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A Comparison of Potential Vorticity-Based and Vorticity-Based Control Variables

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Abstract

In most operational weather forecasting centres variational data assimilation is performed using a different set of variables from the actual model variables The transformation of variables simplifies the problem by assuming that the errors in the transformed variables are uncorrelated The validity of this hypothesis is key to the accuracy of the data assimilation Recently a potential vorticity (PV based set of variables has been proposed These new variables are thought to exploit more accurately important dynamical properties of the atmosphere Here we present new results obtained with a simplified 2D shallow water model comparing the PV based variables to the vorticity based variables currently used at operational weather forecasting centres including the Met Office The validity of the fundamental assumption that the errors in the transformed variables are uncorrelated is tested in a variety of dynamical regimes The results

1 Introduction

Data assimilation is a process for finding initial conditions for numerical weather prediction (NWP) models. By combining observational data, statistical data, knowledge of atmospheric dynamics and a previous short forecast the best estimate, or *analysis*, of the state of the atmosphere is found. Due to the chaotic nature of the governing equations any errors in the initial conditions may grow rapidly in the forecast and thus data assimilation forms a vital part of NWP. The assimilation problem is huge, with typically 10^7 variables, and special methods need to be found to make the problem practical to solve.

At the Met Office the data assimilation is performed using a different set of variables to the model variables. These variables are the control variables and the choice of these is key to the data assimilation system performance. The transformation of variables simplifies the problem by assuming that the errors in the new variables are uncorrelated. One way that is thought to do this accurately is by using *balanced* control variables. Here an attempt is made to separate the balanced and unbalanced modes as it is thought there is little or no interaction between these flows and so their errors are uncorrelated. The use of control variables in this way was first introduced in [8]. Here balance between mass and momentum is implicitly introduced by combining the balanced parts of mass and momentum fields in a single variable.

The current control variables used at the Met Office are vorticity-based and do not represent the separation of balanced and unbalanced modes in all flow regimes. Recently a new set of control variables has been proposed [2] that should be valid across all regimes. The new variables use a conserved quantity, the potential vorticity (PV), to capture the balanced mode. In [14] the PV-based approach is developed for the 2D shallow water equations on a sphere and the potential benefits are demonstrated theoretically and experimentally. These initial results are encouraging. In this study we analyse the vorticity-based and PV-based variables in the context of a simplified

1D shallow water equation model and investigate the validity of the fundamental assumption that the errors in the control variables are uncorrelated in various flow regimes.

We start by introducing the theoretical aspects of control variable transforms as they apply to four dimensional variational data assimilation (4D-VAR). We then derive the vorticity-based and PV-based transforms for the simplified shallow water equation model. In this simplified context the implications of each transform are examined. We first derive the background error covariance matrices implied by each control variable transform. This highlights a key difference between the transforms; whilst the vorticity-based transform implies static background error statistics the implied background error statistics of the PV-based transform are state-dependent. Next we test the validity of the fundamental assumption that the errors in the control variables are uncorrelated. We test whether the assumption holds as we change the dynamical regime. We also propose an approximate form of the PV-based transform and examine the consequences of this approximation on the error correlations between the approximated variables. From these results we are able to draw conclusions regarding the effectiveness of each transform.

2 Control Variable Transforms in 4D-VAR

model space to observational space. The background error covariance matrix is defined by B, typically of size O($10^7 \times 10^7$), and R_i is the observation error covariance matrix, generally of size O($10^6 \times 10^6$). This is a non-linear least squares minimisation problem and is usually solved incrementally as discussed in [1].

Incremental 4D-VAR minimises a series of approximate convex quadratic cost functions for an increment x'_0

$$
\begin{aligned}
\mathrm{J}'^{(k)}[\mathrm{x}'^{(k)}_0] &= \frac{1}{2}(\mathrm{x}'^{(k)}_0 - \mathrm{x}'^{b})^T \mathrm{B}^{-1}(\mathrm{x}'^{(k)}_0 - \mathrm{x}'^{b}) \\
&+ \frac{1}{2}\sum_{i=0}^{n}(\mathrm{H}_i \mathrm{x}'^{(k)}_i - \mathrm{d}_i)^T \mathrm{R}_i^{-1}(\mathrm{H}_i \mathrm{x}'^{(k)}_i - \mathrm{d}_i), \qquad (2)
\end{aligned}
$$

