Diagnosis and Dynamics of Forecast Error Growth

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ABSTRACT

Consideration is given to the diagnosis and dynamics of synoptic and subsynoptic forecast error from a potential vorticity (PV) perspective. A depiction of the extratropical “forecast minus analysis” PV pattern on a cross-tropopause isentropic surface serves to illustrate characteristic features of the PV-error field, and these features relate both to the instigation, development, and breaking of Rossby waves at the tropopause, and to surface cyclones and anticyclones. An outline is provided of a three-component diagnostic approach for studying PV forecast error. The approach exploits the quintessential PV concepts of quasi conservation, inversion, and attribution, and its essence is illustrated qualitatively by reference to one particular synoptic sequence over the North Atlantic. It also provides a framework for assessing the dynamics of possible mechanisms for generating realized PV-error features. The approach offers a conceptually attractive and diagnostically useful method of analyzing, assessing, and understanding the dynamics of forecast error growth.

1. Introduction

Deterministic numerical weather prediction (NWP) for forecasts of up to seven days has improved remarkably over the last quarter of a century (Thorpe 2004; Shapiro et al. 2010), and it has been paralleled by the complementary development of ensemble procedures to assess the contemporaneous forecast uncertainty (Leutbecher and Palmer 2008). Further improvement of the deterministic component of NWP will in part hinge upon the determination, detailed assessment, and physical understanding of the remaining causes for forecast failure. Likewise refinements of the strategy for ensemble forecasting should reflect extant analysis and model shortcomings as well as taking into account the flow’s intrinsic unpredictability. A range of novel approaches for examining and ameliorating forecast errors have been adopted including adjusting for known model biases (e.g., Danforth et al. 2007) and detecting the influence of errors propagating from the far field (Jung 2011).

In this study an outline is provided of an approach to diagnosing the dynamics of forecast error growth with particular emphasis being placed upon flow features at tropopause elevations. A study of the error dynamics could in principle provide the following: an improved assessment of the performance of an NWP system, a physically meaningful diagnosis of the error field’s character, a tailored aid to pinpointing the cause(s)/source(s) of error growth, and an insightful guide to the performance and design of ensemble strategies.

To examine the nature of the error dynamics and to explore the validity of the foregoing assertions we adopt a potential vorticity (PV) perspective, and examine the structure and evolution of the PV-error field. For examining the dynamics of synoptic-scale flow, the perspective’s value (Hoskins et al. 1985) stems from its compact and coherent theoretical framework, its ability to identify salient flow features, and ultimately its provision of insightful dynamical diagnoses. To this end it utilizes the concepts of PV conservation, inversion, and partition and attribution (Hoskins et al. 1985). Furthermore it can be employed to detect the occurrence, and examine the impact, of nonconservative effects (see e.g., Davis and Emanuel 1991; Davis 1992; Wernli and Davies 1997).

Likewise for examining the dynamics of forecast error growth, the perspective’s value will hinge upon whether it provides a ready framework for identifying the structure and analyzing the dynamics of the key error features, and whether the aforementioned core PV concepts are also insightful for examining the PV-error field and its evolution.
The perspective’s potential for studying forecast error has already been mooted (McIntyre 1988, 1999; Caron et al. 2007; Gold and Nielsen-Gammon 2008), and early pointers of its value include the demonstration that for some events the pattern and structure of the PV distribution at tropopause elevations was key to achieving a successful forecast (Fehlmann and Davies 1997; Fehlmann et al. 2000). Moreover it has been shown (Dirren et al. 2003; Rodwell 2006) that both the PV-error pattern and error metrics based upon that pattern provide insight on the nature of the forecast error and its evolution.

The paper is arranged as follows. In section 2 a synoptic sequence is used to identify, illustrate, and signal the significance of characteristic and salient features of the PV forecast error. In section 3 an outline is given of the rationale for, and the ingredients of, a three component PV-based approach to studying the error. Thereafter, some ingredients of the approach are illustrated with reference to the selected synoptic sequence (section 4), and they are also exploited to qualitatively assess the dynamics of various hypotheses and mechanisms for generating realized PV-error features (section 5). In a final section inferences are drawn regarding the approach’s utility and the attendant implications for NWP.

2. Features of the error fields

a. Characteristic PV-error features

Consideration of one particular synoptic setting will serve to highlight the essence of upper-troposphere PV-error patterns and point to accompanying dynamical issues. To this end Fig. 1, derived from the European Centre for Medium-Range Weather Forecasts (ECMWF) operational fields, depicts the PV distributions on the 320-K isentropic surface for 1200 UTC 16 January 2002. The top panel shows the analyzed PV distribution at this time and the bottom panel shows the contemporaneous “forecast minus analysis” difference field for a 96-h forecast to the verification time. Note that the displayed 320-K surface bisects both the extratropical tropopause break and the collocated jet stream, and that a proxy for the location of these two features is the highlighted 2-PVU isoline [note 1 potential vorticity unit (PVU) = $10^{-6}$ m$^2$ s$^{-1}$ K kg$^{-1}$; and see e.g., Hoskins et al. 1985; Martius et al. 2010].

The “analysis” field (Fig. 1a) shows large-scale Rossby wave undulations of the 2-PVU isoline over the central Atlantic, and signatures of wave breaking (W-B), PV filaments (F), and PV cutoffs (C-F) over the eastern Pacific, eastern Atlantic, and Asia.

The “forecast analysis” field (Fig. 1b) shows coherent and distinctive features that tend to be closely aligned to the mismatch in the location of the 2-PVU contours for the analysis (black contour line) and forecast (red contour line) fields. Hereafter we refer to the difference field as the “error,” but will later comment on the appropriateness of this designation. The error features include the inadequate development of the Rossby wave undulations over the central Atlantic as evidenced by the train of alternating blue and yellow signatures, amplitude and/or phase differences of the stratosphere-to-troposphere
filament in the eastern Pacific and the cutoff in the eastern Atlantic, and a discrepancy in the location and form of the troposphere-to-stratosphere filament and the two cutoffs over Asia. These features are synoptic and subsynoptic in scale and their amplitude is comparable to that of the ambient atmosphere. The accompanying velocity and thermal error signatures of these structures, obtained from coinspection of the analysis and forecast fields, amount to typically $\sim 10 \text{ m s}^{-1}$ and $\sim 3 \text{ K}$. These amplitudes indicate that the features are significant from the standpoint both of dynamics and of forecast failure.

