligned} \tag{82}$$

Integrate over the full thickness of the model and assume that the second term is negligible,

$$\int_{z=0}^{z_{top}} \mathrm{d}z \frac{\partial \theta'}{\partial t} + \int_{z=0}^{z_{top}} \mathrm{d}z w' \frac{\partial \theta_0}{\partial z} = 0. \tag{83}$$

We would like to use the continuity equation to eliminate w' in Eq. (83). Return to Eq. (73) but instead of integrating it over the entire thickness of the atmosphere as for the missing PV mode 1, integrate from the ground up to height z,

$$\int_{z'=0}^{z} \mathrm{d}z' \frac{\partial \rho'}{\partial t} + \int_{z'=0}^{z} \mathrm{d}z' \rho_0 \delta' + \int_{z'=0}^{z} \mathrm{d}z' \mathbf{u}'_{\mathbf{h}} \cdot \nabla_z \rho_0 + \rho_0(z) w'(z) = 0, \tag{84}$$

(zero vertical motion has been assumed at the bottom). Eliminate the third term which is assumed to be negligible and rearrange for w',

$$w'(z) = -\frac{1}{\rho_0(z)} \left(\int_{z'=0}^{z} \mathrm{d}z' \frac{\partial \rho'}{\partial t} + \int_{z'=0}^{z} \mathrm{d}z' \rho_0 \delta' \right). \tag{85}$$

$$\int_{z=0}^{z_{top}} \mathrm{d}z \frac{\partial \theta'}{\partial t} - \int_{z=0}^{z_{top}} \mathrm{d}z \frac{\partial \theta_0}{\partial z} \frac{1}{\rho_0} \left(\int_{z'=0}^{z} \mathrm{d}z' \frac{\partial \rho'}{\partial t} + \int_{z'=0}^{z} \mathrm{d}z' \rho_0 \delta' \right) = 0. \tag{86}$$

Just as for mode 1, the important term to eliminate is the divergence increment. This is eliminated with the vorticity equation (Eq. (77) with terms dropped that are assumed small),

$$\frac{\partial \zeta'}{\partial t} + \delta' f = 0, \tag{87}$$

which, when substituted into Eq. (86) gives,

$$\int_{z=0}^{z_{top}} \mathrm{d}z \frac{\partial \theta'}{\partial t} - \int_{z=0}^{z_{top}} \mathrm{d}z \frac{\partial \theta_0}{\partial z} \frac{1}{\rho_0} \left(\int_{z'=0}^{z} \mathrm{d}z' \frac{\partial \rho'}{\partial t} - \int_{z'=0}^{z} \mathrm{d}z' \frac{\rho_0}{f} \frac{\partial \zeta'}{\partial t} \right) = 0. \tag{88}$$

Taking the time derivative operator outside of the integrals (assuming that the linearization state quantities are slowly varying) reveals the second PV-like quantity,

$$\frac{\partial}{\partial t} \left(\int_{z=0}^{z_{top}} \mathrm{d}z \theta' - \int_{z=0}^{z_{top}} \mathrm{d}z \frac{\partial \theta_0}{\partial z} \frac{1}{\rho_0} \int_{z'=0}^{z} \mathrm{d}z' \rho' + \int_{z=0}^{z_{top}} \mathrm{d}z \frac{\partial \theta_0}{\partial z} \frac{1}{\rho_0} \int_{z'=0}^{z} \mathrm{d}z' \frac{\rho_0}{f} \zeta' \right) = 0, \tag{89}$$

where the quantity inside the brackets is PV_2'. We wish to write all mass increments (θ' and ρ') in terms of pressure. Density is related to the pressure by Eq. (108), and potential temperature via Eq. (107). Substituting these equations into PV_2 gives,

$$\begin{aligned} PV_2' &= f \int_{z=0}^{z_{top}} \mathrm{d}z \theta' - f \int_{z=0}^{z_{top}} \mathrm{d}z \frac{\partial \theta_0}{\partial z} \frac{1}{\rho_0} \int_{z'=0}^{z} \mathrm{d}z' \rho' + \int_{z=0}^{z_{top}} \mathrm{d}z \frac{\partial \theta_0}{\partial z} \frac{1}{\rho_0} \int_{z'=0}^{z} \mathrm{d}z' \rho_0 \zeta' && (90) \\ &= f \int_{z=0}^{z_{top}} \mathrm{d}z \overbrace{\frac{1}{\Pi_{0z}} \left\{ \theta_0 \frac{\partial}{\partial z} \left(\kappa \frac{\Pi_0}{p_0} p' \right) \right\}} - \\ &\quad f \int_{z=0}^{z_{top}} \mathrm{d}z \frac{\theta_{0z}}{\rho_0} \int_{z'=0}^{z} \mathrm{d}z' \left\{ \frac{1-\kappa}{R \Pi_0 \hat{\theta}_0} p' + \frac{\rho_0}{\hat{\theta}_0} \overbrace{\frac{1}{\Pi_{0z}} \left\{ \theta_0 \frac{\partial}{\partial z} \left(\kappa \frac{\Pi_0}{p_0} p' \right) \right\}} \right\} + \\ &\quad \int_{z=0}^{z_{top}} \mathrm{d}z \frac{\theta_{0z}}{\rho_0} \int_{z'=0}^{z} \mathrm{d}z' \rho_0 \zeta'. && (91) \end{aligned}$$

In the above definition of PV_2, we have multiplied by f to remove the $1/f$ factor in the last term.

It is found that PV_1 and PV_2 have almost identical structures, dominated by the vorticity field. Differences in the two structures emerge when PV_1 and PV_2 are partially orthogonalised. To do this we make a modification to PV_2. To understand how to make this modification first assume that (a) vorticity increments dominate the two quantities and (b) vorticity is independent of height (call ζ'). PV_1 and PV_2 then approximate to,

$$\begin{aligned} PV_1' &\approx \zeta' \int_{z'=0}^{z_{top}} \mathrm{d}z' \rho_0, && (92) \\ PV_2' &\approx \int_{z=0}^{z_{top}} \mathrm{d}z \frac{1}{\rho_0} \frac{\partial \theta_0}{\partial z} \left\{ \zeta' \int_{z'=0}^{z} \mathrm{d}z' \rho_0 \right\}. && (93) \end{aligned}$$

The part of Eq. (93) inside the curly braces may be replicated from Eq. (92) as,

$$\int_{z'=0}^{z} \mathrm{d}z' \rho_0 \zeta' \approx \frac{PV_1' \int_{z'=0}^{z} \mathrm{d}z' \rho_0}{\int_{z'=0}^{z_{top}} \mathrm{d}z' \rho_0}. \tag{94}$$