where k is the iteration count and H_i is the linearised observation operator. Here $\mathrm{x}'^{(k)}_i = \mathrm{M}(t_i, t_0, \mathrm{x}^{(k)})\mathrm{x}'^{(k)}_0$, where $\mathrm{M}(t_i, t_0, \mathrm{x}^{(k)}) \equiv \mathrm{M}_i$ denotes the linear evolution operator from t_0 to t_i of the tangent linear model (TLM). The TLM is a linearisation of the non-linear model about the current guess trajectory. The background increment, x'^{b}, is given by $\mathrm{x}'^{b} = \mathrm{x}^b - \mathrm{x}^{(k)}_0$ and the innovation vector, d_i, by $\mathrm{d}_i = \mathrm{y}^o_i - \mathcal{H}_i[\mathrm{x}^{(k)}_i]$.

Further simplification is now needed to handle the background error covariance matrix, B, which cannot be stored in memory. This is done by transforming from model variables to new *control variables* to perform the data assimilation. The errors in these control variables are considered to be uncorrelated with each other and thus the background error covariance matrix becomes block diagonal and the size of the data assimilation problem is greatly reduced. The block components of the transformed matrix specify the auto-correlations of each variable. Effectively the problem of modelling and storing the m6 of modeion o;

and its inverse,

$$\mathbf{z}' = \mathbf{T}\mathbf{x}', \tag{4}$$

is known as the T-transform. Here $\mathbf{z}'$ are the control variable increments and $\mathbf{x}'$ the model variable increments. Substituting into the incremental cost function (2) we obtain,

$$J^{(k)}[\mathbf{z}_0'^{(k)}] = \frac{1}{2}(\mathbf{z}_0'^{(k)} - \mathbf{z}'^{b})^T \mathbf{U}^T \mathbf{B}^{-1} \mathbf{U}(\mathbf{z}_0'^{(k)} - \mathbf{z}'^{b})$$
$$+ \frac{1}{2}\sum_{i=0}^{n}(\mathbf{H}_i(\mathbf{M}_i\mathbf{U}\mathbf{z}_0'^{(k)}) - \mathbf{d}_i)^T \mathbf{R}_i^{-1}(\mathbf{H}_i(\mathbf{M}_i\mathbf{U}\mathbf{z}_0'^{(k)}) - \mathbf{d}_i), \tag{5}$$

where $\mathbf{U}$ is the U-transform on iteration k and $(\mathbf{M}_i\mathbf{U}\mathbf{z}_0'^{(k)})$ represents the control variable increment at the initial time transformed to model space and evolved by the TLM to time t_i. It is necessary to transform $\mathbf{z}_0'^{(k)}$ in the observation term of (5) as the linearised observation operator $\mathbf{H}_i$ and the linear model operator $\mathbf{M}_i$ act on model variables and not control variables.

If we now choose $\mathbf{U}$ such that

$$\mathbf{U}^T\mathbf{B}^{-1}\mathbf{U} = \Lambda^{-1},$$

where Λ

$\mathbf{B}$ $\mathbf{U}$ $\mathbf{U}^T\mathbf{U}$

observation is assimilated. Even in this simple scenario it can be shown that the analysis increment

$$\mathrm{x}^a - \mathrm{x}^b \propto \mathrm{B}(:, j) = (\mathrm{U}\Lambda\mathrm{U}^T)(:, j),$$

where x^a is the model state at time $t = 0$ that minimises the cost function (1), $\mathrm{B}(:, j)$ is the jth column of the background error covariance matrix B and a single observation is located at a point j.

In order to identify possible control variables, we use dynamical properties of the system. Two types of atmospheric motion can be identified as normal modes of the primitive equations used in numerical weather prediction (NWP), linearised about a simple basic state [3]. One of these motions is slow and corresponds to a Rossby wave, whilst the others are fast and correspond to inertial-gravity waves. The slow mode is referred to as *balanced*, and the fast as *unbalanced*. This is because in the linear analysis the slow mode satisfies a linear balance condition. For the most part it is the balanced motion that is of meteorological significance. It is thought that a good choice of control variables will involve capturing the balanced and unbalanced modes in separate control variables since we assume that there is little or no interaction between these flows. In the linear case the modes evolve independently and therefore there is no interaction. In the non-linear case the degree of this interaction will depend in some sense on the degree of non-linearity.