The appearance of these coherent and distinctive features in the PV-error pattern is linked to the atmosphere’s characteristic PV distribution with its large gradient across the tropopause. It follows that this gradient is large on isentropic surfaces that cross the tropopause near the jet stream (Davies and Rossa 1998; Martius et al. 2010), and in regions where these surfaces transect across breaking waves, filaments, and cutoffs. Hence, a misplacement of such features in the forecast will result in large PV errors. In effect these are generic error features also evident on other tropopause-crossing isentropic surfaces. They occur regularly (see e.g., Dirren et al. 2003; Didone 2006) and, furthermore, are also characteristic and distinctive features of the difference between members of a forecast ensemble.

b. Relationship to lower-level error features

To examine the relationship of these error features with error features at a lower level consider the corresponding analysis and error fields at 1200 UTC 16 January 2002 for the 500-hPa height (Fig. 2) and the sea level pressure fields (Fig. 3), respectively.

The midtroposphere analysis field (Fig. 2a) shows a large-amplitude cutoff low over the Kamchatka peninsula and a major ridge over the eastern Pacific, shorter wavelength and weaker in amplitude undulations over the Atlantic, and cutoff features over northeastern Canada and poleward of Siberia. Many of these features are mirrored in the SLP field (Fig. 3a) and include a major low–high pressure pattern in the Pacific, a prototypical low off the New England coast, a deep low over the Irminger Sea between Iceland and Greenland, and a farther low over central Asia. For the present purposes we note that these lower-level fields (Figs. 2a and 3a) display vestiges of the overlying tropopause-level PV features (Fig. 1a).

The 500-hPa geopotential error field (Fig. 2b) indicates misforecasts of the trough–ridge pattern over the Pacific, the wave undulations over the Atlantic, and the aforementioned cutoffs. Likewise at the surface (Fig. 3b) the major cyclone over the Bering Sea is mislocated, the incipient low off the New England coast is both misplaced and significantly underdeveloped, and there are major errors over North America, Greenland, Scandinavia, and central Asia. These are notable errors with the amplitude of some features in excess of 20 hPa, and hence their origin clearly merits consideration.

Again most of these lower-level error features are approximately collocated with, and bear traces of, features evident in the tropopause-level PV-error field. For example, over the Atlantic the analyzed SLP pattern and the accompanying error pattern are aligned with the upper-level Rossby wave and wave-breaking error signatures, respectively. This interlevel correspondence is in harmony with the quintessential PV concept of the

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**FIG. 2.** As in Fig. 1, but now displaying the geopotential height pattern on the 500-hPa surface.
far-field influence of isolated PV anomalies. This in turn suggests that consideration of the PV-error features can shed light on the overall forecasted error fields.

c. A selected synoptic sequence

In subsequent sections we illustrate the rudiments of a PV-based approach to examining the error by focusing attention on the synoptic sequence of events that resulted in the wave-undulation and wave-breaking features over the Atlantic on 16 January (Fig. 1a), and the accompanying error pattern in the 96-h forecast for that time (Fig. 1b).

A cursory overview of the synoptic activity during the preceding 96 h is provided in Figs. 4 and 5, which are derived from the ECMWF’s Re-Analysis Interim (ERA-Interim) dataset. The surface pressure pattern and the 500-hPa geopotential height distribution for 1200 UTC 12, 14, and 15 January (Fig. 4) indicates that this was an active synoptic period over the Atlantic with a succession of developing cyclones (L₁, L₂) evident off the eastern seaboard of North America on 12 and 14 January. The first progressed toward Iceland merging with a preexisting system (L₀) by 14 January, and the second followed the same track. Also a weak, incipient, and diffuse low (L₃) present over the Great Lakes on 15 January underwent rapid cyclogenesis in the subsequent 24 h. It was this latter system that was poorly forecasted on 16 January (see Fig. 1b). In contrast a surface anticyclone developed and prevailed during the period over the Atlantic–European sector.

Aloft on the 500-hPa surface, the surface lows L₁ and L₂ were linked on 12 and 14 January with troughs, T₁ and T₂, respectively, located somewhat upstream, and hence in a configuration favorable for baroclinic development. Over Europe a wave-breaking event led to a significant blocked flow regime by 15 January. Also on 15 January the incipient low L₃ was surmounted by a moderate westerly flow that was itself located on the southern rim of a weak trough (T₃).

A complementary picture of the synoptic sequence is provided by the temporally corresponding charts for the 800-hPa thermal field (Figs. 5a–c) and the PV pattern on the 315-K isentropic surface (Figs. 5d–f). The thermal field over the Atlantic exhibits a wave pattern consistent with the underlying translating surface low pressure systems. Over the Atlantic on the 315-K surface, two PV filaments plunge southward and track eastward during the period, and from a PV perspective their location relative to the lower-level θ fields is suitable for promoting baroclinic growth. Over Europe an omega-shaped PV pattern emerges characteristic of a block (Croci-Maspoli et al. 2007), while above the Great Lakes on 15 January an intense but localized positive PV anomaly is evident and located over the ambient low-level baroclinic zone. Other notable features are the narrow and elongated bands of anomalously low PV (the blue dashed arcs in Figs. 5d–f).

3. Diagnosis: Outline of a framework

a. Evolution equation for PV error

The first component of our diagnostic approach is based upon examining the space–time evolution of the flow on an isentropic surface. In this framework the evolution equation for the PV of hydrostatic, frictionless but diabatic flow takes the following form:

\[
\frac{D}{Dt}(PV) = \Pi + R. \tag{1}
\]
Here the operator \((D/Dt)\) refers to the material (i.e., Lagrangian) rate of change expressed in isentropic coordinates, so that

\[
(D/Dt) = \frac{\partial}{\partial t} [\bar{u} + (\bar{v} \cdot \nabla) + \bar{Q} \frac{\partial \theta}{\partial t}],
\]

(2)

where the \(\theta\) subscript refers to temporal and horizontal derivatives evaluated on an isentropic surface, \(v = (u, v)\) refers to the horizontal vector velocity, and \(Q\)—the diabatic contribution to a fluid parcel’s change of \(\theta\)—serves as a pseudovertical velocity. In effect the Lagrangian derivative, \((D/Dt)\), involves both adiabatic “advection” on an isentropic surface and diabatic “convection” through the surface. Furthermore, note that \(PV = \{(\zeta + f)/(\sigma)\}\) is the hydrostatic form of Ertel’s potential vorticity with \(\zeta\) denoting the vertical component of the relative vorticity on an isentropic surface, and \(\sigma = -g^{-1}(\partial p/\partial \theta)\).