The approximate forms of PV_1 and PV_2 have been used to derive this result, which is now used to try to orthogonalize the missing PV terms in their exact forms, Eqs. (80) and (91). PV_1 stays the same, but PV_2 has the following adjustment, based on the result in Eq. (94),

$$\begin{aligned} PV_2' &= f \int_{z=0}^{z_{top}} \mathrm{d}z \overbrace{\frac{1}{\Pi_{0z}} \left\{ \theta_0 \frac{\partial}{\partial z} \left(\kappa \frac{\Pi_0}{p_0} p' \right) \right\}} - \\ &\quad f \int_{z=0}^{z_{top}} \mathrm{d}z \frac{\theta_{0z}}{\rho_0} \int_{z'=0}^{z} \mathrm{d}z' \left\{ \frac{1-\kappa}{R \Pi_0 \hat{\theta}_0} p' + \frac{\rho_0}{\hat{\theta}_0} \overbrace{\frac{1}{\Pi_{0z}} \left\{ \theta_0 \frac{\partial}{\partial z} \left(\kappa \frac{\Pi_0}{p_0} p' \right) \right\}} \right\} + \\ &\quad \int_{z=0}^{z_{top}} \mathrm{d}z \frac{\theta_{0z}}{\rho_0} \left\{ \int_{z'=0}^{z} \mathrm{d}z' \rho_0 \zeta' - \frac{PV_1' \int_{z'=0}^{z} \mathrm{d}z' \rho_0}{\int_{z'=0}^{z_{top}} \mathrm{d}z' \rho_0} \right\}, && (95) \end{aligned}$$

The first term is a single integral and is performed using a low-order integral scheme where the contribution of $I(z)$ from a layer is simply $I(z)\delta z$ (this might be called the "rectangle rule"). Where double integrals are performed (the last two terms), the inner integral is performed using the rectangle rule, and the outer integral is performed using the trapezium rule. The reason for this difference is due to the vertical staggering. Since the inner integrals sum quantities held at p-levels, a rectangle rule integration will give a result on θ-levels (see Fig. (2), right-hand panel). The outer integrals then sum quantities held on θ-levels, and the result is also on θ-levels. The trapezium rule achieves this (see Fig. (2), left-hand panel). More details are given in appendix E which is concerned with discretization. How the expressions for PV_1' and PV_2' are used in the transforms is explained in the text.

8 Appendix C: Useful Relations between Variables

8.1 Relations between full model variables

The relationship between temperature, T and potential temperature, θ is expressed as,

$$\hat{T} = \Pi\hat{\theta}, \tag{96}$$

where the exner pressure, Π is,

$$\Pi = \left(\frac{p}{p_{1000}}\right)^{\kappa}. \tag{97}$$

Here p is pressure, $p_{1000} = 1000\text{hPa}$ is a reference pressure, and κ is the dimensionless constant, $\kappa = R/c_p$ (R is the specific gas constant ($R = c_p - c_v$), and c_p (c_v) is the specific heat capacity at constant pressure (volume)). Some quantities in Eq. (96) have been assigned a hat, $\hat{}$. This denotes that, due to the grid staggering, vertical interpolation has to be performed to estimate the quantity at an intermediate level. In Eq. (96), temperature and potential temperature are situated on θ-levels and pressure and exner pressure on p-levels (see Fig. (1)), and so for the relation to hold, vertical interpolation of T and θ has to be performed to the p-level of Π.

Differentiating Eq. (97) with respect to height yields, on θ-levels,

$$\begin{aligned} \frac{\partial\Pi}{\partial z} &= \kappa\left(\frac{\hat{p}}{p_{1000}}\right)^{\kappa-1}\frac{1}{p_{1000}}\frac{\partial p}{\partial z}, \\ &= \kappa\frac{\hat{\Pi}}{\hat{p}}\frac{\partial p}{\partial z}, \end{aligned} \tag{98}$$

Differentiation of Π in Eq. (97) with respect to p yields,

$$\frac{\mathrm{d}\Pi}{\mathrm{d}p} = \kappa\frac{\Pi}{p}. \tag{99}$$

The ideal gas equation of state on θ- and p-levels respectively, and developed from (p, ρ, T) to (p, Π, ρ, θ) using Eq. (96) is,

$$\begin{aligned} &\theta\text{-levels}: \\ &\qquad \hat{p} = R\hat{\rho}T, \\ &\qquad\quad = R\hat{\rho}\hat{\Pi}\theta, \end{aligned} \tag{100}$$

$$\begin{aligned} &p\text{-levels}: \\ &\qquad p = R\rho\Pi\hat{\theta}. \end{aligned} \tag{101}$$

The familiar hydrostatic relation, written on θ-levels (Eq. (102) below) may be developed in terms of Π and θ using the above equations,

$$\frac{\partial p}{\partial z} = -\hat{\rho}g = -\frac{\hat{p}g}{R\hat{\Pi}\theta}, \tag{102}$$

$$\theta\frac{\partial\Pi}{\partial z} = -\frac{g}{c_p} \tag{103}$$

balance. This equation will be used to derive relations between incremental quantities (see below), which *are* assumed to be in hydrostatic balance, in line with the Var. convention.

Differentiate Eq. (103) with respect to height (divide by $\partial\Pi/\partial z$ first), and give the result on p-levels,

$$\begin{aligned}
\theta &= -\frac{g}{c_p}\left(\frac{\partial \Pi}{\partial z}\right)^{-1}, \\
\frac{\partial \theta}{\partial z} &= \frac{g}{c_p}\left(\frac{\widehat{\partial \Pi}}{\partial z}\right)^{-2}\frac{\partial^2 \Pi}{\partial z^2}.
\end{aligned} \tag{104}$$

8.2 Relations between increments

The above equations allow us to relate incremental quantities to other incremental quantites, while taking into account the grid staggering.

To write ρ increments in terms of other increments, develop the equation of state. Start with Eq. (101) and then write in incremental form,

$$\begin{aligned}
p &= R\rho\Pi\hat{\theta}, \\
p' &= R\rho\Pi\hat{\theta}' + R\rho\hat{\theta}\Pi' + R\Pi\hat{\theta}\rho', \\
&= R\rho\Pi\hat{\theta}' + \kappa p' + R\Pi\hat{\theta}\rho', \\
\therefore \rho' &= \frac{1-\kappa}{R\Pi\hat{\theta}}p' - \frac{\rho}{\hat{\theta}}\hat{\theta}',
\end{aligned} \tag{105}$$

where, for the third line in the above, we have written Π' in terms of p' using Eqs. (99) and (101).