In the following section we present the current vorticity-based control variables and an alternative version of control variables based on the potential

The balance equation is a fundamental component of both the vorticity and the PV-based transforms and is applied to increments in a linearised form. We let $u(x,t) = \bar{u}(x,t) + u'(x,t)$, $v(x,t) = \bar{v}(x,t) + v'(x,t)$ and $h(x,t) = \bar{h}(x,t) + h'(x,t)$, where $\bar{u}(x,t)$, $\bar{v}(x,t)$ and $\bar{h}(x,t)$ are reference states. If we assume that the reference states satisfy the balance equation (10) to first order accuracy, then we obtain a corresponding first-order linear balance equation for the increments, given by

$$fv' - g\frac{\partial h'}{\partial x} = 0. \tag{12}$$

The quantity

$$q = \frac{1}{h}\left(f + \frac{\partial v}{\partial x}\right), \tag{13}$$

or the potential vorticity (PV), is conserved in the simplified SWEs. It can also be shown that the simplified SWEs, linearised about a simple reference state, have three normal modes: one slow and two fast. The slow, or balanced mode satisfies linear balance and is characterised by a linearised form of the PV. The remaining two fast modes can be related to the geostrophic departure, ${}_a\zeta'$, defined by

$${}_a\zeta' = f\frac{\partial v'}{\partial x} - g\frac{\partial^2 h'}{\partial x^2}, \tag{14}$$

and the divergence

$$D' = \frac{\partial u'}{\partial x}, \tag{15}$$

where we recall that, in the system defined by (7)–(9), the model variables do not vary in the y-direction.

Another important dimensionless parameter used to characterise the flow regime is the Burger number,

$$B_u = \frac{\sqrt{gH}}{fL}, \tag{16}$$

where H is a characteristic depth scale. The Burger number is a measure of the relative importance of rotation and stratification in the flow. It is the ratio of the Rossby number and the Froude number,

$$F_r = \frac{U}{\sqrt{gH}}. \tag{17}$$

The Froude number is the ratio of the advective velocity to the gravity wave speed, $c_g = \sqrt{gH}$. In most deep atmospheric motions F_r is small, i.e. the advective velocity is much less than the gravity wave speed.

We now derive the vorticity-based and PV-based transforms for the simplified SWE model.

3.1 Vorticity-Based Transform

The vorticity-based control variables are the streamfunction ψ', velocity potential χ' and 'unbalanced pressure' or, in the case of the SWEs, the residual unbalanced height h'_{res}. Here the rotational wind is assumed to be totally balanced. The Helmholtz decomposition is used to separate velocities into rotational and divergent parts. In 1D the Helmholtz decomposition reduces to the equations

$$\zeta' = \frac{\partial v'}{\partial x} = \frac{\partial^2 \psi'}{\partial x^2}, \tag{18}$$

and

$$D' = \frac{\partial u'}{\partial x} = \frac{\partial^2 \chi'}{\partial x^2}. \tag{19}$$

The velocities u' and v' are given by

$$u' = \frac{\partial \chi'}{\partial x}, \tag{20}$$

and

$$v' = \frac{\partial \psi'}{\partial x}. \tag{21}$$

The linearised balance relationship used in the vorticity-based transform, in terms of the increments ψ' and h', is found by differentiating (12) with respect to x and regarding all of v' as 'balanced'. Thus we obtain

$$f\frac{\partial^2 \psi'}{\partial x^2} - g\frac{\partial^2 h'_b}{\partial x^2} = 0, \tag{22}$$

Step 3 **Solve**

$$\frac{\partial^2 \chi'}{\partial x^2} = D' \tag{25}$$

for χ' subject to periodic boundary conditions. The solution is unique up to an additive constant.

Step 4 **Store mean values of u' and v'. These are otherwise lost through differentiation.**

Equations (23) for ψ' and (25) for χ' are solved with periodic boundary conditions. The solutions are unique up to an additive constant provided the right hand side has a zero mean value. In both cases the right hand sides are derivatives of periodic functions and therefore will always have a zero mean value. The solutions are therefore unique up to a constant and we choose this constant such that the mean value $<\psi'>$ of ψ' is zero and the mean value $<\chi'>$ of χ' is also zero, where $<\cdot>$ indicates the mean of the variable.

In solving (23) for ψ'

Step 2

where the reference states $\bar{v}, \bar{h}$ and $\bar{q}$ are either the first guess, or background states, on the first outer loop of the incremental 4D-VAR, or updates to the background on subsequent outer loops.