Finally \(II\) and \(R\) represent the diabatic and frictional contribution, respectively, to the change of a parcel’s PV. The diabatic contribution can be formulated compactly as follows (Hoskins et al. 1985):

\[
II = -[(\bar{v} \cdot \nabla + f) \cdot (\nabla Q)]/\sigma, \quad (3a)
\]

or alternatively, splitting it into its vertical and horizontal components, in the following form:

\[
II = +PV(\partial Q/\partial \theta) - \{(kV(\partial \omega/\partial \theta)) \cdot (Q V)\}/\sigma. \quad (3b)
\]

Thus, the equation for the evolution of PV can be written in the following form:

\[
(D/Dt)(PV) = +PV(\partial Q/\partial \theta) - \{(kV(\partial \omega/\partial \theta)) \cdot (Q V)\}/\sigma + R. \quad (4)
\]

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**FIG. 4.** (a),(b),(c) Sea level pressure and (d),(e),(f) geopotential height field on the 500-hPa surface at 1200 UTC (a),(d) 12 Jan 2002; (b),(e) 14 Jan; and (c),(f) 15 Jan. Isobars are displayed at contour intervals of 8 hPa, and the height at intervals of 100 gpm. The symbols \(L_0, L_1, H\) and \(T_0, T_1, R\), etc. are synoptic features referred to in the text.
For adiabatic ($Q = 0$) and frictionless ($R = 0$) flow we have the standard result that the PV of an air parcel is conserved as it is advected on an isentropic surface. In the presence of diabatic effects the equation bears comparison with the traditional equation for the vertical component of the vorticity. The pseudovertical velocity $Q$ serves to (i) transfer a fluid parcel's PV from one $\theta$ surface to another (the pseudoconvection effect noted above), (ii) modify the parcel's PV by altering the separation of the isentropes by “vertical stretching” (the $\partial Q/\partial \theta$ term), and (iii) “tilt” the horizontal vorticity (the $\partial v/\partial \theta$ term) into the vertical.

Order of magnitude considerations suggest that the tilting term is comparatively small for synoptic-scale flow. This is also the case for subsynoptic frontal regions provided the diabatically active region is aligned along the front but not coincident with a strong baroclinic zone.

An equation for the evolution of the PV error can be derived directly from Eq. (4). Consider a realized atmospheric flow evolution represented by the space–time distribution of $(PV, V, Q)$ and a corresponding forecasted evolution represented by $(PV, v, Q)$, such that

$$(PV, v, Q) = (PV, V, Q) + (PV*, v*, Q*).$$  \hspace{1cm} (5)

In effect $(PV*, v*, Q*)$ denotes the error field or more precisely the departure of the forecast from the “true” evolution.

An evolution equation for $PV*$ is obtained by substituting separately the forecast and true fields of Eq. (5) into Eq. (4). The resulting evolution equation can be written in the following form:

$$(D/Dt)_{true}(PV*) = I + II + III + IV + R*,$$  \hspace{1cm} (6)

**Fig. 5.** As in Fig. 4, but the displayed fields are the temperature on the (a)–(c) 800-hPa surface and (d)–(f) the potential vorticity on the 315-K isentropic surface. The isentropes are displayed at contour intervals of 5 K, and the PV at 1-PVU intervals. The symbols C and W refer to local regions of comparatively cold and warm air, respectively; and PV+ and PV− designations refer to local regions of comparatively high and low PV, respectively. The blue dashed arcs in (d)–(f) highlight bands of anomalously low PV.
where \((D/Dt)_{\text{true}}\) denotes the material derivative following the realized flow, so that

\[
(D/Dt)_{\text{true}} = \left[ \frac{\partial}{\partial t} + (\mathbf{V} \cdot \nabla) \right] + Q \frac{\partial}{\partial \theta},
\]

and

\[
I = -(v^* \cdot V_0)(PV),
\]

\[
II = -(Q^* \frac{\partial}{\partial \theta})(PV + PV^*),
\]

\[
III = -\frac{\partial (PV)}{\partial \theta}(PV^*) + (PV^* \frac{\partial}{\partial \theta}) (Q + Q^*),
\]

and \(R^*\) is a net residual error that incorporates effects attributable to nonhydrostatic, tilting, and frictional effects.

Consider these contributions to the Lagrangian rate of change of an air parcel’s PV*. Term I, \([- (v^* \cdot V_0)(PV)]\), is the adiabatic contribution due to the isentropic advection of the true \(PV\) field by the isentropic error flow \(v^*\). This contribution can be large in the vicinity of strong isentropic \(PV\) gradients such as the vicinity of the jet stream and collocated tropopause break, and as noted earlier this is consistent with the large-amplitude PV errors aligned along the 2-PVU contour in Fig. 1b.

Term II, \([- (v^* \cdot V_0)(PV^*)]\), is the nonlinear adiabatic contribution due to the isentropic advection of the PV* field by the corresponding isentropic error flow \(v^*\). The amplitude of the PV* field is large and comparable in value to that of the ambient environment (see Fig. 1), and could conceivably play a significant role provided \(v^*\) is not aligned along the PV* contours. (Note that the sum of terms I and II is equivalent to the isentropic advection of the forecasted PV field by the error flow \(v^*\).)

Term III, \([- (Q^* \frac{\partial}{\partial \theta})(PV + PV^*)]\), is “diabatic convection” by the pseudo-cross-isentropic error flow \(Q^*\). For deep penetrative convection this term would either be a single convective shaft provided the location of the convection is forecasted correctly, or otherwise a double shaft. The vertical structure of tropopause-spanning diabatic heating is likely to render \(Q^*\) large in the midto upper troposphere where \(\partial PV/\partial \theta\) is comparatively small, whereas \(Q^*\) will be smaller nearer the tropopause where \(\partial PV/\partial \theta\) is expected to be large. However, a forecast with both a misplaced convective region and an incorrect altitude for the tropopause itself could render the term large. It follows that the amplitude and sign of this term, although conceivably comparatively small, will depend sensitively upon the forecast model’s physical representation of deep convection and its dynamical representation of tropopause undulations.