It is often necessary to write θ increments in terms of p increments. We use the hydrostatic relation, Eq. (103), for this purpose. This is written in terms of increments below,

$$\begin{aligned}
\theta\frac{\partial \Pi}{\partial z} &= -\frac{g}{c_p}, \\
\theta\frac{\partial \Pi'}{\partial z} + \frac{\partial \Pi}{\partial z}\theta' &= 0, \\
\theta\frac{\partial}{\partial z}\left(\kappa\frac{\Pi}{p}p'\right) + \frac{\partial \Pi}{\partial z}\theta' &= 0,
\end{aligned} \tag{106}$$

where Eq. (99) has been used for the last line. We wish to elliminate θ' between Eqs. (105) and (106). In order to do this, we must first compute $\hat{\theta}'$ from Eq. (106), which involves further vertical interpolation,

$$\hat{\theta}' = -\overbrace{\left(\frac{\partial \Pi}{\partial z}\right)^{-1}\left\{\theta\frac{\partial}{\partial z}\left(\kappa\frac{\Pi}{p}p'\right)\right\}}, \tag{107}$$

where the overbrace represents a hat acting on the entire right hand side. This equation is now substituted into Eq. (105),

$$\rho' = \frac{1-\kappa}{R\Pi\hat{\theta}}p' + \frac{\rho}{\hat{\theta}}\overbrace{\left(\frac{\partial \Pi}{\partial z}\right)^{-1}\left\{\theta\frac{\partial}{\partial z}\left(\kappa\frac{\Pi}{p}p'\right)\right\}}. \tag{108}$$

This gives density in terms of p and p_z increments. Note that if it were not for the vertical interpolation, there would be much cancelling and ρ' would have been written in terms of p_z increments only.

Increments of $\partial\theta/\partial z$ in terms of p increments are also required. Writing the incremental form of Eq. (104) in p-levels gives,

$$\begin{aligned}
\frac{\partial \theta'}{\partial z} &= \frac{g}{c_p}\left\{\left(\frac{\widehat{\partial \Pi}}{\partial z}\right)^{-2}\frac{\partial^2 \Pi'}{\partial z^2} - 2\left(\frac{\widehat{\partial \Pi}}{\partial z}\right)^{-3}\frac{\partial^2 \Pi}{\partial z^2}\frac{\widehat{\partial \Pi'}}{\partial z}\right\}, \\
&= \frac{g}{c_p}\left\{\left(\frac{\widehat{\partial \Pi}}{\partial z}\right)^{-2}\frac{\partial^2}{\partial z^2}\left(\kappa\frac{\Pi}{p}p'\right) - 2\left(\frac{\widehat{\partial \Pi}}{\partial z}\right)^{-3}\frac{\partial^2 \Pi}{\partial z^2}\overbrace{\frac{\partial}{\partial z}\left(\kappa\frac{\Pi}{p}p'\right)}\right\},
\end{aligned} \tag{109}$$

where, for the last line, Eq. (99) has been used.

The Met Office 'new dynamics' grid is an Arakawa 'C' grid in the horizontal and a Charney-Phillips grid in the vertical (see Fig. (1)). The position of parameters is labeled as coincident with u, v, ψ, p or θ. It has been decided to store the new parameters introduced in this work at the points outlined in table (I).

Parameter	Staggering
PV'	ψ
$\bar{PV}'$	p
$\nabla_z \cdot \mathbf{u_h}'$	p
s'	ψ
${}^{U}p$	p
χ	p

Table I: Staggering of dual space and control parameters.

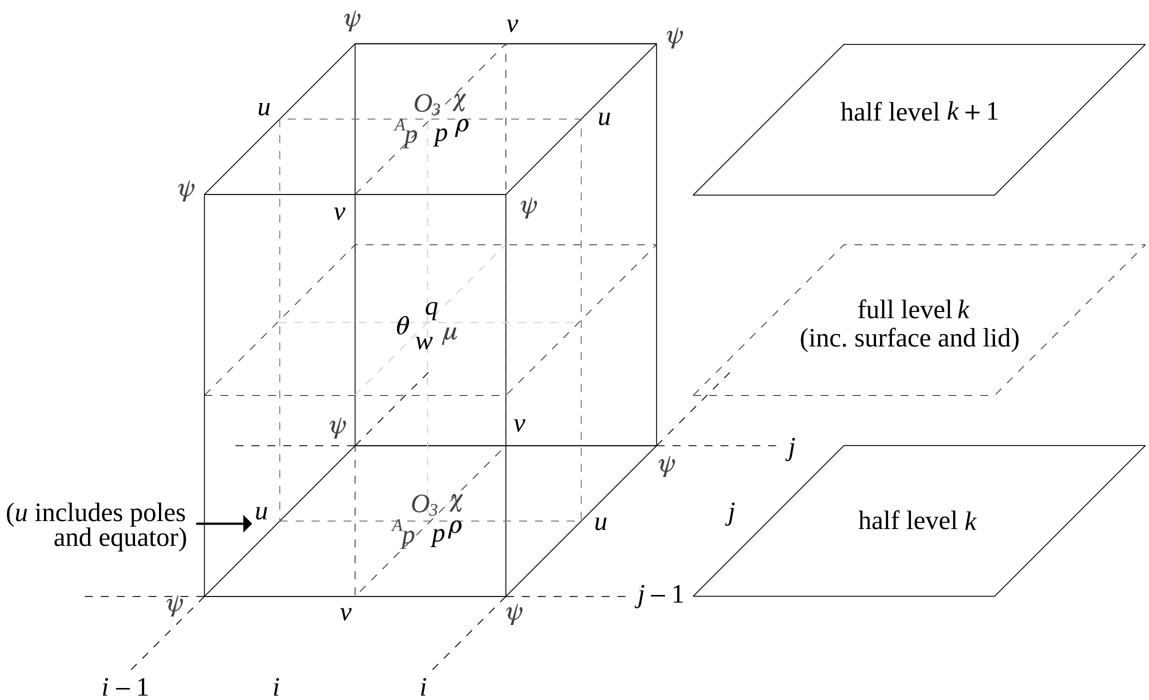

Figure 1: The Met Office 'new dynamics' grid staggering.

10 Appendix E: Discretization and finite differencing

Here we develop finite difference formulae for the important expressions in our scheme. We use spherical coordinates throughout this appendix.

10.1 Notation

Refer to the table II below for the meaning of symbols that do horizontal or vertical interpolation.

The α_1, β_1, α_2 and β_2 are vertical interpolation coefficients used for this purpose, as in the new dynamics formulation. These coefficients are position dependent, although for compactness the position dependence has been dropped in the above formulae). For interpolation from full (θ) levels to half (p)

Horizontal (p-to-ψ)	$\tilde{A}(i,j,k) = \frac{1}{4}(A(i,j,k) + A(i,j+1,k) + A(i+1,j,k) + A(i+1,j+1,k))$	$\overline{\text{long expression}}$
Horizontal (ψ-to-p)	$\tilde{A}(i,j,k) = \frac{1}{4}(A(i,j,k) + A(i,j-1,k) + A(i-1,j,k) + A(i-1,j-1,k))$	$\overline{\text{long expression}}$
Vertical (θ-to-p)	$\hat{B}(i,j,k) = \alpha_1 B(i,j,k) + \beta_1 B(i,j,k-1)$	$\overbrace{\text{long expression}}$
Vertical (p-to-θ)	$\hat{C}(i,j,k) = \alpha_2 C(i,j,k+1) + \beta_2 C(i,j,k)$	$\overbrace{\text{long expression}}$

Table II: Notation for horizontal and vertical interpolation.