For the PV-based transform we define the balanced variables v'_b and h'_b such that they satisfy the linear balance equation

$$f v'_b - g \frac{\partial h'_b}{\partial x} = 0 \tag{32}$$

and the linearised PV equation. To derive the linearised PV equation we follow [13] and start by linearising (31) around a varying reference state

$$q(x, t$$

and

$$\frac{\partial v'_u}{\partial x} - \overline{q}h'_u = 0, \tag{36}$$

i.e. the unbalanced variables do not contribute to the PV increment.

Re-writing these equations using the balanced and unbalanced stream-functions ψ'_b and ψ'_u gives the following four equations

$$\begin{aligned} f\frac{\partial^2\psi'_b}{\partial x^2} - g\frac{\partial^2 h'_b}{\partial x^2} &= 0, & (37)\\ \frac{\partial^2\psi'_b}{\partial x^2} - \overline{q}h'_b &= q'\overline{h}, & (38)\\ f\frac{\partial^2\psi'_u}{\partial x^2} - g\frac{\partial^2 h'_u}{\partial x^2} &= {}_a\zeta', & (39)\\ \frac{\partial^2\psi'_u}{\partial x^2} - \overline{q}h'_u &= 0, & (40)\end{aligned}$$

where ${}_a\zeta'$ is defined by (14). These equations, with appropriate boundary conditions specified later in this report, define four variables ψ'_b, ψ'_u, h'_b and h'_u.

We can now derive the PV-based transform in the context of the model (7) to (9) using equations (37) to (40) and the divergence equation (19). We have five variables ψ'_b

with

$$\mathbf{x}' = \begin{pmatrix} u' \\ v' \\ h' \end{pmatrix},$$

and

$$\mathbf{z}' = \begin{pmatrix} \psi_b' \\ h_u' \\ \chi' \end{pmatrix}$$

is given by solving the following sequence of equations:

Step 1 Solve

$$\frac{\partial^2 \psi_b'}{\partial x^2} - \frac{f\bar{q}}{g}\psi_b' = q'\bar{h} \tag{41}$$

for ψ_b' subject to periodic boundary conditions. The right hand side is known from the model variable increment fields. The equation has a unique solution provided $\bar{q} > 0$.

Step 2 Solve

$$f\bar{q}h_u' - g\frac{\partial^2 h_u'}{\partial x^2} = {}_a\zeta' \tag{42}$$

for h_u' subject to periodic boundary conditions. As before the right hand side is known from the model variable increment fields and the equation has a unique solution provided $\bar{q} > 0$.

Step 3 Solve

$$\frac{\partial^2 \chi'}{\partial x^2} = D' \tag{43}$$

for χ' subject to periodic boundary conditions. The solution is unique up to an additive constant.

Step 4 Store mean values of u' and v'. These are otherwise lost through differentiation.

Equation (41) is found by substituting $h_b' = \frac{f}{g}\psi_b'$ from (37), the linear balance equation, into equation (38). Here we have integrated (37) twice with both constants of integration defined to be zero, as was done for the

Met O□ce variables. Equation (42) is found by substituting $\nabla^2\psi'_u$ from equation (40) into equation (39).

Equation (43) is solved with periodic boundary conditions for χ' and has a unique solution up to an additive constant provided the right hand side has a zero mean value. The right hand side is a derivative of a perio

the practical implementation of the U-transform in the incremental 4D-VAR algorithm.

In equation (46) the unbalanced streamfunction ψ'_u is found by solving (44). The right hand side of (44) is known and must have a mean value of zero for the equation to have a solution. In the optimisation algorithm we minimise the cost function in control space and therefore the condition that the mean of $\bar{q}h'_u$ is zero may not be satisfied unless explicitly enforced. It is not straightforward to do this, since $\bar{q}$ is varying in x and is modified on every outer iteration. However, it is possible to adjust the mean of h'_u, $< h'_u >$, on *each inner iteration* so that $< \bar{q}h'_u >$ is zero. This can be achieved since we are always able to subtract a constant from h'_u such that $< \bar{q}h'_u >$ is zero. Note that it is not a simple case of setting $< h'_u > = 0$; $< h'_u >$ will be non-zero and change on each inner iteration. The constant then must be added to h'_b to preserve the degrees of freedom in h'. The mean of the full height increment is therefore split between h'_b and h'_u.

