

New PV-based control variables for Met Office VAR.

Ross Bannister*, Mike Cullen†

Version 07. Last revised 24th September 2009

A set of new, potential vorticity (PV)-based control variables is introduced for use in the Met Office's VAR scheme. This set has advantages over that currently used operationally. The choice of new variables, of which a PV-related field is the leading variable, is described together with the strategy for its implementation. The transformation from the PV-based set to model variables (the \mathbf{U}_p -transform) and its inverse (the \mathbf{T}_p -transform) are described.

Contents

1. Introduction
2. Mathematical framework
3. Forms of the dual parameters, PV' , D' and $\bar{P}V'$
4. The \mathbf{U}_p transform
5. The \mathbf{T}_p transform
6. Appendix A: Useful relations between variables
7. Appendix B: Ertel PV in height co-ordinates
8. Appendix C: Grid staggering
9. Appendix D: Finite differencing

*Data Assimilation Research Centre (DARC) and National Centre for Earth Observation (NCEO), Dept. of Meteorology, Univ. of Reading, Reading, RG6 6BB, UK

†Met Office, Fitzroy Road, Exeter, Devon, EX1 3PB, UK

1 Introduction

All information that goes into VAR has uncertainties, and these uncertainties are very important to quantify. In current VAR systems, uncertainty is accounted for with Gaussian probability density functions (PDFs). The background error covariance matrix, \mathbf{B}_x , characterizes the shape of the PDF associated with the forecast (or background) state. \mathbf{B}_x appears in the cost function, which itself is minimized in VAR. The model state space is typically very large (10^6 - 10^7 variables) and so we cannot represent the background error covariance matrix explicitly.

As with other assimilation schemes, Met Office VAR does not perform the minimization process in terms of model variables, but instead minimizes in terms of special control parameters. Let a perturbation in model space be \mathbf{x}' and let the equivalent perturbation in terms of control parameters be \mathbf{v}'_p . Let the two representations be related via the linear transform \mathbf{U}_p , ie $\mathbf{x}' = \mathbf{U}_p \mathbf{v}'_p$ and let the background error covariance matrix in terms of parameters be \mathbf{B}_v . The control parameters are chosen on the basis that they are thought to have the following properties.

- Errors in the background between different control parameters are uncorrelated. This means that \mathbf{B}_v has block-diagonal structure and so is easier to represent than \mathbf{B}_x .
- Components of \mathbf{v}'_p may be labelled as either 'balanced' or 'unbalanced'. Balanced and unbalanced variables have different error covariances, and so it is useful to deal with each separately (via the block-diagonal matrices in \mathbf{B}_v).
- Balance relationships may be built-into \mathbf{U}_p . This ensures that covariances between errors of model variables - which are implied from those of control parameters, $\mathbf{B}_x = \mathbf{U}_p \mathbf{B}_v \mathbf{U}_p^T$ - are suitably balanced.
- The \mathbf{U}_p -transform is extended with further transformations to relate \mathbf{x}' to completely uncorrelated variables using so-called vertical and horizontal transforms [10, 11, 12, 1]). VAR minimization is performed in terms of these completely uncorrelated variables allowing potential improvements in the conditioning of the minimization (compared to minimization with respect to model variables). Here though we are only concerned with the parameter transform.

A potential vorticity (PV)-based set of control parameters which attempts to achieve these benefits has already been investigated in the ECMWF VAR system [9]. This paper is about a PV-based set of control parameters for the Met Office VAR system. This includes a discussion of the transformation \mathbf{U}_p and its pseudo inverse, \mathbf{T}_p . The new control parameters that make up \mathbf{v}'_p are introduced in Sec. 2 and related so-called dual parameters which are given in Sec. 3. The development of the \mathbf{U}_p and \mathbf{T}_p -transforms are shown in Secs. 4 and 5 respectively. This document contains some useful appendices: App. A gives some physical relationships between variables, App. B gives a discussion of Ertel potential vorticity, App. C gives details of the grid staggering used and App. D gives some finite difference formulae. The scientific case for the use of PV-based control variables is discussed elsewhere [9, 3, 4] and a user guide to the Met Office PV code (including discussion of the new namelist variables) is available [8].

The standard Met Office control parameters are streamfunction (ψ'), velocity potential (χ'), and geostrophically unbalanced (i.e. ageostrophic) pressure (p'_A) [10] (this latter variable is sometimes called the residual pressure, p'_r , which is arguably a better description of it). Other parameters related to humidity and ozone, etc. are not modified here and so are not discussed.

2 Mathematical Framework

Fields are described as deviations from a reference state. These deviations (or increments) are denoted by primes. Let the state \mathbf{x}' be the vector of model variable increments of zonal velocity, meridional velocity and pressure

$$\mathbf{x}' = \begin{pmatrix} u' \\ v' \\ p' \end{pmatrix}. \quad (1)$$

Elements of \mathbf{x}' are fields that are a function of longitude, latitude and height (they are stored in the PF structure in the code). \mathbf{x}' has a vector property because it represents a number of fields. A temperature field is missing from (1), but it can be derived diagnostically from fields in (1) (see (49) of App. A). The

control parameters of the PV-based scheme are described by the vector \mathbf{v}'_p

$$\mathbf{v}'_p = \begin{pmatrix} \psi'_b \\ \chi' \\ p'_u \end{pmatrix}, \quad (2)$$

where ψ'_b is the balanced part of the streamfunction (this parameter is related to the potential vorticity), χ' is the velocity potential pertaining to the divergent component of the flow (this is unchanged from the standard formulation), and p'_u is the unbalanced pressure (this parameter is related to a new quantity called the anti-potential vorticity - see below). Unlike p'_A of the standard formulation, p'_u is a true unbalance pressure over a wider range of flow regimes [3]. Parameters remain a function of longitude, latitude and height and are stored in the Vp structure in the code (ψ'_b uses the existing Vp % psi array in the code and is not renamed, e.g. Vp % psib; and p_u uses the existing Vp % Ap array). It is also useful to define a dual representation, \mathbf{d}' of the increments. Let this have components of potential vorticity (PV), horizontal divergence, D' and anti-potential vorticity ($\bar{P}V'$)

$$\mathbf{d}' = \begin{pmatrix} PV' \\ D' \\ \bar{P}V' \end{pmatrix}. \quad (3)$$

These dual parameters are defined in Sec. 3. Each component in \mathbf{d}' corresponds exclusively to each component in \mathbf{v}'_p (ie PV' is a function of ψ'_b only, D' is a function of χ' only and $\bar{P}V'$ is a function of p'_u only). Arrays for these fields are declared as and when they are needed in the code.

2.1 The \mathbf{U}_p -transform formalism

The transform that produces \mathbf{x}' from \mathbf{v}'_p is \mathbf{U}_p

$$\mathbf{x}' = \mathbf{U}_p \mathbf{v}'_p, \quad (4)$$

$$\begin{pmatrix} u' \\ v' \\ p' \end{pmatrix} = \begin{pmatrix} \mathbf{U}_{11} & \mathbf{U}_{12} & \mathbf{U}_{13} \\ \mathbf{U}_{21} & \mathbf{U}_{22} & \mathbf{U}_{23} \\ \mathbf{U}_{31} & \mathbf{U}_{32} & \mathbf{U}_{33} \end{pmatrix} \begin{pmatrix} \psi'_b \\ \chi' \\ p'_u \end{pmatrix}. \quad (5)$$

The forms of the component \mathbf{U}_{ij} -operators are developed in Sec. 4. The respective columns of \mathbf{U}_p give the balanced, divergent and unbalanced contributions to \mathbf{x}' .