levels, as in the second row of table II the coefficents are,

$$\alpha_1(i,j,k) = \frac{r_0^p(i,j,k) - r_0^\theta(i,j,k-1)}{r_0^\theta(i,j,k) - r_0^\theta(i,j,k-1)}, \tag{110}$$

$$\beta_1(i,j,k) = \frac{r_0^\theta(i,j,k) - r_0^p(i,j,k)}{r_0^\theta(i,j,k) - r_0^\theta(i,j,k-1)}, \tag{111}$$

and for interpolation from half (p) levels to full (θ) levels, as in the last row of the table the coefficents are,

$$\alpha_2(i,j,k) = \frac{r_0^\theta(i,j,k) - r_0^p(i,j,k)}{r_0^p(i,j,k+1) - r_0^p(i,j,k)}, \tag{112}$$

$$\beta_2(i,j,k) = \frac{r_0^p(i,j,k+1) - r_0^\theta(i,j,k)}{r_0^p(i,j,k+1) - r_0^p(i,j,k)}. \tag{113}$$

10.2 Potential vorticity increment, PV'

10.2.1 Bulk potential vorticity

We choose PV' (Eq. (18)) to be represented on a ψ-point. Evaluating it with respect to a zonal-mean linearisation state gives the following finite difference formula,

$$\begin{aligned} PV'(i,j,k) \;=\;& \overline{\frac{\theta_{0z}(j,k)}{\rho_0(j,k)}} \zeta'(i,j,k) - \\ & \overline{\frac{f_u(j)\theta_{0z}(j,k)}{\rho_0^2(j,k)} \frac{1-\kappa}{R\Pi_0(j,k)\hat{\theta}_0(j,k)} p'(i,j,k)} - \overline{\frac{f_u(j)\theta_{0z}(j,k)}{\rho_0^2(j,k)} \frac{\rho_0(j,k)}{\hat{\theta}_0(j,k)} \hat{Q}(i,j,k)} + \\ & \overline{\frac{f_u(j)}{\rho_0(j,k)} \frac{g}{c_p} \frac{1}{\hat{\Pi}_{0z}^2(j,k)} R(i,j,k)} - \overline{\frac{f_u(j)}{\rho_0(j,k)} \frac{g}{c_p} \frac{2\Pi_{0zz}(j,k)}{\hat{\Pi}_{0z}^3(j,k)} \hat{S}(i,j,k)}. \end{aligned} \tag{114}$$

In Eq. (114) there are new symbols introduced for convenience. These are defined as the following (absence of a zonal index, i, $i+1$, etc, in reference state quantities implies that the quantity has been

$$
\begin{aligned}
\theta_{0z}(i,j,k) &= \frac{\theta_0(i,j,k)-\theta_0(i,j,k-1)}{r_0^\theta(i,j,k)-r_0^\theta(i,j,k-1)}, && (115)\\
\zeta'(i,j,k) &= \frac{1}{r\cos\phi}\left(\frac{\partial v'}{\partial\lambda}-\frac{\partial(u'\cos\phi)}{\partial\phi}\right),\\
&= \frac{v'(i+1,j,k)-v'(i,j,k)}{r\cos\phi_v(j)\delta\lambda}-\frac{u'(i,j+1,k)\cos\phi_u(j+1)-u'(i,j,k)\cos\phi_u(j)}{r\cos\phi_v(j)\delta\phi}, && (116)\\
Q(i,j,k) &= \frac{r_0^p(i,j,k+1)-r_0^p(i,j,k)}{\Pi_0(j,k+1)-\Pi_0(j,k)}\theta_0(j,k)\frac{\Pi'(i,j,k+1)-\Pi'(i,j,k)}{r_0^p(i,j,k+1)-r_0^p(i,j,k)},\\
&= \frac{1}{\Pi_0(j,k+1)-\Pi_0(j,k)}\theta_0(j,k)\left(\Pi'(i,j,k+1)-\Pi'(i,j,k)\right), && (117)\\
R(i,j,k) &= \frac{1}{r_0^\theta(i,j,k)-r_0^\theta(i,j,k-1)}\left(\frac{\Pi'(i,j,k+1)-\Pi'(i,j,k)}{r_0^p(i,j,k+1)-r_0^p(i,j,k)}-\frac{\Pi'(i,j,k)-\Pi'(i,j,k-1)}{r_0^p(i,j,k)-r_0^p(i,j,k-1)}\right), && (118)\\
S(i,j,k) &= \frac{\Pi'(i,j,k+1)-\Pi'(i,j,k)}{r_0^p(i,j,k+1)-r_0^p(i,j,k)}, && (119)\\
\Pi'(i,j,k) &= \kappa\frac{\Pi_0(j,k)}{p_0(j,k)}p'(i,j,k), && (120)\\
\hat{\Pi}_{0z}(i,j,k) &= \frac{\Pi_0(i,j,k+1)-\Pi_0(i,j,k)}{r_0^p(i,j,k+1)-r_0^p(i,j,k)}, && (121)\\
\Pi_{0zz}(i,j,k) &= \frac{1}{r_0^\theta(i,j,k)-r_0^\theta(i,j,k-1)}\left(\frac{\Pi_0(i,j,k+1)-\Pi_0(i,j,k)}{r_0^p(i,j,k+1)-r_0^p(i,j,k)}-\frac{\Pi_0(i,j,k)-\Pi_0(i,j,k-1)}{r_0^p(i,j,k)-r_0^p(i,j,k-1)}\right). && (122)
\end{aligned}
$$

10.2.2 Vertical boundary 'potential vorticity'

The quantities PV_1' and PV_2' are both two dimensional fields, stored at ψ points. They replace PV which cannot be defined at the boundaries. Although PV_1' and PV_2' do not correspond respectively to the bottom and top, we plan to store them at these locations in the PV field in the code. This will simplify the logistics of information transfer in the Var. scheme.

PV_1' (to be stored at level '1' in the PV array) is,

$$
PV_1'(i,j,1) = I_A(i,j,N) - f_v(j)\tilde{I}_B(i,j,N), \tag{123}
$$

where there are N half-levels in the model grid (there is one more full-level than half-level which has index 0). By the rectangle integration rule (see Fig. (2), right panel), $I_A(i,j,N)$ and $I_B(i,j,N)$ are,

$$
\begin{aligned}
I_A(i,j,N) &= \sum_{k=1}^{N}\zeta'(i,j,k)\overline{\rho_0(j,k)(r_0^\theta(i,j,k)-r_0^\theta(i,j,k-1))}, && (124)\\
I_B(i,j,N) &= \sum_{k=1}^{N}\left(\frac{1-\kappa}{R\Pi_0(j,k)\hat{\theta}_0(j,k)}p'(i,j,k)+\frac{\rho_0(j,k)}{\hat{\theta}_0(j,k)}\hat{Q}(i,j,k)\right)(r_0^\theta(i,j,k)-r_0^\theta(i,j,k-1)). && (125)
\end{aligned}
$$

In these equations, the argument N is there to emphasise the fact that the integrals are performed over all N vertical levels. Later, we shall integrate the same integrands over partial vertical domains.