The problem could be avoided by choosing to approximate $\bar{q}$ by a constant. An approximation of this sort was made in [2]. In the simplified SWEs context this would mean that we are simply able to explicitly set $< h'_u > = 0$ and so $\bar{q}h'_u$ will always have a zero mean value. We then store the mean of the full height increment solely in h'_b. This approximation is also desirable from an operational perspective since the transform would be less computationally demanding. In the following section we consider the possible implications of making this approximation in the PV-based transform. We note that approximating $\bar{q}$ to any constant would achieve this type of simplification. We therefore choose to approximate $\bar{q} = f / < \bar{h} >$, where $< \bar{h} >$ is the mean of the linearisation state fluid depth.

COV (h', h') and COV (v', v'). The statistical model is much more complicated for the PV-based variables and, whilst B_V is static, the PV-based implied background error statistics include the linearised PV $\bar{q}$. Thus the PV-based transforms have introduced state-dependence into the implied background error statistics.

4.2 The Correlation of Control Variables

We now test the assumption that the errors in the vorticity and PV-based control variables are uncorrelated. If the control variables are indeed representing the balanced and unbalanced flows, then we should see very little correlation between the balanced and unbalanced variables. However, if the vorticity-based variables are not representing the balanced flow well in the low Burger regime we would expect to see a correlation between ψ' and h'_{res}.

We are also in a position to consider the consequences of using an approximate $\bar{q} = f / < \bar{h} >$ in the PV-based transforms. This can be achieved by looking at the correlation of the approximated PV-based variables.

We start by briefly introducing the two-time-level semi-impli

and

$$\varphi = gh.$$

This form of the equations is chosen as it is a more convenient when applying the SISL scheme [11].

Applying the SISL scheme as in [5] to the equations (50)–(52) gives the following time-discrete equations

$$\frac{\mathbf{u}_a^{n+1} - \mathbf{u}_d^n}{\Delta t} + \alpha_1 \quad \varphi_x + g$$

parameter $f = 0.01s^{-1}$. The orography is given by

$$\tilde{H}(x) = H_c \left(1 - \frac{x^2}{a^2}\right) \quad \text{for} \quad -a \leq x \leq a \tag{56}$$

$$= 0 \quad \text{otherwise} \tag{57}$$

with $a = 40\Delta x$, $H_c = 7.6$m in the high Burger regime and $H_c = 0.019$m in the low Burger regime. For the high Burger experiments the mean depth $< h > \approx 40$m and for the low Burger experiments $< h > \approx 0.1$m.

4.2.2 Correlation Experiment: Method

It is assumed in the data assimilation that the errors in the control variables are uncorrelated. We now investigate the truth of this assumption. We look at correlations of the errors in the vorticity and PV-based control variables where we fix the Burger number to be either high or low and vary the Rossby

and

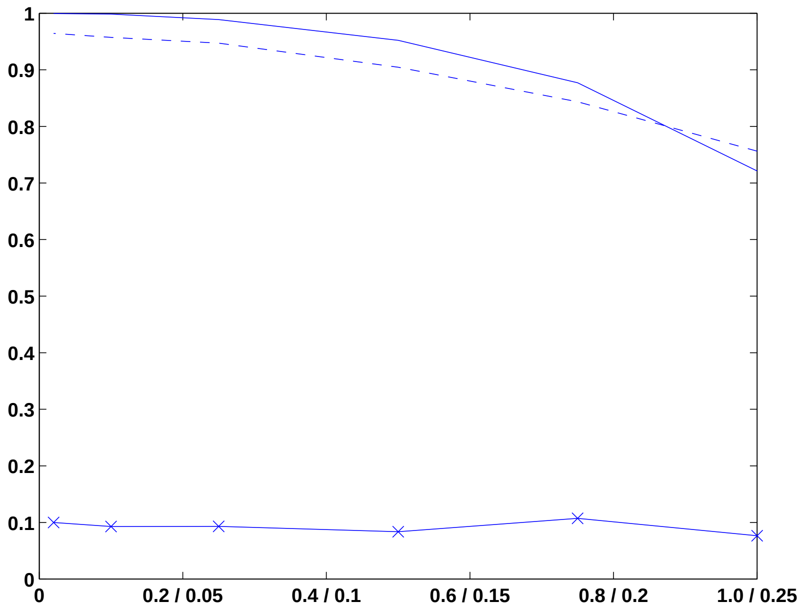
$$< \psi^{\square} > = \frac{\psi_1^{\square} + \ldots + \psi_{N \times M}^{\square}}{N \times M}; \qquad (61)$$

also

$$< \psi^{\square} h^{\square} > = (\psi_1^{\square} h_1^{\square} + \ldots + \psi_{N \times M}^{\square} h^{\square}$$

In the high Burger case the fast gravity waves cover the length of the domain in time $\frac{N\Delta x}{\sqrt{gH}}$s. We choose to remove this signal from the time-difference fields by choosing a time interval of $\frac{N\Delta x}{\sqrt{gH}}$s.