2.2 The \mathbf{T}_p -transform formalism

The transform that produces \mathbf{v}' from \mathbf{x}' is \mathbf{T}_p . Is is the pseudo inverse of \mathbf{U}_p . Unlike for \mathbf{U}_p , we find that it is generally not possible to write down an explicit form for \mathbf{T}_p . It will be helpful however to define a dual operator, \mathbf{A} , as a first step to achieving the inverse operation. The dual operator produces the dual parameters, \mathbf{d}' from \mathbf{x}'

$$\mathbf{d}' = \mathbf{A} \mathbf{x}', \quad (6)$$

$$\begin{pmatrix} PV' \\ D' \\ \bar{P}V' \end{pmatrix} = \begin{pmatrix} \mathbf{P}V \\ \mathbf{D} \\ \mathbf{P}\bar{V} \end{pmatrix} \mathbf{x}'. \quad (7)$$

Each side of (4) is a state of model variables and so we can operate on each side with \mathbf{A}

$$\mathbf{A} \mathbf{x}' = \mathbf{A} \mathbf{U}_p \mathbf{v}'_p. \quad (8)$$

Since each dual space parameter is designed to be associated exclusively with each control parameter, the combined operator $\mathbf{A} \mathbf{U}_p$ is block-diagonal. This yields a set of three equations that we can use as a basis for doing the inverse operation

$$\mathbf{P}V(\mathbf{x}') = \mathbf{P}V \begin{pmatrix} \mathbf{U}_{11} \psi'_b \\ \mathbf{U}_{21} \psi'_b \\ \mathbf{U}_{31} \psi'_b \end{pmatrix}, \quad \mathbf{D}(\mathbf{x}') = \mathbf{D} \begin{pmatrix} \mathbf{U}_{12} \chi' \\ \mathbf{U}_{22} \chi' \\ \mathbf{U}_{32} \chi' \end{pmatrix}, \quad \mathbf{P}\bar{V}(\mathbf{x}') = \mathbf{P}\bar{V} \begin{pmatrix} \mathbf{U}_{13} p'_u \\ \mathbf{U}_{23} p'_u \\ \mathbf{U}_{33} p'_u \end{pmatrix}. \quad (9)$$

3 Forms of the dual parameters, PV' , D' and $\bar{P}V'$

Forms of the three dual parameters are given here before discussion of the \mathbf{U}_p and \mathbf{T}_p -transforms.

3.1 The potential vorticity for the balanced equation

PV' is associated with the balanced part of the flow and hence with the balanced parameter ψ'_b . The incremental form of the PV' is now developed starting with the Ertel PV in height co-ordinates as follows

$$PV = \frac{\zeta_0 + f}{\rho_0} \frac{\partial \theta_0}{\partial z}, \quad (10)$$

(see first term of (55) of Appendix B) 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 this work the reference state quantities shall be averaged zonally, and so they become a function of latitude and height only. The zonal mean reference state is a new substructure of LS, e.g. `LS % LSzm % u(:,:)`, where the two arguments correspond to latitude and model level respectively (all zonal mean data correspond to $t = 0$).

Equation (10) is a non-linear function of model variables. For the transformations, the equations should be linear so that an incremental form can be written. Linearising (10) about a chosen state, $\mathbf{x}_0 = (u_0, v_0, p_0)^T$, can be done systematically by the following expansion

$$PV' = \left. \frac{\partial PV}{\partial \zeta} \right|_0 \zeta' + \left. \frac{\partial PV}{\partial \rho} \right|_0 \rho' + \left. \frac{\partial PV}{\partial (\partial_z \theta)} \right|_0 \partial_z \theta', \quad (11)$$

where primed quantities denote deviation from the reference state (e.g. $\zeta' = \zeta_0 + \zeta'$) and ∂_z is compact notation for $\partial/\partial z$. Note that the basic state for vorticity, ζ_0 follows from u_0 and v_0 as $\zeta_0 = \mathbf{k} \cdot (\nabla_h \times \mathbf{u}_{0h}) = (\partial_x v_0)_z - (\partial_y u_0)_z$ (where subscript 'h' stands for horizontal and subscript 'z' outside of the brackets stands for the derivative calculated at constant z). The partial derivatives in (11) are

$$\left. \frac{\partial PV'}{\partial \zeta} \right|_0 = \frac{1}{\rho_0} \frac{\partial \theta_0}{\partial z}, \quad (12)$$

$$\left. \frac{\partial PV'}{\partial \rho} \right|_0 = -\frac{\zeta_0 + f}{\rho_0^2} \frac{\partial \theta_0}{\partial z}, \quad (13)$$

$$\left. \frac{\partial PV'}{\partial (\partial_z \theta)} \right|_0 = \frac{\zeta_0 + f}{\rho_0}. \quad (14)$$

The density increments in the above can be written in terms of pressure increments using (50) of App. A. The $\partial_z \theta'$ increments can also be written in terms of pressure increments using (51). Substituting into (11) and assuming small Rossby number ($f \gg \zeta_0$) gives

$$\begin{aligned} PV' &= \frac{1}{\rho_0} \frac{\partial \theta_0}{\partial z} \zeta' - \\ &\frac{f}{\rho_0^2} \frac{\partial \theta_0}{\partial z} \left\{ \frac{1 - \kappa}{R \Pi_0 \hat{\theta}_0} p' + \frac{\rho_0}{\hat{\theta}_0} \overbrace{\left(\frac{\partial \Pi_0}{\partial z} \right)^{-1} \theta_0 \frac{\partial}{\partial z} \left(\kappa \frac{\Pi_0}{p_0} p' \right)} \right\} + \\ &\frac{f}{\rho_0} \frac{g}{c_p} \left\{ \overbrace{\left(\frac{\partial \Pi_0}{\partial z} \right)^{-2}} \frac{\partial^2}{\partial z^2} \left(\kappa \frac{\Pi_0}{p_0} p' \right) - 2 \frac{\partial^2 \Pi_0}{\partial z^2} \overbrace{\left(\frac{\partial \Pi_0}{\partial z} \right)^{-3} \frac{\partial}{\partial z} \left(\kappa \frac{\Pi_0}{p_0} p' \right)} \right\}, \quad (15) \end{aligned}$$

$$= \frac{1}{\rho_0} \frac{\partial \theta_0}{\partial z} \zeta' - \frac{f}{\rho_0^2} \frac{\partial \theta_0}{\partial z} \left\{ \frac{1 - \kappa}{R \Pi_0 \hat{\theta}_0} p' + \frac{\rho_0}{\hat{\theta}_0} \hat{Q} \right\} + \frac{f}{\rho_0} \frac{g}{c_p} \left\{ \overbrace{\left(\frac{\partial \Pi_0}{\partial z} \right)^{-2}} R - 2 \frac{\partial^2 \Pi_0}{\partial z^2} \overbrace{\left(\frac{\partial \Pi_0}{\partial z} \right)^{-3}} \hat{S} \right\} \quad (16)$$

where the following substitutions have been made to write (16)

$$Q = \left(\frac{\partial \Pi_0}{\partial z} \right)^{-1} \theta_0 \frac{\partial}{\partial z} \left(\kappa \frac{\Pi_0}{p_0} p' \right), \quad (17)$$

$$R = \frac{\partial^2}{\partial z^2} \left(\kappa \frac{\Pi_0}{p_0} p' \right), \quad (18)$$

$$S = \frac{\partial}{\partial z} \left(\kappa \frac{\Pi_0}{p_0} p' \right). \quad (19)$$

Each term in (11) falls naturally on ρ -levels (called 'half'-levels) in the vertical (see Fig. 1). This is not true in (15) where some of the terms fall naturally on θ -levels ('full'-levels), e.g. the vertical derivative of Π . Such terms need to be vertically interpolated to ρ -levels. For individual variables in (15), this interpolation is denoted by a hat $\hat{\cdot}$ and for groups of terms it is denoted by an overbrace. (Note generally this notation indicates that vertical interpolation is performed to levels not natural to the quantity in question; this could be θ -to- ρ -levels, as above, or the other way around). It is important to respect the vertical grid staggering in this way to minimize numerical problems. Horizontal grid staggering is not considered at this stage as this is less important (it is considered when the equations are discretized fully - see App. D).

3.2 The divergence parameter for the irrotational equation

D' is associated with the irrotational part of the flow and hence with the irrotational parameter χ' . The incremental form of the divergence, D' , is standard as follows

$$D' = \nabla_{\text{h}} \cdot \mathbf{u}'_{\text{h}}. \quad (20)$$

3.3 The anti-potential vorticity for the unbalanced equation

$\bar{P}V'$ is associated with the unbalanced part of the flow and hence with the unbalanced parameter p'_{u} . The incremental form of the $\bar{P}V'$ is now given (the reason why this is the form of $\bar{P}V'$ is evident from Secs. 4.1 and 4.3).

$$\bar{P}V' = \nabla_{\text{h}} \cdot (f \rho_0 \nabla_{\text{h}} \psi') - \nabla_{\text{h}}^2 p'. \quad (21)$$

3.4 Summary of the 'dual' parameters

The dual parameters PV' , D' and $\bar{P}V'$ are associated with the balanced (ψ'_{b}), irrotational (χ') and rotational unbalanced (p'_{u}) components of the flow respectively. They are useful because each can be calculated from the same basic increments u' , v' and p' . They are mutually independent in the sense that ψ'_{b} is associated with $D' = 0$ and $\bar{P}V' = 0$, χ' is associated with $PV' = 0$ and $\bar{P}V' = 0$, and p'_{u} is associated with $PV' = 0$ and $D' = 0$. These properties are used in Sec. 5 when constructing the \mathbf{T}_{p} transform.