PV_2' contains double integrals. The integrands of the inner integrals are on p-levels, and the result of the inner integrals is required on θ-levels. The rectangle integration rule achieves this (see Fig. (2), right panel). The outer integrals thus have integrands on θ-levels, and the result is also required on θ-levels (covering the entire vertical domain of the model). The trapezium integration rule achieves this (Fig. (2), middle panel). For the first term of PV_2, which is only a single integral, the rectangle

$$
\begin{aligned}
PV_2'(i,j,N) \quad = \quad & f_v(j)\overline{\sum_{k=1}^{N}\hat{Q}(i,j,k)(r_0^\theta(i,j,k)-r_0^\theta(i,j,k-1))} - \\
& f_v(j)\overline{\sum_{k=0}^{N-1}\frac{1}{2}\left(\frac{\overbrace{\theta_{0z}(j,k)}}{\rho_0(j,k)}I_B(i,j,k)+\frac{\overbrace{\theta_{0z}(j,k+1)}}{\rho_0(j,k+1)}I_B(i,j,k+1)\right)(r_0^\theta(i,j,k+1)-r_0^\theta(i,j,k))} + \\
& \sum_{k=0}^{N-1}\frac{1}{2}\left(\overline{\frac{\overbrace{\theta_{0z}(j,k)}}{\rho_0(j,k)}(r_0^\theta(i,j,k+1)-r_0^\theta(i,j,k))I_A(i,j,k)} + \right. \\
& \left.\overline{\frac{\overbrace{\theta_{0z}(j,k+1)}}{\rho_0(j,k+1)}(r_0^\theta(i,j,k+1)-r_0^\theta(i,j,k))I_A(i,j,k+1)}\right) - \\
& PV_1'(i,j)\overline{\frac{1}{I_\rho(i,j,N)}\sum_{k=0}^{N-1}\frac{1}{2}\left(\frac{\overbrace{\theta_{0z}(j,k+1)}}{\rho_0(j,k+1)}I_\rho(i,j,k+1)+\frac{\overbrace{\theta_{0z}(j,k)}}{\rho_0(j,k)}I_\rho(i,j,k)\right)} \\
& \overline{(r_0^\theta(i,j,k+1)-r_0^\theta(i,j,k))}, \qquad (126)
\end{aligned}
$$

where the integrals I_A and I_B are similar to Eqs. (124) and (125), but are instead integrated only up to level k. I_ρ is,

$$
I_\rho(i,j,k) = \sum_{k'=1}^{k}\rho_0(k)(r_0^\theta(i,j,k)-r_0^\theta(i,j,k-1))(1-\delta_{k0}). \qquad (127)
$$

I_A, I_B and I_ρ are specified in discretized form as Eqs. (129), (130) and (127) below where they have been evaluated using the rectangle integration rule, making them valid at θ-levels (as required for Eq. (126)).

There are an number of changes to be made to Eq. (126) to allow easier coding. Firstly, take the two terms of the summation on the second line (involving I_B) and the two terms of the summation spanning the third and fourth lines (involving I_A), and write these as separate summations. For the first term of each summation, the lower summation limit can be changed from $k=0$ to $k=1$ since the $k=0$ contribution is zero (due to the $1-\delta_{k0}$ prefactors in Eqs. (129) and (130)). For the remaining, second terms, re-index the summations by replacing k with $k-1$. The result is the following,

$$
\begin{aligned}
PV_2'(i,j,N) \quad = \quad & f_v(j)\overline{\sum_{k=1}^{N}\hat{Q}(i,j,k)(r_0^\theta(i,j,k)-r_0^\theta(i,j,k-1))} - \\
& \frac{f_v(j)}{2}\overline{\sum_{k=1}^{N-1}\frac{\overbrace{\theta_{0z}(j,k)}}{\rho_0(j,k)}I_B(i,j,k)(r_0^\theta(i,j,k+1)-r_0^\theta(i,j,k))} - \\
& \frac{f_v(j)}{2}\overline{\sum_{k=1}^{N}\frac{\overbrace{\theta_{0z}(j,k)}}{\rho_0(j,k)}I_B(i,j,k)(r_0^\theta(i,j,k)-r_0^\theta(i,j,k-1))} + \\
& \frac{1}{2}\overline{\sum_{k=1}^{N-1}\frac{\overbrace{\theta_{0z}(j,k)}}{\rho_0(j,k)}(r_0^\theta(i,j,k+1)-r_0^\theta(i,j,k))I_A(i,j,k)} + \\
& \frac{1}{2}\overline{\sum_{k=1}^{N}\frac{\overbrace{\theta_{0z}(j,k)}}{\rho_0(j,k)}(r_0^\theta(i,j,k)-r_0^\theta(i,j,k-1))I_A(i,j,k)} - \\
& \frac{PV_1'(i,j)}{2}\overline{\frac{1}{I_\rho(i,j,N)}\left\{\sum_{k=1}^{N}\frac{\overbrace{\theta_{0z}(j,k)}}{\rho_0(j,k)}I_\rho(i,j,k)(r_0^\theta(i,j,k)-r_0^\theta(i,j,k-1))+\right.} \\
& \overline{\left.\sum_{k=1}^{N-1}\frac{\overbrace{\theta_{0z}(j,k)}}{\rho_0(j,k)}I_\rho(i,j,k)(r_0^\theta(i,j,k+1)-r_0^\theta(i,j,k))\right\}}. \qquad (128)
\end{aligned}
$$

$$I_A(i,j,k) = (1-\delta_{k0}) \sum_{k'=1}^{k} \zeta'(i,j,k') \overline{\rho_0(j,k')(r_0^\theta(i,j,k') - r_0^\theta(i,j,k'-1))}, \tag{129}$$

$$I_B(i,j,k) = (1-\delta_{k0}) \sum_{k'=1}^{k} \left(\frac{1-\kappa}{R\Pi_0(j,k')\hat{\theta}_0(j,k')} p'(i,j,k') + \frac{\rho_0(j,k')}{\hat{\theta}_0(j,k')} \hat{Q}(i,j,k') \right) (r_0^\theta(i,j,k') - r_0^\theta(i,j,k'-1)). \tag{130}$$

The $(1-\delta_{k0})$ multiple in I_A and I_B reminds us that the summations are not computed when $k=0$. Remember that the values of these integrals fall on θ-levels and that the vertical interpolation needed to evaluate the prefactors of I_A and I_B in Eq. (126) goes from p- to θ-levels (use the formula in the last row of table II).