Term IV, \([(PV \frac{\partial}{\partial \theta})(Q^*) + (PV^* \frac{\partial}{\partial \theta})(Q + Q^*)]\), is the sum of PV* tendencies due to vertical stretching effects. The dependencies upon \(Q^*\) and PV* again renders the term sensitive to model physics and dynamics.

It follows from the above that estimating the model-sensitive cloud-diabatic contributions (terms III and IV) from the available true and “forecasted” fields poses a formidable challenge, but this is alleviated by a major redeeming factor. On an isentropic surface in the vicinity of the tropopause, the direct cloud-diabatic contribution to the PV* tendency after a misforecast of a deep convective event will be effectively zero, whereas the indirect effect due to earlier diabatic generation of PV* will remain present. Later we indicate an alternative approach to assessing the impact of diabatic effects (see section 3c).

b. Partition and attribution

The traditional adoption of the PV concepts of partition and attribution is meaningful when the flow is characterized by distinctive PV structures. Inversion of such a feature yields the accompanying flow field, and thereby an assessment of the feature’s contribution to the flow development.

The adoption of these concepts to the PV-error field is prompted by the coherency of the error structures and their confinement to predominantly near-tropopause elevations. This invites performing a layer-wise PV inversion of the near-tropopause PV-error distribution to determine its contribution to the error velocity \(v^*\). Likewise, inverting the \(\theta\)-error distribution at a near-surface level would indicate its contribution to the error velocity. The derived results can then be utilized to formally examine the nature of single and interlevel interactions.

A qualitative indication of the interactions can be obtained by inferring the form of the aforementioned velocity contributions, and this is facilitated by noting that LPV, where LPV = ln PV, is related approximately to the corresponding quasigeostrophic PV (Martius et al. 2010).

c. PV and parcel trajectories

Given both the analyzed and forecasted Eulerian space–time distribution of the meteorological variables, backward trajectories from a specified point can be computed for both the true and the forecast flow. Also the accompanying values of \(PV\) and PV along the respective tracks can be calculated from the corresponding Eulerian datasets. In effect this procedure circumvents undertaking the Lagrangian-time integral of Eq. (1) over a time interval \(\tau = [0, T]\).

\[
P V|_T = PV\|_0 + \int_T^0 (II + R) d\tau, \tag{7}
\]

by merely calculating PV\|_T and PV\|_0 directly from the available Eulerian fields.
Hence, backward trajectories provide the Lagrangian time history of the parcels arriving at the specified point for both the true and forecasted flow evolutions. Moreover trajectories calculated backward from domains of large PV error can shed light on the origin of the accompanying PV* error by documenting the different trajectories followed by key true and forecasted air parcels, providing information on the space–time distribution of the (possibly) differing nonconservative contributions experienced by those parcels, and thereby helping pinpoint aspects of the error growth.

d. A diagnostic framework

The previous subsections set out the ingredients for a comparatively simple three-component approach for studying error growth. First the PV perspective serves to direct attention to errors in the neighborhood of the jet stream and the tropopause. As noted earlier, at these elevations and away from the limited regions influenced by a misforecasted diabatic event, the Lagrangian PV* tendency is determined essentially by adiabatic advective processes [terms I and II of Eq. (6)]. Moreover the influence of these two terms upon the Lagrangian tendency can be estimated quantitatively from, or inferred qualitatively by inspecting, charts displaying the error flow v* and the true PV field and the error PV* field.

Second, application of the concepts of partition and attribution enables the prevailing adiabatic contribution to the PV-error tendency near the tropopause to be linked to purely upper-level dynamics and/or interlevel dynamical interactions. Third, computation of backward trajectories and the evaluation of the along-track variations in PV and θ for both the observed and forecast flows from the identified regions of large PV error provide further pointers to the origin and cause of the errors.

e. Comments and caveats

The present approach is avowedly deterministic in character. However, it does not exclude consideration of error growth due to “chaotic” development arising from a small initial error, and, hence, it can also shed light on the dynamics whereby members of a forecast ensemble diverge from one another. In effect the present approach can point to and shed insight on the deterministic pathway resulting from such an initial error. Indeed the relative configuration of the forecasted and realized 2-PVU isolines in Fig. 2 is very reminiscent of the relative configuration that often characterizes different ensemble members. It is in this context that the present approach could also have ramifications for the design of ensemble procedures.

The approach set out here also majors on examining the Lagrangian tendency of the PV error between the forecast and the true evolution, and the Lagrangian history of key air parcels in both the analysis and the forecast fields. Below we comment in turn upon these two aspects.

Equation (6) is formulated in terms of the Lagrangian rate of change of the error following the realized flow. Hence, the interpretative focus is on the dynamics of forecast’s deviation away from the true flow. Alternatively, but more unconventionally, one could consider the Lagrangian rate of change of the error following the forecasted flow, and thereby examine the true evolution’s departure way from the forecasted evolution. In this context note that Eq. (6) can be rearranged to the following form:

\[
\frac{D}{Dt}_{\text{for}}(\text{PV}^*) = -(\mathbf{v}^* \cdot \nabla_\theta)(\text{PV}) - Q^* \frac{\partial}{\partial \theta}(\text{PV}) + IV + R^*,
\]

where \( \frac{D}{Dt}_{\text{for}} \) denotes the material derivative following the forecasted flow, so that

\[
\frac{D}{Dt}_{\text{for}} = \left[ \frac{\partial}{\partial t} + (\mathbf{v} \cdot \nabla_\theta) + Q \frac{\partial}{\partial \theta} \right],
\]

with \( \mathbf{v} \) and \( Q \) now referring to the forecast fields.

Again the formulation of Eq. (6) lays stress upon the Lagrangian of the PV* error tendency rather than an in situ budget calculation. At the elevation of the jet stream a local budget calculation would inevitably be sensitive to the potentially small difference between the inflow and outflow contributions associated with the advection of errors by the flow field itself. Also, as noted earlier, applying the Lagrangian approach to assessing the PV-error tendency at tropopause elevations partially circumvents the need to, and the lack of data for, evaluating the diabatic contributions.