4 Formulating the Equations for the \mathbf{U}_{p} -Transform

4.1 The first \mathbf{U}_{p} -transform (the balanced equation)

In (15) and (16) a small Rossby number has been assumed, i.e. that $f \gg \zeta_0$. Also valid in this domain is the linear balance relationship which relates balanced mass and balanced wind fields

$$\nabla_{\text{h}} \cdot (f \rho_0 \nabla_{\text{h}} \psi'_{\text{b}}) - \nabla_{\text{h}}^2 p'_{\text{b}} = 0, \quad (22)$$

where p'_{b} is the balanced pressure increment. Notice that the definition of $\bar{P}V'$ in (21) has the same structure as the linear balance equation (22). Equation (22) then enforces the condition that the balanced components ψ'_{b} and p'_{b} should together have no $\bar{P}V'$ (as stated in Sec. 3.4).

The standard relationship between streamfunction and horizontal velocity is (written below for balanced and incremental variables)

$$\mathbf{v}'_{\text{b}} = \mathbf{k} \times \nabla_{\text{h}} \psi'_{\text{b}}. \quad (23)$$

These last two equations can be used to yield the part of the \mathbf{U}_p -operator that gives the balanced increments, \mathbf{x}'_b , from ψ'_b

$$\mathbf{x}'_b = \begin{pmatrix} \mathbf{U}_{11} \\ \mathbf{U}_{21} \\ \mathbf{U}_{31} \end{pmatrix} \psi'_b = \begin{pmatrix} -\partial/\partial y \\ \partial/\partial x \\ \nabla_h^{-2} \nabla_h \cdot (f \rho_0 \nabla_h) \end{pmatrix} \psi'_b. \quad (24)$$

The velocity components (first two rows) are specified in local Cartesian coordinates, 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. This transform is essentially the same one used in standard VAR, except that the argument is ψ'_b instead of ψ' .

4.2 The second \mathbf{U}_p -transform (the irrotational equation)

The second control variable is velocity potential increment, χ' , which describes the irrotational component to the flow. For the \mathbf{U}_p transform, the operator associated with this variable has the simplest structure of the three variables. The divergent flow is given by the divergence operator (this transform has zero pressure increment)

$$\mathbf{x}'_{\text{div}} = \begin{pmatrix} \mathbf{U}_{12} \\ \mathbf{U}_{22} \\ \mathbf{U}_{32} \end{pmatrix} \chi' = \begin{pmatrix} \partial/\partial x \\ \partial/\partial y \\ 0 \end{pmatrix} \chi', \quad (25)$$

which is again, for simplicity, written in local Cartesian coordinates. This transform is the same one used in standard VAR.

4.3 The third \mathbf{U}_p -transform (the unbalanced equation)

The total rotational part of the flow is not exclusively balanced and so ψ'_b does not describe completely the rotational flow. The unbalanced part of the pressure is described by p'_u , which is the third control parameter. Just as the balanced increments in the first \mathbf{U}_p -transform have no PV' (the PV' has been designed so this is the case), the unbalanced increment is designed to have no PV . This is the strategy for developing the third \mathbf{U}_p -transform. The unbalanced transform is performed by the following prescription.

1. Setting $PV' = 0$ using (15) yields an anti-balance relationship between pressure and vorticity. This is the equation that will be used to gain a set of wind increments (via vorticity) from p'_u . Given this unbalanced pressure increment, the unbalanced vorticity increment is ζ'_u , and is found from (15) set to zero for unbalanced flow

$$\zeta'_u = \frac{f}{\rho_0} \left\{ \frac{1 - \kappa}{R\Pi_0 \hat{\theta}_0} p'_u + \frac{\rho_0}{\hat{\theta}_0} \overbrace{\left(\frac{\partial \Pi_0}{\partial z} \right)^{-1} \theta_0 \frac{\partial}{\partial z} \left(\kappa \frac{\Pi_0}{p_0} p'_u \right)} \right\} - \frac{fg}{c_p} \left(\frac{\partial \theta_0}{\partial z} \right)^{-1} \left\{ \overbrace{\left(\frac{\partial \Pi_0}{\partial z} \right)^{-2} \frac{\partial^2}{\partial z^2} \left(\kappa \frac{\Pi_0}{p_0} p'_u \right)} - 2 \frac{\partial^2 \Pi_0}{\partial z^2} \overbrace{\left(\frac{\partial \Pi_0}{\partial z} \right)^{-3} \frac{\partial}{\partial z} \left(\kappa \frac{\Pi_0}{p_0} p'_u \right)} \right\}. \quad (26)$$

Note: Vorticity on the left hand side is normally stored on ψ - points (Fig. 1), but the right hand side of the above is suited to ρ -points. For the third \mathbf{U}_p -transform, (26) is calculated on ρ -points and the interpolation is done later.

2. The unbalanced vorticity increment is decomposed into velocity increments. Unbalanced streamfunction, ψ'_u , is derived from unbalanced vorticity, ζ'_u , by solving one horizontal Poisson equation per model level

$$\zeta'_u = \nabla_h^2 \psi'_u, \quad (27)$$

with both quantities (ζ'_u and ψ'_u) held on ρ -points. After streamfunction is determined on ρ -points, it is interpolated to its desired position (ψ -points) where the unbalanced velocity components follow

$$\mathbf{u}'_u = \mathbf{k} \times \nabla_h \psi'_u \\ \begin{pmatrix} u'_u \\ v'_u \end{pmatrix} = \begin{pmatrix} -\partial \psi'_u / \partial y \\ \partial \psi'_u / \partial x \end{pmatrix}. \quad (28)$$

The pressure increment due to the third control variable is the control variable itself. This, and (28), allow the third set of model increments to be written

$$\begin{aligned}
\mathbf{x}'_{\mathbf{u}} &= \begin{pmatrix} \mathbf{U}_{13} \\ \mathbf{U}_{23} \\ \mathbf{U}_{33} \end{pmatrix} p'_{\mathbf{u}} \\
&= \begin{pmatrix} -\frac{\partial}{\partial y} \nabla_{\mathbf{h}}^{-2} \left[\frac{f}{\rho_0} \left\{ \frac{1-\kappa}{R\Pi_0\theta_0} \star + \frac{\rho_0}{\theta_0} \overbrace{\left(\frac{\partial\Pi_0}{\partial z} \right)^{-1} \theta_0 \frac{\partial}{\partial z} \left(\kappa \frac{\Pi_0}{p_0} \star \right)} \right\} - \right. \\ \left. \frac{fg}{c_p} \left(\frac{\partial\theta_0}{\partial z} \right)^{-1} \left\{ \overbrace{\left(\frac{\partial\Pi_0}{\partial z} \right)^{-2} \frac{\partial^2}{\partial z^2} \left(\kappa \frac{\Pi_0}{p_0} \star \right)} - 2 \frac{\partial^2 \Pi_0}{\partial z^2} \overbrace{\left(\frac{\partial\Pi_0}{\partial z} \right)^{-3} \frac{\partial}{\partial z} \left(\kappa \frac{\Pi_0}{p_0} \star \right)} \right\} \right] \\ \\ \left. \frac{\partial}{\partial x} \nabla_{\mathbf{h}}^{-2} \left[\frac{f}{\rho_0} \left\{ \frac{1-\kappa}{R\Pi_0\theta_0} \star + \frac{\rho_0}{\theta_0} \overbrace{\left(\frac{\partial\Pi_0}{\partial z} \right)^{-1} \theta_0 \frac{\partial}{\partial z} \left(\kappa \frac{\Pi_0}{p_0} \star \right)} \right\} - \right. \right. \\ \left. \left. \frac{fg}{c_p} \left(\frac{\partial\theta_0}{\partial z} \right)^{-1} \left\{ \overbrace{\left(\frac{\partial\Pi_0}{\partial z} \right)^{-2} \frac{\partial^2}{\partial z^2} \left(\kappa \frac{\Pi_0}{p_0} \star \right)} - 2 \frac{\partial^2 \Pi_0}{\partial z^2} \overbrace{\left(\frac{\partial\Pi_0}{\partial z} \right)^{-3} \frac{\partial}{\partial z} \left(\kappa \frac{\Pi_0}{p_0} \star \right)} \right\} \right] \right] \times p'_{\mathbf{u}}, \quad (29)
\end{pmatrix}
\end{aligned}$$

where, for clarity, $p'_{\mathbf{u}}$ appears where there is a star, \star . As in previous equations, Cartesian components have been used for illustration, but spherical coordinates would be used in practice (see App. D which is concerned with discretization).

Knowing (24), (25), and (29), we can now compute all three sets of increments from the three control parameters, $\mathbf{x}' = \mathbf{x}'_{\mathbf{b}} + \mathbf{x}'_{\mathbf{div}} + \mathbf{x}'_{\mathbf{u}}$.