In the low Burger number experiments the dominant gravity wave is actually stationary and tied to the orography, as we discuss in S


1
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0.4
0.3
0.2
0.1
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0.2 / 0.05
0.4 / 0.1
0.6 / 0.15
0.8 / 0.2
1.0 / 0.25

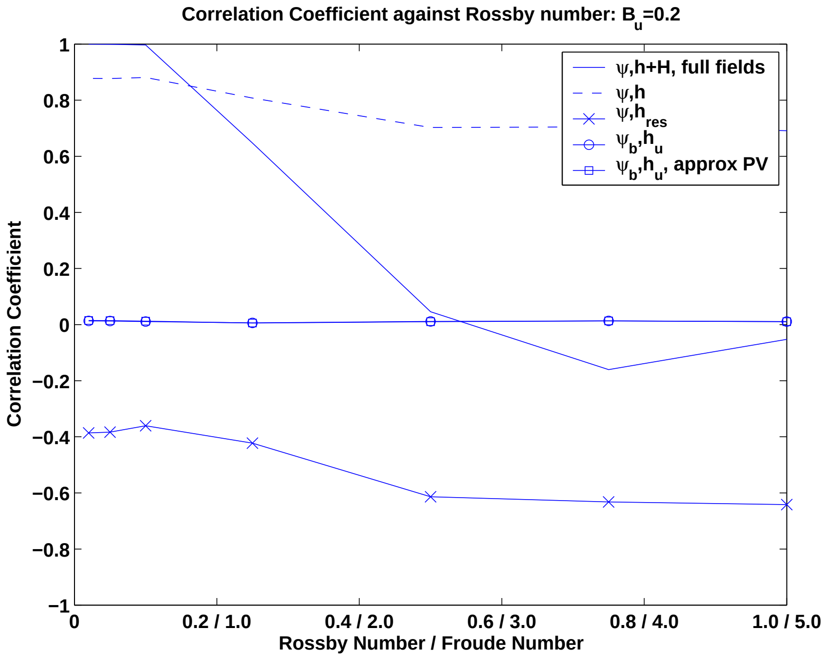

Figure 2: Plot of correlation coe cient against Rossby number for B_u = 0.2. The solid line is the correlation for full model field ψ and h + H, the dashed line for model field time di erences ψ′ and h′. Vorticity-based control variable correlations ψ B_u

5 Summary and Conclusions

Control variable transforms in data assimilation have a dual function. Firstly they are a necessity due to the size of the background error covariance matrix. Secondly, they are used to introduce important physical relationships into the data assimilation. We show how the control variable transform is used in 4D-VAR and that the key assumption is that the errors in the control variables are uncorrelated. This simplifies the data assimilation problem but also implicitly models the background errors as

$$\mathrm{B} = \mathrm{U}\Lambda\mathrm{U}^T.$$

We then derive two sets of control variables for a simplified SWE model, the vorticity-based and the PV-based versions, which attempt to exploit properties of balance. We are then able to derive, in this simple case, the implied background statistics for each transform. This highlights several key di□erences in the two transforms. Most importantly that the implied background statistics for the vorticity-based transforms are static whilst the PV-based transforms are state-dependent as they involve the linearised form of the PV.

We then test the assumption that the errors in the control variables are uncorrelated. We are able to validate our hypothesis that the PV-based variables capture the balanced motion in both high and low Burger regimes, whilst the vorticity-based transforms fail in the low Burger regime. This suggests that the PV-based control variables are a much better choioe. Tch

These results suggest that the PV-based variables are superior to the vorticity-based variables in several vital areas: the PV-based variables imply a state-dependent matrix B and the assumption that the errors in the PV-based variables are uncorrelated is valid in all regimes tested.

The obvious next step is to compare control variables in assimilation experiments. This would involve identical twin 4D-VAR experiments using single and incomplete sets of observations. The success of the experiment should be assessed against how well the balanced flow is represented in the analysis. To do this we can look at the PV in each analysis and compare this to the true PV. This work is currently being carried out as part of a PhD research project and will be published in a subsequent report.

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