Consideration of the Lagrangian history of air parcels [Eq. (7)] for a prescribed flow evolution can be undertaken in two ways. The direct approach is to evaluate the source terms on the right-hand side of Eq. (4) (see, e.g., Rodwell and Hoskins 1995; Morgenstern 1998). In practice this approach is complex requiring detailed information on, and the evaluation of, the diabatic processes including cloud microphysics and radiative effects. For a realized, as opposed to simulated, flow the available data would generally be inadequate.

The indirect approach is to compute air parcel trajectories using the available Eulerian data and recording the accompanying change in the PV as evidenced by the realized change in the flow variables. In effect this approach merely infers the net effect of the physics along the trajectory.
Herein we need perforce to consider the true flow evolution, and hence we pursue the latter approach. To this end we apply the Lagrangian tracking technique of Wernli and Davies (1997) to the 6-hourly ECMWF analysis and forecast fields. The technique’s accuracy relative to other schemes has been evaluated independently (Stohl et al. 2001), and its utility is well attested and extensively used for a range of tracking purposes including deep convection in the extratropics (e.g., Hegglin et al. 2004; Eckhardt et al. 2004).

In the present context a key dynamical factor is the PV of an air parcel deposited at tropopause elevations following ascent within a deep convective updraft from the lower troposphere. A parcel’s PV will be related to Lagrangian time history of the \( \partial Q / \partial \theta \) [Eq. (4)]. For quasi-vertical shaft of convection there will be compensation as the parcel traverses through regions of oppositely signed \( \partial Q / \partial \theta \) within the cloud-diabatic domain, while within the core of a band of slantwise convection \( \partial Q / \partial \theta \) will tend to be comparatively small throughout the ascent. Thus, despite the complexity of cloud processes, the net PV change might not be large. Nevertheless the mere deposition of low-tropospheric air with low PV at tropopause levels would be dynamically significant because it could constitute a major negative PV anomaly relative to the ambient upper-level air (see, e.g., bands of low PV highlighted in Fig. 5).

4. Diagnosis: Qualitative Illustrations

Here we consider the various ingredients of the diagnostic approach outlined in the previous section in the context of the synoptic sequence introduced in section 2. The focus will be primarily, but not exclusively, on the nature of the error in the 96-h forecast for 1200 UTC 16 January. This choice is consistent with our stipulated objective of illustrating qualitative aspects of the dynamics of PV-error growth. Clearly the examination of a particular forecast for some specific purpose might warrant selecting a different lead time.

a. Adiabatic contributions to the PV-error tendency

The adiabatic contribution to the Lagrangian PV\(^*\) tendency is given by term I, \(- (v^* \cdot V_o) (PV)\), and term II, \(- (v^* \cdot V_o) (PV^*)\), of Eq. (6). Qualitative inferences of term I’s structure and amplitude over the Atlantic at 1200 UTC 16 January can be gleaned from Fig. 6a. It shows the true \( PV \) field and the \( v^* \) field on the 320-K isentropic surface at the stipulated time. Positive (negative) tendencies of PV\(^*\) prevail where \( v^* \) is directed down (up) the gradient of the \( PV \) field. It follows that there are significant negative PV\(^*\) tendencies within domain \( A \), and contrariwise significant positive tendencies within domain \( B \). Both these contributions are significant, \(-5 \text{ PVU day}^{-1}\), and connote a westward shift of the major positive error feature in the mid-Atlantic (the feature labeled C in Fig. 6b) in opposition to the eastward advection of this error feature by the prevailing large-scale flow. This is consistent with a Rossby wave–like propagation of the PV\(^*\) error on the gradient of the ambient \( PV \) field. Also at the crest of the 2-PVU isoline immediately west of domain \( A \) and at the trough west of \( B \), the PV\(^*\) tendencies equate respectively to a modest decay and growth \((<1 \text{ PVU day}^{-1})\) of the in situ PV errors.

Likewise qualitative inferences on the structure and amplitude of term II can be drawn from Fig. 6b, which displays the corresponding PV\(^*\) error field and again the \( v^* \) error field. Now a positive (negative) tendency of PV\(^*\) prevails where \( v^* \) is directed down (up) the gradient of the PV\(^*\) field. This contribution has a rich structure as indicated by the open “+” and “–” symbols for the tendency. This pattern is consistent with a reduction in amplitude \((\sim 1 \text{ PVU day}^{-1})\) within the core of the positive error feature C, and an amplitude increase \((\sim 5 \text{ PVU day}^{-1})\) on its southwesternmost tip. Together these tendencies connote a southwestward shift of feature C. Likewise at the southern tip of the negative error feature located upstream of C there is a strong negative tendency \((\sim 5 \text{ PVU day}^{-1})\) that is consistent with in situ error growth. Overall the error tendency pattern indicates that the Rossby-like wave undulation of the PV\(^*\) error field is undergoing a further nonlinear distortion that is consistent with the subsequent occurrence of wave breaking and streamer formation at the trough in the 2-PVU isoline in the western Atlantic. Hence, the forecast, having failed to adequately capture the realized wave-undulations (Fig. 1b), continues to underdevelop the further distortion of the undulations.

The above discussion related solely to the flow on the 320-K isentropic surface. Its representivity can be gleaned from inspection of Fig. 7, which shows the longitude–height cross section of the PV error between 80° and 40°W along 42°N latitude. (The cross-section’s location coincides with the purple line in Fig. 6b.) The analyzed tropopause height (i.e., 2-PVU isoline) descends to the 500-hPa level at 64°W, whereas in the 96-h forecast the descent is only to 400 hPa and occurs at 49°W. The sharp rise in tropopause height to the east of these minima corresponds to the true and forecasted tropopause-break and jet stream location. In harmony with this difference there are deep and vertically coherent positive and negative PV-error features located to the east and west of the true break resulting directly from the horizontal misplacement and inadequate downward intrusion of the tropopause in the forecast.
field. Forecast errors of this form are commonplace although usually smaller in amplitude.