5 Formulating the Equations for the \mathbf{T}_p Transform

The objective of the \mathbf{T}_p transform is to determine the fields of the control parameters, $\psi'_{\mathbf{b}}$, χ' , and $p'_{\mathbf{u}}$ from 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 the outer loop is implemented). We discuss below, in turn, the equations needed to determine each field. Equations (9) are three independent equations for the three unknowns $\psi'_{\mathbf{b}}$, χ' , and $p'_{\mathbf{u}}$.

5.1 The first equation for ψ'_b

To form the equation that we wish to solve for the balanced variable, substitute the balanced components from (24) into PV' (15), noting that here $\zeta' = \nabla_h^2 \psi'_b$

$$\begin{aligned}
PV' = & \frac{1}{\rho_0} \frac{\partial \theta_0}{\partial z} \nabla_h^2 \psi'_b - \\
& \frac{f}{\rho_0^2} \frac{\partial \theta_0}{\partial z} \left\{ \frac{1 - \kappa}{R \Pi_0 \hat{\theta}_0} \nabla_h^{-2} \nabla_h \cdot (f \rho_0 \nabla_h \psi'_b) + \right. \\
& \left. \frac{\rho_0}{\hat{\theta}_0} \left(\frac{\partial \Pi_0}{\partial z} \right)^{-1} \theta_0 \frac{\partial}{\partial z} \left(\kappa \frac{\Pi_0}{p_0} \nabla_h^{-2} \nabla_h \cdot (f \rho_0 \nabla_h \psi'_b) \right) \right\} + \\
& \frac{fg}{\rho_0 c_p} \left\{ \left(\frac{\partial \Pi_0}{\partial z} \right)^{-2} \frac{\partial^2}{\partial z^2} \left(\kappa \frac{\Pi_0}{p_0} \nabla_h^{-2} \nabla_h \cdot (f \rho_0 \nabla_h \psi'_b) \right) - \right. \\
& \left. 2 \frac{\partial^2 \Pi_0}{\partial z^2} \left(\frac{\partial \Pi_0}{\partial z} \right)^{-3} \frac{\partial}{\partial z} \left(\kappa \frac{\Pi_0}{p_0} \nabla_h^{-2} \nabla_h \cdot (f \rho_0 \nabla_h \psi'_b) \right) \right\}. \tag{30}
\end{aligned}$$

Notice that PV' is calculated from the full increment, \vec{X}' , even though we are solving for the balanced part of the flow only. This is the case because the divergent and unbalanced components of the flow have no PV' by design of the transforms. Equation (30) is solved using an iterative generalized conjugate residual (GCR) algorithm e.g. [13, 2] using appropriate preconditioning [5, 6, 7].

There is a potential problem when solving (30). The balanced pressure, $\nabla_h^{-2} \rho_0 \nabla_h \cdot (f \nabla_h \psi'_b)$, is the solution of a horizontal Poisson equation, and consequently the solution (of the Poisson equation) must have a horizontal global mean of zero. This requirement may be thought of as a level-by-level adjustment of balanced pressure. In (30), however, this balanced pressure (multiplied by $\kappa \Pi_0 / p_0$) is differentiated once and twice in the vertical, which may be strongly affected by the (effective) adjustment. Practically there is no clear solution of this potential problem, but the method adopted is to ensure that the PV' calculated from the full increment is found using a pressure that itself has been adjusted to have zero global mean in the horizontal.

5.2 The second equation for χ

The contribution to the flow from the χ' control variable is found by computing the divergence of u_2 and v_2 from (20) and (25)

$$\nabla_h \cdot \mathbf{u}_h' = \nabla_h^2 \chi'. \tag{31}$$

Notice that, as for PV , the divergence is calculated from the full increment, \vec{X}' , even though we are solving for the divergent part of the flow only. This is the case because the balanced and unbalanced components of the flow each have no divergence by design of the transforms.

5.3 The third equation, p'_u

There are two alternative ways of solving for p'_u . Method 1 is a fit of p'_u to $\bar{P}\bar{V}$ in a similar way to the fit of ψ_b to PV . Here though the anti-balance relation (26) is used instead of the balance relation (22). Method 2 involves no use of $\bar{P}\bar{V}$, but a direct inversion of (26). Each method is described below.

5.3.1 Method 1 for p'_u : using $\bar{P}\bar{V}$

In this approach, the equation that we wish to solve for the unbalanced variable is formed by substituting the unbalanced components from (29) into $\bar{P}\bar{V}'$ (21)

$$\begin{aligned} \bar{P}\bar{V}' = & \left(f\rho_0 + \frac{d(f\rho_0)}{dy} \frac{\partial}{\partial y} \nabla_h^{-2} \right) \times \\ & \left[\frac{f}{\rho_0} \left\{ \frac{1-\kappa}{R\Pi_0\hat{\theta}_0} p'_u + \frac{\rho_0}{\hat{\theta}_0} \overbrace{\left(\frac{\partial\Pi_0}{\partial z} \right)^{-1} \theta_0 \frac{\partial}{\partial z} \left(\kappa \frac{\Pi_0}{p_0} p'_u \right)} \right\} - \right. \\ & \left. \frac{fg}{c_p} \left(\frac{\partial\theta_0}{\partial z} \right)^{-1} \left\{ \left(\frac{\partial\Pi_0}{\partial z} \right)^{-2} \frac{\partial^2}{\partial z^2} \left(\kappa \frac{\Pi_0}{p_0} p'_u \right) - 2 \frac{\partial^2\Pi_0}{\partial z^2} \left(\frac{\partial\Pi_0}{\partial z} \right)^{-3} \overbrace{\frac{\partial}{\partial z} \left(\kappa \frac{\Pi_0}{p_0} p'_u \right)} \right\} \right] - \\ & \nabla_h^2 p'_u, \end{aligned} \quad (32)$$

Notice that, as for PV and divergence, $\bar{P}\bar{V}'$ is calculated from the full increment, \bar{X}' , even though we are solving for the unbalanced part of the flow only. This is the case because the balanced and divergent components of the flow each have no $\bar{P}\bar{V}'$ by design of the transforms. Equation (32) is solved using an iterative generalized conjugate residual (GCR) algorithm e.g. [13, 2] using appropriate preconditioning using appropriate preconditioning [5, 6, 7].

5.3.2 Method 2 for p'_u : direct inversion of the anti-balance equation (no $\bar{P}\bar{V}$ used)

There are two problems associated with solution of ψ'_b and p'_u by iterative solvers that solve (30) and (32).

- The third unbalanced \mathbf{U}_p -transform (26) amplifies modes of p'_u that have small vertical scales (and when transforming from ζ'_u to ψ'_u via (27) also amplifies modes of p'_u that have large horizontal scales). In order to prevent these scales from flooding the unbalanced wind fields (32) must be solved adequately so that p'_u contains only very small weight in these scales. In practice it is found that (32) is not solved adequately to achieve this.
- The combined solution of (30) and (32) must satisfy $\psi' = \psi'_b + \psi'_u$ and $p' = p'_b + p'_u$. There is nothing in the solution to ensure this, especially if (30) and (32) are not solved adequately.

These problems show up in failures of so-called inverse tests, where $\mathbf{U}_p \mathbf{T}_p = \mathbf{I}$ is tested.

The first problem can be solved in principle by inverting (26) directly in the following way. First solve for ψ'_b by solving (30) as normal. Next calculate ψ'_u as a residual, $\psi'_u = \psi' - \psi'_b$. ψ'_u may then be used to compute p'_u by inverting (26) column-by-column. This alternative procedure to calculate p'_u no longer needs (32) nor $\bar{P}\bar{V}'$.

This does not solve the second problem. Although the direct inversion procedure ensures roughly that $\psi' = \psi'_b + \psi'_u$, it does not ensure that $p' = p'_b + p'_u$. Additionally a couple of steps exist in this procedure that introduce errors (interpolation of ψ'_u from ψ to ρ -points and the inability to invert (26) at the equator).

6 Appendix A: Useful Relations between variables

6.1 Standard relationships for wind variables

The relationship between horizontal rotational wind and the vertical component of vorticity is

$$\zeta = \mathbf{k} \cdot \nabla \times \mathbf{u}_h, \quad (33)$$

where \mathbf{k} is the vertical unit vector and ∇ is the three-dimensional differential operator. The relationship between the vertical component of vorticity and streamfunction is

$$\zeta = \nabla_h^2 \psi, \quad (34)$$

where ∇_h is the horizontal differential operator. The relationship between horizontal rotational wind and streamfunction is

$$\mathbf{u}_h = \mathbf{k} \times \nabla \psi. \quad (35)$$

The relationship between horizontal divergent wind and velocity potential is

$$\mathbf{u}_h = \nabla_h \chi, \quad (36)$$

and the relationship between horizontal divergence, $\nabla_h \cdot \mathbf{u}_h$, and velocity potential is

$$\nabla_h \cdot \mathbf{u}_h = \nabla_h^2 \chi. \quad (37)$$

6.2 Relations between full model variables

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

$$\hat{T} = \Pi \hat{\theta}, \quad (38)$$

where the exner pressure, Π is

$$\Pi = \left(\frac{p}{p_{1000}} \right)^\kappa. \quad (39)$$

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 (38) have been assigned a hat, $\hat{\cdot}$. This denotes that, due to the grid staggering, vertical interpolation has to be performed to estimate the quantity at an intermediate level. In (38), temperature and potential temperature are situated on θ -levels and pressure and exner pressure on ρ -levels (see Fig. 1), and so for the relation to hold, vertical interpolation of T and θ has to be performed to the ρ -level of Π .