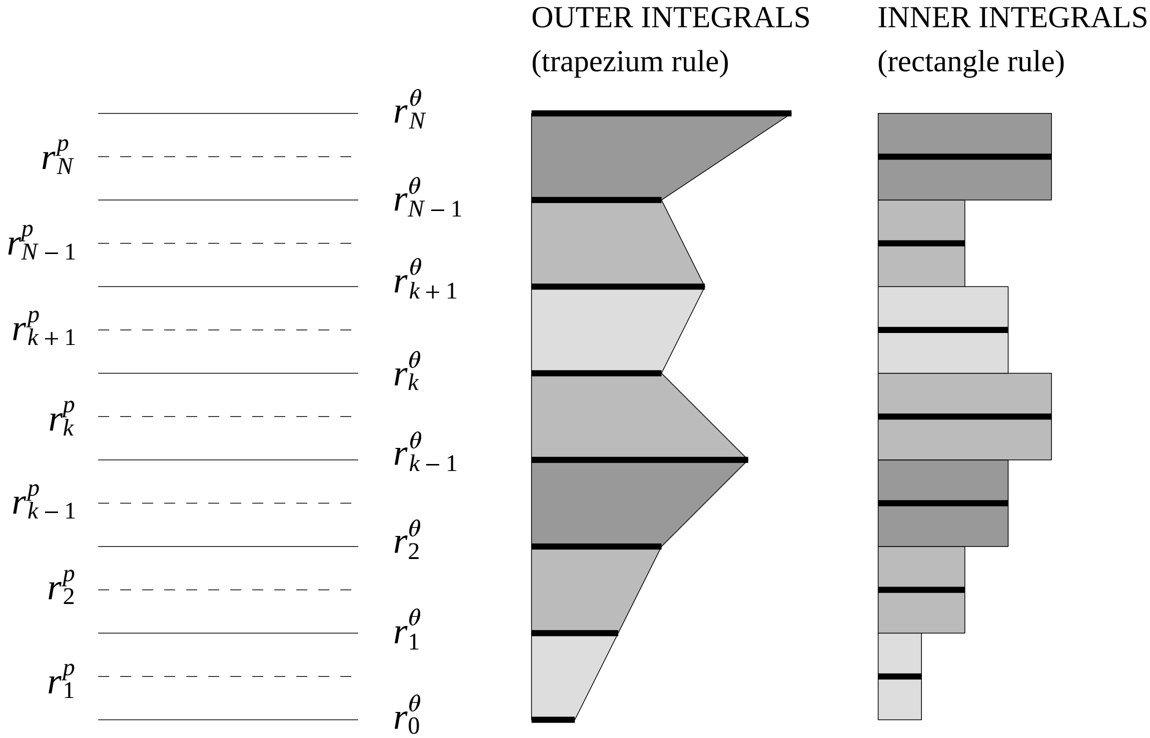

Figure 2: The schemes used to perform the inner and outer integrations. The left panel denotes the full- (θ) and half- (p) levels in the vertical. When evaluating the integrals in Eq. (128), we find it convenient to use different schemes for the inner and outer integrals which are consistent with the Charney-Phillips discretization. The remaining two panels show the schemes used. Shaded areas denote the areas that are summed, which approximate the integrals, and the thick horizontal lines denote where the quantities of the vertical profiles are stored (showing whether the quantity is on θ- or p-levels). Inner integrals use the 'rectangle rule', giving results on θ levels (right panel). These are summed in the outer integrals using the trapezium rule (middle panel). Note that inner integrals do not always sum to the top of the model domain as shown.

The formula, Eq. (117), for $Q(i,j,1)$ and $Q(i,j,N)$ cannot be evaluated exactly as vertical derivatives of Π_0 and Π' have to be evaluated at the top and bottom. Only $\hat{Q}$ (i.e. not Q) is used in the expressions above - PV' in Eq. (114) and I_B in Eqs. (125) and (130). $\hat{Q}$ (held on p-levels) is the vertical interpolation of Q (held on θ-levels), and so instead of trying to calculate Q at the top and bottom θ-levels (which is not possible due to the lack of information available), we approximate $\hat{Q}$ directly at the top and bottom p-levels. The following finite-difference formulae estimate $\hat{Q}$ in these cases,

$$\hat{Q}(i,j,N) = \frac{1}{\Pi_0(j,N) - \Pi_0(j,N-1)} \left(\alpha_1\theta_0(j,N) + \beta_1\theta_0(j,N-1)\right) \left(\Pi'(i,j,N) - \Pi'(i,j,N-1)\right), \tag{131}$$

$$\hat{Q}(i,j,1) = \frac{1}{\Pi_0(j,2) - \Pi_0(j,1)} \left(\alpha_1\theta_0(j,1) + \beta_1\theta_0(j,0)\right) \left(\Pi'(i,j,2) - \Pi'(i,j,1)\right). \tag{132}$$

approximate its value to be $\theta_0(j,0) \approx \theta_0(j,1)$. Since then we are interpolating between two idential values, replace $\alpha_1\theta_1(j,1) + \beta_1\theta_0(j,0)$ in Eq. (132) with simply $\theta_0(j,1)$.

10.3 Anti-potential vorticity increment, $\bar{PV}'$

We choose $\bar{PV}'$ to be represented on a p-point. Equation (30) for $\bar{PV}'$ has the following finite difference form,

$$
\begin{aligned}
\bar{PV}'(i,j,k) &= f(\nabla_z f\rho_0)\cdot(\nabla_z\psi') + f^2\rho_0\nabla_z^2\psi' - f\nabla_z^2 p', \qquad (133)\\
&= -f(\nabla_z f\rho_0)\cdot(\mathbf{k}\times\mathbf{u_h}') + f^2\rho_0\zeta' - f\nabla_z^2 p',\\
&= -\frac{f_u(j)\tilde{u}'(i,j,k)}{r}\left\{2\Omega\cos\phi_u(j)\rho_0(j,k) + f_u(j)\frac{\rho_0(j+1,k)-\rho_0(j-1,k)}{2\delta\phi}\right\} +\\
&\quad f_u^2(j)\rho_0(j,k)\left\{\left(\frac{v'(i+1,j,k)-v'(i,j,k)}{r\cos\phi_v(j)\delta\lambda}\right) - \right.\\
&\quad \left.\left(\frac{u'(i,j+1,k)\cos\phi_u(j+1) - u'(i,j,k)\cos\phi_u(j)}{r\cos\phi_v(j)\delta\phi}\right)\right\} -\\
&\quad f_u(j)\left\{\frac{(p'(i+1,j,k)-2p'(i,j,k)+p'(i-1,j,k))}{\delta\lambda^2 r^2\cos^2(\phi_u(j))} + \right.\\
&\quad \left.\frac{(p'(i,j+1,k)-p'(i,j,k))\cos\phi_v(j) - (p'(i,j,k)-p'(i,j-1,k))\cos\phi_v(j-1)}{\delta\phi^2 r^2\cos\phi_u(j)}\right\},
\end{aligned}
\tag{134}
$$

$$
\begin{aligned}
\text{noting that } \nabla_z\psi' &= -\mathbf{k}\times\mathbf{u_h}',\\
\mathbf{k}\times\mathbf{u_h}' &= \begin{pmatrix} -v \\ u \\ 0 \end{pmatrix},\\
\text{and } \zeta' &= \mathbf{k}\cdot\nabla\times\mathbf{u_h}'.
\end{aligned}
$$

There is a complication when evaluating $\bar{PV}$ at the poles. The poles lie on a u-point, and since $\cos(\pi/2) = 0$, there is a division by zero in the third term of $\bar{PV}$ there (see the last two lines of Eq. (134), which is the last term of Eq. 133).