For the present purpose we note that the 320-K surface samples the core of the major error features, and, hence, gives added weight to the earlier inference that the forecast continues to misrepresent the realized flow development.

b. Interlevel interaction

Here we exploit the partition and attribution concepts to examine qualitatively the relative contribution of the upper-level PV and the lower-level $\theta$ field to the PV* error tendency on the 320-K surface. To this end we show in Fig. 8 the pattern of the PV and $v^*$ error fields on the 320-K isentropic surface (top panel), and the $\theta$ and $v^*$ error fields on the 800-hPa surface (bottom panel).

Quasigeostrophic (QG) theory indicates that a compact ellipsoidal PV feature, (cf. the major positive error region depicted in Figs. 7 and 8a) is accompanied by an azimuthal geostrophic velocity ($v^*_{\text{PV}}$) in the far field of the following form:

$$v^*_{\text{PV}} \sim \frac{1}{3} \left( \frac{\Delta q}{\theta^2 + (N f_0)^2 (z - d)^2} \right)^{1/2} \frac{r}{\rho},$$  \hspace{1cm} (9)

where $\Delta q$ is the feature’s mean quasigeostrophic potential vorticity, $a$ and $d$ are the half-width of the feature.
and its height above the surface, and \( r \) denotes radial distance. Likewise QG theory shows that a local symmetric surface \( \theta \) anomaly (cf. the negative error region depicted in the center of Fig. 8b) is accompanied (cf. Schär and Davies 1988; Davies and Schär 1991) by an azimuthal geostrophic velocity (\( v^* \)) in the far field of the following form:

\[
v^* \sim \frac{g}{N} \Delta \theta \left( \frac{1}{N} \right) \left( \frac{b}{r^2} + \left( \frac{N}{f_0} \right)^2 \frac{z^2}{2} \right)^{1/2} \left( \frac{r}{b} \right),
\]

where \( \Delta \theta \) denote the mean background potential temperature and the anomaly’s amplitude, respectively; \( N \) is the Brunt–Väisälä frequency; and \( (b, r) \) denote the half-width and radial distance.

For the extant PV and \( \theta \) error features of Fig. 8, the foregoing equations [Eqs. (9) and (10)] indicate that \( v^*_{\text{PV}} \sim v^* \sim 15 \text{ m s}^{-1} \) at their respective levels, and their respective north–south velocity signatures are indicated schematically by the heavy black arrows (top panel) and the open arrows (bottom panel) in the figure. However, the above formulas [Eqs. (9) and (10)] also indicate that the \( v^*_{\text{PV}} \) signature at the 800-hPa level and the \( v^* \) signature on the 320-K surface are smaller by a factor of \( \sim 0.8 \).

Now consider the contribution of the lower-level thermal error pattern to the velocity on the surmounting isentropic surface. The phasing of its \( v^* \) velocity field relative to the wave pattern of the PV error aloft is aligned so as to increase the latter’s amplitude. However, the aforementioned reduction in amplitude of \( v^* \) indicates that its contribution to the error tendency is comparatively small compared with extant value (see section 3e). This in turn points to the dominance of nonlinear upper-level effects at this stage of error development.

c. Lagrangian trajectories

Ensembles of 96-h backward air parcel trajectories are computed for the true and the simulated flow from two specified three-dimensional regions. The regions compose the core of the major positive and negative PV-error structures present along the jet over the Atlantic at 1200 UTC 16 January. The fields for the computation are the 6-hourly ECMWF analyses and contemporaneous 96-h forecast fields.

The resulting trajectories are depicted in Fig. 9. It shows the ensemble of trajectories derived from the positive and negative error regions using the analysis fields (Figs. 9a,b) and forecast fields (Figs. 9c,d). The insets in the bottom panel display the initial portion of the tracks superimposed upon a depiction of the
analyzed PV field on the 330-K surface for the start time of the backward trajectories.

For the trajectories from the negative PV-error feature (Figs. 9b,d) the two ensembles are somewhat similar and originate predominantly from, and remain on, the poleward side of the jet at tropopause levels. Irrespective of their origin in the stratosphere (light blue colored tracks) or upper troposphere (yellow colored tracks), they retain PV values characteristic of their origin.

For the positive PV-error feature (Figs. 9a,c) the two ensembles show a marked difference in origin, track, and physics. For the realized flow the tracks indicate that a significant fraction of the air originated at low levels over and to the west of the Caribbean, remained at comparatively low levels as the air advected toward a major surface depression (not shown), participated in deep moist diabatic ascent ahead of and along a surface front some 24–30 h prior to the verification time, and ascended rapidly to near-tropopause levels. For the forecast flow the tracks indicate that the air originated for the most part in the lower stratosphere, and advected isentropically into the region of the pronounced PV error. This absence of tropospheric-spanning trajectories is in part linked to the misforecast of a trough over the United States on 15 January.

Thus, these highly differentiated ensembles of trajectories suggest that the upper-level PV* pattern at the verification time was impacted significantly by both the misforecast of an earlier dynamical feature and subsequent diabatic effects.

5. Dynamics of PV-error growth

It has been shown that the PV framework can shed light on the dynamics of the error growth. In particular for the selected synoptic sequence, the PV-error pattern on the 320-K surface (Fig. 1b) is indicative of an inadequate representation in the forecast of the following:
rapid cyclogenesis off the eastern seaboard of North America, major synoptic-scale wave undulations over the mid-Atlantic, and Rossby wave breaking and block formation over Europe. Moreover, consideration of the PV*-error tendency and air parcel trajectories links the inadequate development of the wave undulations to quasi-linear and nonlinear adiabatic effects, modest interlevel interaction, and the failure to capture a significant cloud-diabatic event.

Here we consider further the dynamics of the error growth by first examining the error in a sequence of forecasts of differing duration to the verification time of 1200 UTC 16 January, and then assessing the efficacy of possible mechanisms for PV-error growth.

a. A sequence of forecasts

Figure 10 shows the time traces of RMS error of four forecasts of different duration all to 1200 UTC 16 January. The verification area is the Euro–Atlantic sector, and the forecasts are of 96-, 72-, 48-, and 24-h duration.