Differentiating (39) with respect to height yields, on θ -levels

$$\begin{aligned} \frac{\partial \Pi}{\partial z} &= \kappa \left(\frac{\hat{p}}{p_{1000}} \right)^{\kappa-1} \frac{1}{p_{1000}} \frac{\partial p}{\partial z}, \\ &= \kappa \frac{\hat{\Pi}}{\hat{p}} \frac{\partial p}{\partial z}. \end{aligned} \quad (40)$$

Differentiation of Π in (39) with respect to p yields

$$\frac{d\Pi}{dp} = \kappa \frac{\Pi}{p}. \quad (41)$$

The ideal gas equation of state on θ - and ρ -levels respectively, and developed from (p, ρ, T) to (p, Π, ρ, θ) using (38) is

$$\begin{aligned} \theta\text{-levels} : \quad \hat{p} &= R\hat{\rho}T, \\ &= R\hat{\rho}\hat{\Pi}\theta, \end{aligned} \quad (42)$$

$$p\text{-levels} : \quad p = R\rho\Pi\hat{\theta}. \quad (43)$$

The familiar hydrostatic relation, written on θ -levels (Eq. (44) below) may be developed in terms of Π and θ using the above equations

$$\frac{\partial p}{\partial z} = -\hat{\rho}g = -\frac{\hat{p}g}{R\hat{\Pi}\theta}, \quad (44)$$

$$\theta \frac{\partial \Pi}{\partial z} = -\frac{g}{c_p}. \quad (45)$$

Although we give the hydrostatic equation, we do not assume that full model fields are in hydrostatic 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 (45) with respect to height (divide by $\partial \Pi / \partial z$ first), and give the result on ρ -levels

$$\begin{aligned} \theta &= -\frac{g}{c_p} \left(\frac{\partial \Pi}{\partial z} \right)^{-1}, \\ \frac{\partial \theta}{\partial z} &= \frac{g}{c_p} \left(\frac{\partial \Pi}{\partial z} \right)^{-2} \frac{\partial^2 \Pi}{\partial z^2}. \end{aligned} \quad (46)$$

6.3 Relations between increments

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

To write ρ increments in terms of other increments, develop the equation of state. Start with (43) and then write in incremental form

$$\begin{aligned} p &= R\rho\Pi\hat{\theta}, \\ p' &= R\rho\Pi\hat{\theta}' + R\rho\hat{\theta}\Pi' + R\Pi\hat{\theta}\rho', \\ &= R\rho\Pi\hat{\theta}' + \kappa p' + R\Pi\hat{\theta}\rho', \\ \therefore \rho' &= \frac{1-\kappa}{R\Pi\hat{\theta}} p' - \frac{\rho}{\hat{\theta}} \hat{\theta}', \end{aligned} \quad (47)$$

where for the third line in the above we have written Π' in terms of p' using (41) and (43). It is often necessary to write θ increments in terms of p increments. We use the hydrostatic relation (45) for this purpose. This is written in terms of increments below

$$\begin{aligned} \theta \frac{\partial \Pi}{\partial z} &= -\frac{g}{c_p}, \\ \theta \frac{\partial \Pi'}{\partial z} + \frac{\partial \Pi}{\partial z} \theta' &= 0, \\ \theta \frac{\partial}{\partial z} \left(\kappa \frac{\Pi}{p} p' \right) + \frac{\partial \Pi}{\partial z} \theta' &= 0, \end{aligned} \quad (48)$$

where (41) has been used for the last line. We wish to eliminate θ' between (47) and (48). In order to do this, we must first compute $\hat{\theta}'$ from (48), which involves further vertical interpolation

$$\hat{\theta}' = -\overbrace{\left(\frac{\partial \Pi}{\partial z} \right)^{-1} \theta \frac{\partial}{\partial z} \left(\kappa \frac{\Pi}{p} p' \right)}^{\text{hat}}, \quad (49)$$

where the overbrace represents a hat acting on the entire right hand side. This equation is now substituted into (47)

$$\rho' = \frac{1-\kappa}{R\Pi\hat{\theta}} p' + \frac{\rho}{\hat{\theta}} \overbrace{\left(\frac{\partial \Pi}{\partial z} \right)^{-1} \theta \frac{\partial}{\partial z} \left(\kappa \frac{\Pi}{p} p' \right)}^{\text{hat}}. \quad (50)$$

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 (46) in ρ -levels gives

$$\begin{aligned}\frac{\partial\theta'}{\partial z} &= \frac{g}{c_p} \left\{ \left(\widehat{\frac{\partial\Pi}{\partial z}} \right)^{-2} \frac{\partial^2\Pi'}{\partial z^2} - 2 \left(\widehat{\frac{\partial\Pi}{\partial z}} \right)^{-3} \frac{\partial^2\Pi}{\partial z^2} \widehat{\frac{\partial\Pi'}{\partial z}} \right\}, \\ &= \frac{g}{c_p} \left\{ \left(\widehat{\frac{\partial\Pi}{\partial z}} \right)^{-2} \frac{\partial^2}{\partial z^2} \left(\kappa \frac{\Pi}{p} p' \right) - 2 \left(\widehat{\frac{\partial\Pi}{\partial z}} \right)^{-3} \frac{\partial^2\Pi}{\partial z^2} \overbrace{\frac{\partial}{\partial z} \left(\kappa \frac{\Pi}{p} p' \right)} \right\},\end{aligned}\quad (51)$$

where for the last line (41) has been used.

7 Appendix B: Ertel PV in Height Co-ordinates

Normally Ertel PV is specified in isentropic co-ordinates

$$Q = \frac{\zeta_\theta + f}{-\frac{1}{g} \frac{\partial p}{\partial \theta}}, \quad (52)$$

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

$$\zeta_\theta = \mathbf{k} \cdot (\nabla_\theta \times \mathbf{u}_h). \quad (53)$$

In (53), \mathbf{k} is the vortical unit vector, ∇_θ is the gradient operator evaluated along isentropic surfaces in the horizontal, and \mathbf{u}_h is the horizontal velocity. In order to transform to height (z) co-ordinates, we make use of the following relations in the vertical and in the horizontal

$$\begin{aligned}\frac{\partial p}{\partial \theta} &= \frac{\partial z}{\partial \theta} \frac{\partial p}{\partial z} = -\frac{\partial z}{\partial \theta} \rho g, \\ \left(\frac{\partial}{\partial x} \right)_z &= \left(\frac{\partial}{\partial x} \right)_\theta + \left(\frac{\partial \theta}{\partial x} \right)_z \frac{\partial}{\partial \theta}, \\ \left(\frac{\partial}{\partial y} \right)_z &= \left(\frac{\partial}{\partial y} \right)_\theta + \left(\frac{\partial \theta}{\partial y} \right)_z \frac{\partial}{\partial \theta}.\end{aligned}\quad (54)$$

By inserting this information into (52) the following emerges

$$PV = \frac{1}{\rho} \left\{ (\zeta + f) \frac{\partial \theta}{\partial z} - \mathbf{k} \cdot \left(\nabla_h \theta \times \frac{\partial \mathbf{u}_h}{\partial z} \right) \right\}, \quad (55)$$

where ζ 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 (55) is much smaller in magnitude than the first.

8 Appendix C: Grid staggering

The Met Office 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 labelled as coincident with u , v , ψ , ρ or θ . The new parameters introduced in this work are stored at the points outlined in Table I.

9 Appendix D: Discretization and finite differencing

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

Parameter	Staggering
PV'	ψ
$\bar{P}V'$	ρ
$\nabla_h \cdot \mathbf{u}'_h$	ρ
ψ'_b	ψ
p'_u	ρ
χ	ρ

Table I: Staggering of dual space and control parameters.