Parameter	North pole	South pole
Δ_1	-1	$+1$
Δ_2	-1	0

Table III: The values of Δ_1 and Δ_2, as used by the application of Gauss' theorem at the poles.

The Laplacian of the pressure increment at the poles can be evaluated with the help of Gauss' theorem in the plane (otherwise known as Green's theorem in the plane), given generically as,

$$\int_{\text{area } ds} \nabla_z\cdot\mathbf{v}ds = \oint \mathbf{v}\cdot\mathbf{n}dl, \tag{135}$$

where $\mathbf{n}$ is a unit vector pointing in the positive meridonal direction for the south pole and the negative meridional direction for the north pole (it points outside of the loop). We shall use Δ_1 in table (III) as a proxy of this in the finite difference form of Eq. (135) below. Let $\mathbf{v}$ be $\nabla_z p'$, ds be an area element of the polar area and dl be a length element of its boundary. Equation (135) can be developed to yield an expression for $\nabla_z^2 p'$ at the poles,

$$
\begin{aligned}
A\nabla_z^2 p'(i,j,k) &= \Delta_1 r\frac{\delta\phi}{2}\delta\lambda\sum_i \frac{1}{r}\frac{\partial p'}{\partial\phi},\\
&= \Delta_1\frac{1}{2}\delta\lambda\sum_i (p'(i,j+\Delta_2+1,k) - p'(i,j+\Delta_2,k)).
\end{aligned}
\tag{136}
$$

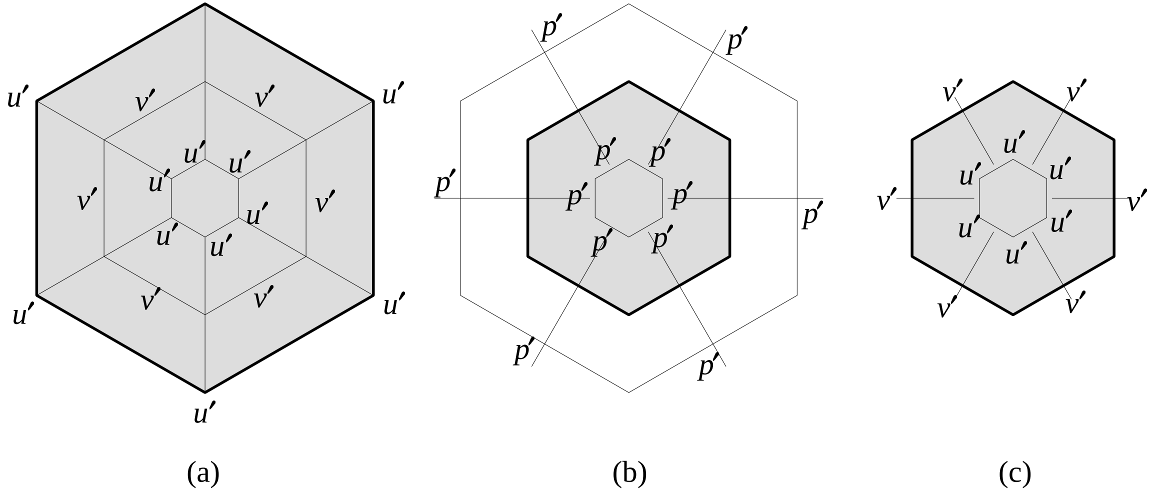

Figure 3: The polar integrals that need to be performed to calculate $\bar{PV}$ (panel b), and $\nabla_z \cdot \mathbf{u_h}'$ (panel c). The thick lines circuling the pole indicate the paths of the loop integrals in each case, and enclose the shaded areas. The shaded areas in panels b and c have an area A (Eq. 137). Note that the polar points ('u' and 'p'-points) have been drawn slightly displaced from the pole for clarity. (Panel a is redundant and was used in a previous version of the code.)

The parameter Δ_2 is used to increment correctly the meridional index of pressure (see table (III)). The sum is performed around the 'v' latitude 'one away' from the pole (see Fig. (3b)). The effective polar area, A is the shaded area in Fig. 3,

$$A \approx \pi (r\delta\phi/2)^2. \tag{137}$$

10.4 Divergence, $\nabla_z \cdot \mathbf{u_h}'$

Horizontal divergence is the simplest of the three dual space parameters to express in finite difference form. It is positioned on a p-point.

$$\begin{aligned}
\nabla_z \cdot \mathbf{u_h}'(i,j,k) &= \frac{1}{r\cos\phi}\frac{\partial u'}{\partial\lambda} + \frac{1}{r\cos\phi}\frac{\partial(v'\cos\phi)}{\partial\phi}, \\
&= \frac{1}{r\cos\phi_u(j)}\frac{u'(i,j,k) - u'(i-1,j,k)}{\delta\lambda} + \\
&\quad \frac{1}{r\cos\phi_u(j)}\frac{v'(i,j,k)\cos\phi_v(j) - v'(i,j-1,k)\cos\phi_v(j-1)}{\delta\phi}.
\end{aligned} \tag{138}$$

Once more we face the pole problem. This can be overcome by using Gauss' divergence theorem in the plane, Eq. (135), and choosing $\mathbf{v} = \mathbf{u_h}'$. Then Gauss' theorem allows us to write,

$$A\nabla_z \cdot \mathbf{u_h}'(i,j,k) = \Delta_1 r\frac{\delta\phi}{2}\delta\lambda \sum_i v'(i,j+\Delta_2,k), \tag{139}$$

where j is the meridional index for either of the poles, and A, Δ_1 and Δ_2 are specified in the discussion about $\bar{PV}'$ above. The sum is performed around the 'v' latitude 'one away' from the pole (see Fig. (3c)).

10.5 The U_1-transform

The leading part of the U-transform - giving the balanced increments, $\vec{X}_1'$, Eq. (29) - has three components. The first two components for u_1' and v_1' are specified in local cartesian co-ordinates in Eq. (29). The general expression $\mathbf{u_h}' = \mathbf{k} \times \nabla s'$ is needed for the spherical expression. Translating this into finite

$$
\begin{aligned}
u' &= -\frac{1}{r}\frac{\partial s'}{\partial \phi}, \\
u'(i,j,k) &= -\frac{1}{r}\frac{s'(i,j,k)-s'(i,j-1,k)}{\delta\phi}, \qquad (140)\\
v' &= \frac{1}{r\cos\phi}\frac{\partial s'}{\partial\lambda}, \\
v'(i,j,k) &= \frac{1}{r\cos\phi_v(j)}\frac{s'(i,j,k)-s'(i-1,j,k)}{\delta\lambda}. \qquad (141)
\end{aligned}
$$

With s' held on 'ψ'-points, the u' and v' variables are positioned correctly.