In Fig. 10a the selected error measure is the mean PV error in the 200–400-hPa layer and this provides an indication of the net upper-level PV error (cf. Fig. 7). The four time traces are similar in form exhibiting an initial significant and quasi-linear increase. For example the PV error in the 96-h duration forecast amplifies by 50% from 24 to 48 h and again from 48 to 72 h. The corresponding traces for the PV error averaged over 200-hPa layers in the middle and lower troposphere (not shown) exhibit a similar form, but their RMS amplitude is less by a factor of 3. This behavior for a single case mirrors that already recorded for PV-related metrics for seasonally averaged RMS and anomaly correlation measures (Dirren et al. 2003; Rodwell 2006).

It is noteworthy that the typical time trace for RMS wind and temperature measures over large domains tend to exhibit an s-shaped profile with an initial exponential growth transiting to a linear phase as the error attains large finite-amplitude values, and then eventual error saturation. A plausible and tentative, but uncomfortable, inference would be that the initial PV error in the analysis is significant.

The corresponding traces for the SLP error (Fig. 10b) bear comparison with those for the PV error. A notable feature is a very large increase of the SLP error during the last 24 h of the 96-h forecast. It is linked to both the misplacement of the rapid cyclogenesis off the eastern seaboard of the United States and the structure and amplitude of the block located west of Spain. There are related error signatures evident at 500 hPa and in the upper-level PV pattern.

Further consideration of the error growth could include examination of the space–time evolution of the error patterns of the individual forecasts and a comparison of
their contemporaneous error structures. For individual forecasts we simply record that the spatial form of the PV-error pattern on the 320-K isentropic surface for the 96-h forecast (not shown) is relatively well established after only 24–30 h, and amplifies quasi linearly thereafter. This would be consistent with a misspecification of the initial state that would serve to trigger effectively or project significantly upon an intrinsic flow instability.

For the comparison of contemporaneous forecasts, consider the PV-error pattern at 1200 UTC 16 January of the four forecasts of differing duration (Fig. 11). The three shorter-duration forecasts show a similar error pattern at the base of the trough over the western Atlantic and at the crest of the wave-breaking ridge in the northeast Atlantic albeit with different amplitude. In the 96-h forecast these features are more intense and a pronounced positive PV-error feature has emerged that is located east of the trough in the western Atlantic.

The replication of similar features, despite the difference in the initial states, is indicative of a systematic failure in capturing the wave development. In general it would point to either systematic deficiencies in the model physics or a consistent misspecification of the initial state that projects onto an intrinsic feature or a sustained instability of the prevailing flow. In either case the error source would need to impact rapidly upon the PV pattern at tropopause elevations. For the physical deficiency possible candidates include the misrepresentation of deep convection and/or in situ radiative effects. For the misspecification in the initial analysis possible candidates include errors in the specification of the location and/or structure of the jet stream or the consistent misrepresentation of a sustained feature that impacts upon the jet stream and its undulations.

The appearance in the 96-h forecast of an additional and major positive PV* feature over the western Atlantic is consistent with this forecast’s aforementioned failure to capture the debouched low-PV anomaly associated with diabatic effects (Fig. 9).

b. Mechanisms of error growth

The structure of the PV-error features in the case study and the replication of same error features in forecasts of different duration prompt questions regarding the dynamics and efficacy of various mechanisms for the growth of PV error. A schematic collage of various possible mechanisms is shown in Fig. 12, and we comment in turn upon their possible contributions to the selected synoptic sequence.

1) LARGE-SCALE DEFORMATION

A large-scale deformation field translating eastward over the Atlantic and with its dilatation axis aligned approximately north–south perpendicular to the jet (Fig. 12a) would enable a preexisting wave to grow in amplitude while concomitantly experiencing a reduction in its wavelength. A horizontally aligned deformation field of strength $D$ acting for a time $T$ would increase the wave amplitude and decrease the wavelength by $\exp(\pm D T)$. For characteristic deformation values of $D \sim 10^{-5} \text{s}^{-1}$ prevailing for $T \sim 2$ days, this equates to changes by factors of $a \sim 5.6$ increase in the amplitude (from say, 100 km to more than a 500 km) and a decrease of $a \sim 0.18$ in the wavelength (from say, 4000 km to around 3200 km), respectively.

If the mechanism were to have prevailed during the event it would require the deformation to have been present in the realized flow but inadequately represented.
in the corresponding initial analysis. Furthermore, in light of Fig. 11, a similar analysis error would need to have been present at subsequent times. However a major and sustained misspecification of the planetary-scale deformation field is unlikely.

Notwithstanding there are more plausible sources of synoptic-scale deformation error. First an elongated along-jet error associated with the misrepresentation of the shear on the jet stream’s flank would constitute a deformation field rotated by 45° relative to the jet, but its effect would not induce the structure of the observed error (cf. Davies et al. 1991). Second an emerging block, composed of localized north–south-aligned PV anomalies (Altendoff et al. 2008), would possess a deformation component in the far field. Such a block appeared over western Europe during the synoptic sequence (Fig. 5d). An underestimate of its strength in the initial analysis would result in an underestimate of the deformation field’s strength, and the impact would be consistent with the observed wave undulations upstream on the jet. Likewise, underestimate of the block’s strength in the initial analyses of subsequent forecasts would connote underestimates of the undulations in the forecasts of shorter duration.

2) BAROCLINIC DEVELOPMENT

From the PV perspective, baroclinic development can be viewed as the codevelopment of tropopause-level PV features with lower-tropospheric PV and surface potential temperature features. Growth ensues when the spatial alignment of the upper- and lower-level features are such that their far-field effects serve to increase the amplitude of the extant features (Fig. 12b). The true flow exhibits the characteristics of a significant baroclinic development over the Atlantic (Figs. 4 and 5) in the 12–16 January time period; hence, the documented PV-error pattern could be viewed as indicative of an inadequate baroclinic development in the forecast.

Our earlier considerations indicate that on 16 January the vertical alignment of the upper-level PV error and the lower-level \( \theta \) error (Fig. 8) remains conducive to continued error growth associated with the lack of baroclinic development. However, the PV-error aloft has by this time achieved nonlinear amplitude (Fig. 6) and provides the dominant contributor to the PV-error tendency.