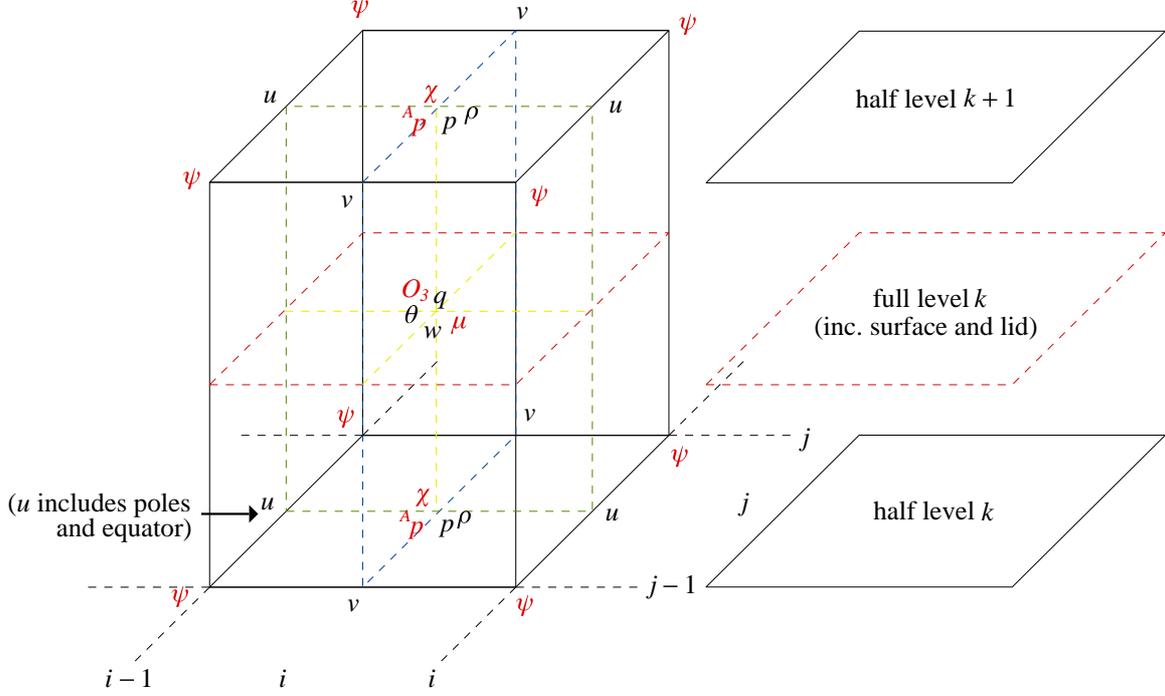


Figure 1: The Met Office 'new dynamics' grid staggering.

9.1 Notation

Refer to 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 (ρ) levels, as in the second row of Table II the coefficients are

$$\alpha_1(i, j, k) = \frac{r_0^\rho(i, j, k) - r_0^\theta(i, j, k-1)}{r_0^\theta(i, j, k) - r_0^\theta(i, j, k-1)}, \quad (56)$$

$$\beta_1(i, j, k) = \frac{r_0^\theta(i, j, k) - r_0^\rho(i, j, k)}{r_0^\theta(i, j, k) - r_0^\theta(i, j, k-1)}, \quad (57)$$

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

$$\alpha_2(i, j, k) = \frac{r_0^\theta(i, j, k) - r_0^\rho(i, j, k)}{r_0^\rho(i, j, k+1) - r_0^\rho(i, j, k)}, \quad (58)$$

$$\beta_2(i, j, k) = \frac{r_0^\rho(i, j, k+1) - r_0^\theta(i, j, k)}{r_0^\rho(i, j, k+1) - r_0^\rho(i, j, k)}. \quad (59)$$

Averaging direction	'Small' symbol	'Large' symbol
Horizontal (ρ -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- ρ)	$\tilde{A}(i, j, k) = \frac{1}{4}(A(i, j, k) + A(i, j - 1, k) + A(i - 1, j, k) + A(i - 1, j - 1, k))$	$\overline{\text{long expression}}$
Vertical (θ -to- ρ)	$\hat{B}(i, j, k) = \alpha_1 B(i, j, k) + \beta_1 B(i, j, k - 1)$	$\overbrace{\text{long expression}}$
(ρ -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.

9.2 Potential vorticity increment, PV'

We choose PV' (15) to be represented on a ψ -point. Evaluating it with respect to a zonal-mean linearisation state gives the following finite difference formula,

$$\begin{aligned}
PV'(i, j, k) &= \frac{\overline{\partial_z \theta_0(j, k)}}{\rho_0(j, k)} \zeta'(i, j, k) - \\
&\frac{\overline{f_u(j) \partial_z \theta_0(j, k)}}{\rho_0^2(j, k)} \frac{1 - \kappa}{R \Pi_0(j, k) \hat{\theta}_0(j, k)} p'(i, j, k) - \frac{\overline{f_u(j) \partial_z \theta_0(j, k)}}{\rho_0^2(j, k)} \frac{\rho_0(j, k)}{\hat{\theta}_0(j, k)} \hat{Q}(i, j, k) + \\
&\frac{\overline{f_u(j) \frac{g}{c_p} \widehat{\partial_z \Pi_0}^{-2}(j, k) R(i, j, k)}}{\rho_0(j, k) c_p} - \frac{\overline{f_u(j) \frac{g}{c_p} 2 \partial_{zz} \Pi_0(j, k) \widehat{\partial_z \Pi_0}^{-3}(j, k) \hat{S}(i, j, k)}}{\rho_0(j, k) c_p},
\end{aligned} \tag{60}$$

where ∂_z and ∂_{zz} are shorthand for $\partial/\partial z$ and $\partial^2/\partial z^2$ respectively. In (60) 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 zonally meaned)

$$\partial_z \theta_0(i, j, k) = \frac{\theta_0(i, j, k) - \theta_0(i, j, k - 1)}{r_0^\theta(i, j, k) - r_0^\theta(i, j, k - 1)}, \tag{61}$$

$$\begin{aligned}
\zeta'(i, j, k) &= \frac{1}{r \cos \phi} \left(\frac{\partial v'}{\partial \lambda} - \frac{\partial(u' \cos \phi)}{\partial \phi} \right), \\
&= \frac{v'(i + 1, j, k) - v'(i, j, k)}{r \cos \phi_v(j) \delta \lambda} - \frac{u'(i, j + 1, k) \cos \phi_u(j + 1) - u'(i, j, k) \cos \phi_u(j)}{r \cos \phi_v(j) \delta \phi},
\end{aligned} \tag{62}$$

$$\begin{aligned}
Q(i, j, k) &= \frac{r_0^p(i, j, k + 1) - r_0^p(i, j, k)}{\Pi_0(j, k + 1) - \Pi_0(j, k)} \theta_0(j, k) \frac{\Pi'(i, j, k + 1) - \Pi'(i, j, k)}{r_0^p(i, j, k + 1) - r_0^p(i, j, k)}, \\
&= \frac{1}{\Pi_0(j, k + 1) - \Pi_0(j, k)} \theta_0(j, k) (\Pi'(i, j, k + 1) - \Pi'(i, j, k)),
\end{aligned} \tag{63}$$

$$R(i, j, k) = \frac{1}{r_0^\theta(i, j, k) - r_0^\theta(i, j, k - 1)} \left(\frac{\Pi'(i, j, k + 1) - \Pi'(i, j, k)}{r_0^p(i, j, k + 1) - r_0^p(i, j, k)} - \frac{\Pi'(i, j, k) - \Pi'(i, j, k - 1)}{r_0^p(i, j, k) - r_0^p(i, j, k - 1)} \right), \tag{64}$$

$$S(i, j, k) = \frac{\Pi'(i, j, k + 1) - \Pi'(i, j, k)}{r_0^p(i, j, k + 1) - r_0^p(i, j, k)}, \tag{65}$$

$$\Pi'(i, j, k) = \kappa \frac{\Pi_0(j, k)}{p_0(j, k)} p'(i, j, k), \tag{66}$$

$$\widehat{\partial_z \Pi_0}(i, j, k) = \frac{\Pi_0(i, j, k + 1) - \Pi_0(i, j, k)}{r_0^p(i, j, k + 1) - r_0^p(i, j, k)}, \tag{67}$$

$$\partial_{zz} \Pi_0(i, j, k) = \frac{1}{r_0^\theta(i, j, k) - r_0^\theta(i, j, k - 1)} \left(\frac{\Pi_0(i, j, k + 1) - \Pi_0(i, j, k)}{r_0^p(i, j, k + 1) - r_0^p(i, j, k)} - \frac{\Pi_0(i, j, k) - \Pi_0(i, j, k - 1)}{r_0^p(i, j, k) - r_0^p(i, j, k - 1)} \right). \tag{68}$$