A poisson equation must be solved for the pressure (third component of Eq. (29)). The finite difference form of the right hand side of the poisson equation is derived in the following,

$$
\begin{aligned}
\nabla_z\cdot(f\rho_0\nabla_z)s' &= \frac{f\rho_0}{r\cos\phi}\frac{\partial(\nabla_z s')_\lambda}{\partial\lambda} + \frac{1}{r\cos\phi}\frac{\partial(\cos\phi(f\rho_0\nabla_z s')_\phi)}{\partial\phi}, \\
&= \frac{f\rho_0}{r^2\cos^2\phi}\frac{\partial}{\partial\lambda}\left(\frac{\partial s'}{\partial\lambda}\right) + \frac{1}{r^2\cos\phi}\frac{\partial}{\partial\phi}\left(f\rho_0\cos\phi\frac{\partial s'}{\partial\phi}\right), \\
\{\nabla_z\cdot(f\rho_0\nabla_z)s'\}(i,j,k) &= \frac{1}{r^2\cos\phi_v(j)}\left\{\frac{f_v(j)\tilde\rho_0(j,k)}{\cos\phi_v(j)}\left(\frac{s'(i+1,j,k)+s'(i-1,j,k)-2s'(i,j,k)}{\delta\lambda^2}\right)+\right. \\
&\quad \frac{1}{\delta\phi}\left(f_u(j+1)\rho_0(j+1,k)\cos\phi_u(j+1)\left(\frac{s'(i,j+1,k)-s'(i,j,k)}{\delta\phi}\right)-\right. \\
&\quad \left.\left. f_u(j)\rho_0(j,k)\cos\phi_u(j)\left(\frac{s'(i,j,k)-s'(i,j-1,k)}{\delta\phi}\right)\right)\right\}, \qquad (142)\\
\text{where } \tilde\rho_0(j,k) &= \frac{1}{2}(\rho_0(j+1,k)+\rho_0(j,k)). \qquad (143)
\end{aligned}
$$

The result of Eq. (142) is stored on 'ψ'-points. Solving the poisson equation yields pressure, also on 'ψ'-points, which must be interpolated to the correct pressure points (see Fig. (1)).

10.6 The U_2-transform

The calculation of the leading unbalanced part of the model fields, $\vec{X}'_2$, from the ubalanced pressure parameter requires the solution of a poisson equation (Eq. (33)), given the vorticity at each level. The vorticity in Eq. (33) at the vertical boundaries is calculated differently that it is in the bulk of the model domain, as discussed in section 3.2, and so we treat each of these cases separately.

10.6.1 The unbalanced vorticity calculation in the bulk

In the bulk, we need to evauate Eq. (31). In this equation, ${}^u p'$ is stored on p-points, but ${}^u\zeta'$ is stored on ψ-points, and so we need to interpolate to ψ-points in the discretized form of the equations. Just as ${}^u\zeta'$ in Eq. (31) has been found by setting $PV'=0$ (PV' given as Eq. (18)), we can find ${}^u\zeta'$ in the finite-difference form of the equations by setting the discretized PV', Eq. (114), to zero, and rearranging for ${}^u\zeta'$,

$$
\begin{aligned}
{}^u\zeta'(i,j,k) &= \overline{\frac{f_u(j)}{\rho_0(j,k)}\left\{\frac{1-\kappa}{R\Pi_0(j,k)\hat\theta_0(j,k)}{}^u p'(i,j,k)+\frac{\rho_0(j,k)}{\hat\theta_0(j,k)}\hat Q(i,j,k)\right\}} - \\
&\quad \overline{\frac{f_u(j)}{\hat\theta_{0z}(j,k)}\frac{g}{c_p}\left\{\frac{1}{\hat{\Pi_{0z}}^2(j,k)}R(i,j,k)-\frac{2\Pi_{0zz}(j,k)}{\hat{\Pi_{0z}}^3(j,k)}\hat S(i,j,k)\right\}}, \qquad (144)
\end{aligned}
$$

where Q, R and S are given in discretized form in Eqs. (117), (118) and (119) respectively, but using the unbalanced pressure parameter instead of the full pressure increment.

10.6.2 The unbalanced vorticity calculation at the vertical boundaries

Vorticity at the boundaries is found from Eqs. (55) and (56). We therefore need to evaulate the I_n and F_n summations in discretized form in line with the vertical integrals performed when discretizing the 'missing' PV' modes as in section 10.1.2.

10.6.3 Computing velocity components

Velocity follows from vorticity in two steps - first by solving the Poisson equation ${}^u\zeta'_z = \nabla_z^{2\,u}\psi'$ for ${}^u\psi'$ followed by a derivative step - Eq. (33). The same calculation is done whether vorticity has been calculated in the bulk or on the vertical boundaries. Although ${}^u\zeta'$ should be stored on ψ-points, in the U_2 transform it falls on p-points, where it is used to find ${}^u\psi'$. ${}^u\psi'$ is then interpolated to ψ-points from which the winds are derived, Eq. (33),

The calculation for ${}^u u'$ in finite difference form is,

$$\begin{aligned} {}^u u'(i,j,k) &= -\frac{1}{r}\frac{\partial^u\psi'}{\partial\phi}, \\ &= -\frac{1}{r}\frac{{}^u\psi'(i,j,k) - {}^u\psi'(i,j-1,k)}{\delta\phi}, \end{aligned} \tag{145}$$

and the calculation for ${}^u v'$ in finite difference form is,

$$\begin{aligned} {}^u v'(i,j,k) &= -\frac{1}{r\cos\phi_v(j)}\frac{\partial^u\psi'}{\partial\lambda}, \\ &= -\frac{1}{r\cos\phi_v(j)}\frac{{}^u\psi'(i,j,k) - {}^u\psi'(i-1,j,k)}{\delta\lambda}. \end{aligned} \tag{146}$$

Note that the pressure contribution from the second transform is the unbalanced pressure itself, and requires no processing.

10.7 The U_3-transform

Once again, the transform, Eq. (57), for the irrotational component, $\vec{X}'_2$ has been expressed in cartesian co-ordinates in the main body of this document. The finite difference forms (below) are in terms of spherical co-ordinates.

$$\begin{aligned} u' &= \frac{1}{r\cos\phi}\frac{\partial\chi'}{\partial\lambda}, \\ u'(i,j,k) &= \frac{1}{r\cos\phi_u(j)}\frac{\chi'(i+1,j,k) - \chi'(i,j,k)}{\delta\lambda}, \end{aligned} \tag{147}$$

$$\begin{aligned} v' &= \frac{1}{r}\frac{\partial\chi'}{\partial\phi}, \\ v'(i,j,k) &= \frac{1}{r}\frac{\chi'(i,j+1,k) - \chi'(i,j,k)}{\delta\phi}. \end{aligned} \tag{148}$$

With χ' held on 'p'-points, the u' and v' variables are positioned correctly.

It looks like there is the common problem in evaluating the zonal wind increment at the poles, since $\cos(\pi/2) = 0$. The zonal wind is meaningless at the poles, and so it is set to zero (all polar points are coincidental and so there is no 'zonal gradient of χ''). This avoids the need to deal with the 'polar problem' using integral techniques as used before.

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