3) A LOWER-STRATOSPHERE PV ANOMALY

An isolated PV anomaly juxtaposed to the jet stream would perturb the jet and induce a wave train on the jet’s band of enhanced lateral PV gradient. The amplitude, wavelength, and phase speed of the resulting wave train depend critically upon the strength and scale of the anomaly, and its location and velocity relative to the jet (Schweirz et al. 2004). In particular, if the anomaly is suitably located relative to the jet so that its eastward translation with the flow matches the Doppler-shifted phase speed of the induced wave on the jet, then a resonance effect will prevail and a wave train will be generated downstream of the anomaly (Fig. 12c). In effect...
such an anomaly could instigate a wave train over the Atlantic.

This mechanism could yield PV-error growth in the realized event provided such an anomaly was present at tropopause-level, retained its identity over several days, possessed an amplitude sufficient to spawn the observed pattern, and crucially was repeatedly missed in successive analyses. Anomalies of the desired scale, amplitude, and duration do exist. Indeed, the lowermost stratosphere poleward of the extratropical jet is often characterized by the presence of numerous isolated positive PV anomalies (Kew et al. 2010). Accurately capturing
the amplitude and structure of such an anomaly over the Atlantic is not straightforward, and the anomaly’s repeated omission from or underestimation in successive initial analyses could result from an over-reliance upon the first guess field in the data-assimilation cycle.

In a similar context we note that if the rapid cyclogenesis off the eastern U.S. seaboard on 16 January was a classic example of the passage aloft of a short mobile trough (i.e., a compact PV anomaly) over a surface frontal zone, then its misforecast would be consistent with the underestimation of the amplitude of the PV anomaly aloft over the Great Lakes the previous day (see Fig. 5f).

4) PV REALIGNMENT AND UNSHIELDING

The determination of the initial flow states for an ensemble forecasting procedure should blend information on the likely structure of the analysis error and on the growth of perturbations of that analyzed state. The present study’s focus on PV-error growth has a bearing upon the interpretation of a perturbation’s growth.

A frequent signature of the most unstable perturbations is that of a richly structured, upstream-slanting, and comparatively narrow band of PV (Fig. 10d) located in the mid- to lower troposphere beneath a prevailing jet stream (Badger and Hoskins 2001; Montani and Thorpe 2002). The selection of such perturbations is predicated upon requiring the perturbation energy to grow rapidly (i.e., in effect maximizing growth of an energy-based metric). Growth ensues as the ambient shear realigns the PV band into a vertical alignment and thereby unshields the initially countering velocity signals of the band (see, e.g., Farrell 1982; Davies and Bishop 1994; Badger and Hoskins 2001; Morgan and Chen 2002).

From the present study’s standpoint three caveats arise regarding such perturbations. First they do not necessarily exhibit significant growth when assessed in terms of a PV-based metric (Kim and Morgan 2002). This raises an issue regarding the physical basis for the choice of an energy-based error metric and/or the appropriateness of the approach pursued in the present study.

Second, although the perturbations are assigned weak velocity and thermal signals, nevertheless their PV amplitude can be significant, and this poses a query regarding their physical realizability. In effect either the analyzed initial state or the ensemble member’s initial state must possess large-amplitude, localized, and highly structured PV features in the midtroposphere. Such features might not prevail on a daily basis. Alternatively it might be argued that the actual PV error will project significantly onto the most-favored pattern for energy growth, but again the regular occurrence of such a circumstance is contestable.

Third the time scale for realignment of the PV band to the vertical by the ambient shear and its subsequent acquisition of a downstream tilt clearly depends upon the strength of the jet and the initial tilt of the band, and moreover it is only transiently during the band’s quasi-vertical alignment that it would exert significant influence upon and serve to trigger a wave undulations on the jet of the observed form (see, e.g., Davies and Bishop 1994; Badger and Hoskins 2001; Morgan and Chen 2002). To be effective the realignment would need to take ~1.5–2 days, yet the observed wavelike structure of the PV error in successive forecasts emerges on a time scale (~24 h).

5) DEEP CONVECTION

Inspection of ECMWF forecasts charts on upper-level isentropic surfaces reveals the frequent emergence of an elongated band of anomalously low PV beneath the tropopause on the equatorward side of the jet. Such bands are highlighted in Fig. 5 and are evident in the insets to Fig. 9. It was noted earlier (section 3e) that deep moist convection can debouch such low PV air from the confined shaft of deep cloud convection into the free atmosphere near the tropopause.

An elongated band of low PV aligned along the equatorward side of the jet stream (Fig. 12e) would act to deflect the jet equatorward on the band’s forward flank. A strong deflection could serve to promote wave breaking, generate a streamer of high PV air extending equatorward on isentropic surfaces, and eventually lead to the formation of a cutoff (cf. Massacand et al. 2001).

Such a sequence of events is evident in Figs. 4 and 5. Moreover diagnosis of cloud-diabatic effects by computing parcel trajectories (section 4c) showed that a significant feature of the PV error resulted from the noncapture of a debouching event in the forecast simulation with a concomitant difference in origin of the air residing in the region of large upper-level PV error.

6. Conclusions

An outline has been provided of a PV-based approach to examining forecast error. It entails examining the Lagrangian tendency of the PV error between the forecast and the true evolution, and evaluating the Lagrangian history of key identified air parcels in both the analysis and the forecast fields. In principle it allows a formal quantitative evaluation to be undertaken. Application to a particular event would be challenging and data demanding because it would require detailed
space–time information both of a realized flow evolution and of a contemporaneous forecast simulation.

However it has also been shown that a qualitative application of the approach to a given synoptic sequence can be illuminating. It provides a physically meaningful and dynamically insightful diagnosis that points to the role of distinctive features of the PV-error pattern, and thereby sheds light on the error field’s origin, character, and evolution.

Concomitantly it singles out particular components of operational analysis-cum-forecasting system that would benefit from further examination and/or improvement. For example it suggests that a PV-based metric of forecast error would be a more sensitive and dynamical meaningful measure of assessing forecast performance. However this suggestion is offset by the study’s hint that the data assimilation cycle might not adequately capture the details of key PV flow features at tropopause elevations in the initial analysis. Again the prevalence of debouched low PV air at tropopause elevations and the significant potential impact of such anomalies upon flow development suggest that an overarching test of cloud representation in NWP models would be the emergence of the correct PV distribution aloft.

In summary the approach offers a conceptually attractive method for analyzing and identifying key features of the error pattern, and for assessing and understanding the dynamics of forecast error growth.

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