9.3 Divergence increment, $\nabla_{\text{h}} \cdot \mathbf{u}'_{\text{h}}$

Horizontal divergence is the simplest of the three dual space parameters to express in finite difference form. It is positioned on a ρ -point and calculated as follows

$$\begin{aligned} \nabla_{\text{h}} \cdot \mathbf{u}'_{\text{h}}(i, j, k) &= \frac{1}{r \cos \phi} \frac{\partial u'}{\partial \lambda} + \frac{1}{r \cos \phi} \frac{\partial(v' \cos \phi)}{\partial \phi}, \\ &= \frac{1}{r \cos \phi_u(j)} \frac{u'(i, j, k) - u'(i-1, j, k)}{\delta \lambda} + \\ &\quad \frac{1}{r \cos \phi_u(j)} \frac{v'(i, j, k) \cos \phi_v(j) - v'(i, j-1, k) \cos \phi_v(j-1)}{\delta \phi}. \end{aligned} \quad (69)$$

There is a problem when evaluating (69) at the poles. Since ρ -points exist at the pole, terms containing $1/\cos \phi_u$, are impossible to evaluate there. This can be overcome by using Gauss' divergence theorem in the plane (otherwise known as Green's theorem in the plane), given generically as,

$$\int_{\text{area } ds} \nabla_{\text{h}} \cdot \mathbf{v} ds = \oint \mathbf{v} \cdot \mathbf{n} dl, \quad (70)$$

where \mathbf{n} is a unit vector pointing in the positive meridional direction for the south pole and the negative meridional direction for the north pole (it points outside of the loop). To apply (70) to (69) let $\mathbf{v} = \mathbf{u}'_{\text{h}}$. Then Gauss' theorem allows us to write

$$A \nabla_{\text{h}} \cdot \mathbf{u}'_{\text{h}}(i, j, k) = \Delta_1 r \frac{\delta \phi}{2} \delta \lambda \sum_i v'(i, j + \Delta_2, k), \quad (71)$$

where j is the meridional index for either of the poles, Δ_1 and Δ_2 are specified in Table III and A is

$$A \approx \pi (r \delta \phi / 2)^2, \quad (72)$$

which is the shaded area in Fig. 2a. The sum is performed around the ' v ' latitude 'one away' from the pole (see Fig. 2a).

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.

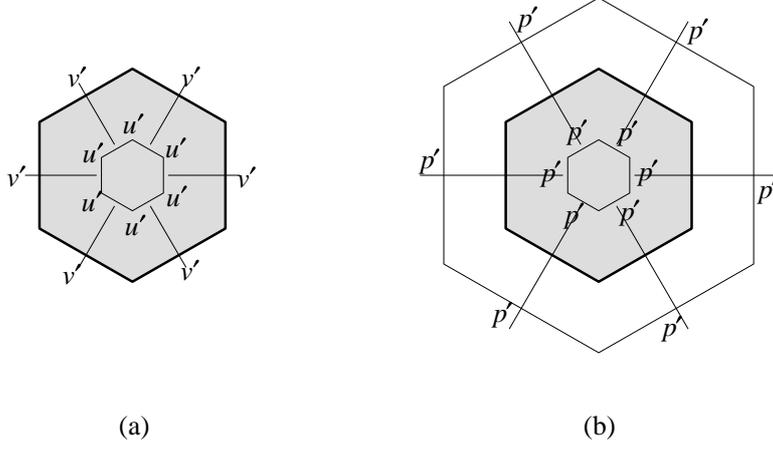


Figure 2: The polar integrals that need to be performed to calculate $\bar{P}\bar{V}$ (panel b), and $\nabla_{\mathbf{h}} \cdot \mathbf{u}'_{\mathbf{h}}$ (panel c). The thick lines circulating the pole indicate the paths of the loop integrals in each case, and enclose the shaded areas. The shaded areas in panels b and c have an area A (72). Note that the polar points ($'u'$ and $'\rho'$ -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.)

9.4 Anti-potential vorticity increment, $\bar{P}\bar{V}'$

We choose $\bar{P}\bar{V}'$ to be represented on a ρ -point. Equation (21) for $\bar{P}\bar{V}'$ has the following finite difference form

$$\begin{aligned}
\bar{P}\bar{V}'(i, j, k) &= (\nabla_{\mathbf{h}} f \rho_0) \cdot (\nabla_{\mathbf{h}} \psi') + f \rho_0 \nabla_{\mathbf{h}}^2 \psi' - \nabla_{\mathbf{h}}^2 p', \\
&= -(\nabla_{\mathbf{h}} f \rho_0) \cdot (\mathbf{k} \times \mathbf{u}'_{\mathbf{h}}) + f \rho_0 \zeta' - \nabla_{\mathbf{h}}^2 p', \\
&= -\frac{\tilde{u}'(i, j, k)}{r} \left\{ 2\Omega \cos \phi_u(j) \rho_0(j, k) + f_u(j) \frac{\rho_0(j+1, k) - \rho_0(j-1, k)}{2\delta\phi} \right\} + \\
&\quad f_u(j) \rho_0(j, k) \left\{ \left(\frac{v'(i+1, j, k) - v'(i, j, k)}{r \cos \phi_v(j) \delta\lambda} \right) - \right. \\
&\quad \left. \left(\frac{u'(i, j+1, k) \cos \phi_u(j+1) - u'(i, j, k) \cos \phi_u(j)}{r \cos \phi_v(j) \delta\phi} \right) \right\} - \\
&\quad \left\{ \frac{(p'(i+1, j, k) - 2p'(i, j, k) + p'(i-1, j, k))}{\delta\lambda^2 r^2 \cos^2(\phi_u(j))} + \right. \\
&\quad \left. \frac{(p'(i, j+1, k) - p'(i, j, k)) \cos \phi_v(j) - (p'(i, j, k) - p'(i, j-1, k)) \cos \phi_v(j-1)}{\delta\phi^2 r^2 \cos \phi_u(j)} \right\},
\end{aligned} \tag{73}$$

noting that $\nabla_{\mathbf{h}} \psi' = -\mathbf{k} \times \mathbf{u}'_{\mathbf{h}}$,

$$\mathbf{k} \times \mathbf{u}'_{\mathbf{h}} = \begin{pmatrix} -v \\ u \\ 0 \end{pmatrix},$$

and $\zeta' = \mathbf{k} \cdot \nabla \times \mathbf{u}'_{\mathbf{h}}$.

As for divergence there is a complication when evaluating $\bar{P}\bar{V}$ at the poles (see the last two lines of (74), which make up the last term of 73). The Laplacian of the pressure increment at the poles can be evaluated with the help of Gauss' theorem. Let \mathbf{v} in (70) be $\nabla_{\mathbf{h}} p'$, ds be an area element of the polar area and dl be a length element of its boundary. Equation (70) can be developed to yield an expression for $\nabla_{\mathbf{h}}^2 p'$ at the poles

$$\begin{aligned}
A \nabla_{\mathbf{h}}^2 p'(i, j, k) &= \Delta_1 r \frac{\delta\phi}{2} \delta\lambda \sum_i \frac{1}{r} \frac{\partial p'}{\partial \phi}, \\
&= \Delta_1 \frac{1}{2} \delta\lambda \sum_i (p'(i, j + \Delta_2 + 1, k) - p'(i, j + \Delta_2, k)).
\end{aligned} \tag{75}$$

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. 2b). The effective polar area, A (72) is the shaded area in Fig. 2b.

9.5 The U_1 -transform

The leading part of the U_p -transform - giving the balanced increments, \mathbf{x}'_b (24) - has three components. The first two components for u'_b and v'_b are specified in local Cartesian co-ordinates in (24). The general expression $\mathbf{u}'_h = \mathbf{k} \times \nabla \psi'_b$ is needed for the spherical expression. Translating this into finite difference form gives rise to the following result on the sphere

$$\begin{aligned} u' &= -\frac{1}{r} \frac{\partial \psi'_b}{\partial \phi}, \\ u'(i, j, k) &= -\frac{1}{r} \frac{\psi'_b(i, j, k) - \psi'_b(i, j - 1, k)}{\delta \phi}, \end{aligned} \quad (76)$$

$$\begin{aligned} v' &= \frac{1}{r \cos \phi} \frac{\partial \psi'_b}{\partial \lambda}, \\ v'(i, j, k) &= \frac{1}{r \cos \phi_v(j)} \frac{\psi'_b(i, j, k) - \psi'_b(i - 1, j, k)}{\delta \lambda}. \end{aligned} \quad (77)$$

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

A Poisson equation must be solved for the pressure (third component of (24)). The finite difference form of the right hand side of the Poisson equation is derived in the following

$$\begin{aligned} \nabla_h \cdot (f \rho_0 \nabla_h) \psi'_b &= \frac{f \rho_0}{r \cos \phi} \frac{\partial (\nabla_h \psi'_b)_\lambda}{\partial \lambda} + \frac{1}{r \cos \phi} \frac{\partial (\cos \phi (f \rho_0 \nabla_h \psi'_b)_\phi)}{\partial \phi}, \\ &= \frac{f \rho_0}{r^2 \cos^2 \phi} \frac{\partial}{\partial \lambda} \left(\frac{\partial \psi'_b}{\partial \lambda} \right) + \frac{1}{r^2 \cos \phi} \frac{\partial}{\partial \phi} \left(f \rho_0 \cos \phi \frac{\partial \psi'_b}{\partial \phi} \right), \\ \{\nabla_h \cdot (f \rho_0 \nabla_h) \psi'_b\}(i, j, k) &= \frac{1}{r^2 \cos \phi_v(j)} \left\{ \frac{f_v(j) \tilde{\rho}_0(j, k)}{\cos \phi_v(j)} \left(\frac{\psi'_b(i + 1, j, k) + \psi'_b(i - 1, j, k) - 2\psi'_b(i, j, k)}{\delta \lambda^2} \right) + \right. \\ &\quad \left. \frac{1}{\delta \phi} \left(f_u(j + 1) \rho_0(j + 1, k) \cos \phi_u(j + 1) \left(\frac{\psi'_b(i, j + 1, k) - \psi'_b(i, j, k)}{\delta \phi} \right) - \right. \right. \\ &\quad \left. \left. f_u(j) \rho_0(j, k) \cos \phi_u(j) \left(\frac{\psi'_b(i, j, k) - \psi'_b(i, j - 1, k)}{\delta \phi} \right) \right) \right\}, \end{aligned} \quad (78)$$

$$\text{where } \tilde{\rho}_0(j, k) = \frac{1}{2}(\rho_0(j + 1, k) + \rho_0(j, k)). \quad (79)$$

The result of (78) is stored on ' ψ '-points. Solving the Poisson equation yields pressure, also on ' ψ '-points, which must be interpolated to the ρ points (see Fig. 1).

9.6 The U_2 -transform

Again the transform (25) for the irrotational component, \mathbf{x}'_{div} 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

$$\begin{aligned} u' &= \frac{1}{r \cos \phi} \frac{\partial \chi'}{\partial \lambda}, \\ u'(i, j, k) &= \frac{1}{r \cos \phi_u(j)} \frac{\chi'(i + 1, j, k) - \chi'(i, j, k)}{\delta \lambda}, \end{aligned} \quad (80)$$

$$\begin{aligned} v' &= \frac{1}{r} \frac{\partial \chi'}{\partial \phi}, \\ v'(i, j, k) &= \frac{1}{r} \frac{\chi'(i, j + 1, k) - \chi'(i, j, k)}{\delta \phi}. \end{aligned} \quad (81)$$

With χ' held on ' ρ '-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 gradient of χ' in the zonal direction). This avoids the need to deal with the 'polar problem' using the integral techniques used before.

9.7 The U_3 -transform

The calculation of the leading unbalanced part of the model fields, \mathbf{x}'_u , from the unbalanced pressure parameter requires the solution of a Poisson equation (28) given the vorticity at each level. We need to evaluate (26). In this equation, p'_u is stored on ρ -points, but ζ'_u is stored on ψ -points, and so we need to interpolate to ψ -points in the discretized form of the equations. Just as ζ'_u in (26) has been found by setting $PV' = 0$ (PV' given as (15)), we can find ζ'_u in the finite-difference form of the equations by setting the discretized PV' , (60), to zero, and rearranging for ζ'_u

$$\zeta'_u(i, j, k) = \frac{f_u(j)}{\rho_0(j, k)} \left\{ \frac{1 - \kappa}{R\Pi_0(j, k)\hat{\theta}_0(j, k)} p'_u(i, j, k) + \frac{\rho_0(j, k)}{\hat{\theta}_0(j, k)} \hat{Q}(i, j, k) \right\} - \frac{f_u(j)(\partial_z \theta_0)^{-1}(j, k) \frac{g}{c_p} \left\{ \overbrace{\partial_z \Pi_0}^{-2}(j, k) R(i, j, k) - 2\partial_{zz} \Pi_0(j, k) \overbrace{\partial_z \Pi_0}^{-3}(j, k) \hat{S}(i, j, k) \right\}}{R\Pi_0(j, k)\hat{\theta}_0(j, k)}, \quad (82)$$

where Q , R and S are given in discretized form in (63), (64) and (65) respectively, but using the unbalanced pressure parameter instead of the full pressure increment.

9.7.1 Computing velocity components

Velocity follows from vorticity in two steps - first by solving the Poisson equation $\zeta'_u = \nabla_h^2 \psi'_u$ for ψ'_u followed by a derivative step (28). The same calculation is done whether vorticity has been calculated in the bulk or on the vertical boundaries. Although ζ'_u should be stored on ψ -points, in the U_2 transform it falls on ρ -points, where it is used to find ψ'_u . ψ'_u is then interpolated to ψ -points from which the winds are derived (28). The calculation for u'_u in finite difference form is

$$\begin{aligned} u'_u(i, j, k) &= -\frac{1}{r} \frac{\partial \psi'_u}{\partial \phi}, \\ &= -\frac{1}{r} \frac{\psi'_u(i, j, k) - \psi'_u(i, j - 1, k)}{\delta \phi}, \end{aligned} \quad (83)$$

and the calculation for v'_u in finite difference form is,

$$\begin{aligned} v'_u(i, j, k) &= -\frac{1}{r \cos \phi_v(j)} \frac{\partial \psi'_u}{\partial \lambda}, \\ &= -\frac{1}{r \cos \phi_v(j)} \frac{\psi'_u(i, j, k) - \psi'_u(i - 1, j, k)}{\delta \lambda}. \end{aligned} \quad (84)$$

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

10 Acknowledgements

We acknowledge useful discussions with Paul Berrisford (Univ. of Reading), Sean Buckeridge (Univ. of Bath), Peter Clark (MetO), Terry Davis (MetO), Mark Dixon (MetO), David Katz (Univ. of Reading), Amos Lawless (Univ. of Reading), Andrew Lorenc (MetO), Stefano Migliorini (Univ. of Reading), Nancy Nichols (Univ. of Reading), Alan O'Neill (Univ. of Reading), Tim Payne (MetO), Ian Roulstone (Univ. of Surrey, formerly MetO), John Thuburn (formerly Univ. of Reading) and Jan Van Lent (Univ. of Bath). Particular thanks go to Marek Wlasak (MetO) for help with implementation of the new variables and for suggesting improvements to this manuscript .

References

- [1] R.N. Bannister (2003), On control variable transforms in the Met Office 3d and 4d Var., and a description of the proposed waveband summation transformation, DARC Internal Report **5**, 45 pp.

- [2] R.N. Bannister (2004), Iterative solvers and minimization algorithms, <http://www.met.rdg.ac.uk/ross/Documents/CG+GCR.pdf>, 15 pp.
- [3] R.N. Bannister, M.J.P. Cullen (2007), A regime-dependent balanced control variable based on potential vorticity, ECMWF workshop on flow-dependent aspects of data assimilation, 11-13 June 2007, 101-112.
- [4] R.N. Bannister, D. Katz, M.J.P. Cullen, A.S. Lawless, N.K. Nichols (2008), Modelling of forecast errors in geophysical fluid flows, *Int. J. Numer. Meth. Fluids* **56** 1147-1153.
- [5] R.N. Bannister, Diagonal preconditioning of the PV equations for preconditioning, <http://www.met.rdg.ac.uk/ross/DARC/PVcv/PreconDiag.pdf>.
- [6] R.N. Bannister, Approximate 'vertical only' preconditioning of the PV equations, <http://www.met.rdg.ac.uk/ross/DARC/PVcv/PreconVert.pdf>.
- [7] R.N. Bannister, ADI preconditioning for the PV equations, <http://www.met.rdg.ac.uk/ross/DARC/PVcv/PreconADI.pdf>.
- [8] R.N. Bannister (2008), The 'potential vorticity'-based control vector project. User's guide for the new code, <http://www.met.rdg.ac.uk/ross/DARC/PVcv/UserGuide.pdf>.
- [9] M.J.P. Cullen (2003), Four-dimensional variational data assimilation: A new formulation of the background-error covariance matrix based on a potential-vorticity representation, *Q.J.R. Meteorol. Soc.* **129** 2777-2796.
- [10] Met Office VAR Scientific Documentation Paper 11, Control variable transforms - parameters.
- [11] Met Office VAR Scientific Documentation Paper 13, Control variable transforms. [Documentation for the vertical transform]
- [12] Met Office VAR Scientific Documentation Paper 14, Horizontal transforms.
- [13] M. Zerroukat (2000), Iterative solvers, Met Office.