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Comments on: "Notes on the appropriateness of 'bred modes' for generating initial perturbations"

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ABSTRACT

We are gratified by Errico and Langland's (EL, 1999) interest in the use of bred vectors (BVs) in ensemble forecasting. Since they offer detailed comments on only 2 of our papers related to breeding, we would like to bring attention to a number of other related papers that are not referenced by EL. In addition to Toth and Kalnay 1997 (TK97), which discussed in detail properties of breeding and its operational implementation at NCEP, these papers cover mathematically-oriented studies (Smith, 1997; Smith and Gilmour, 1998), experiments with low- or intermediate-dimensional models (Houtekamer and Derome, 1994; Swanson et al., 1998; Noone and Simmonds, 1998), and the use and verification of ensemble forecasts with operational numerical weather prediction models (Rennick, 1995; Barker, 1998; Atger, 1999; Zhu et al., 1996; Toth et al., 1996, 1997, 1998). With respect to EL's comments, we agree with many of their points in which they restate important and basic information available from different sources. We read with interest about EL's ideas and experiments regarding the geostrophic balance (or lack of it) of the total energy based (TE) singular vectors (SVs). We are grateful to the authors for helping us find 2 minor inconsistencies in the paper by Szunyogh et al. (SKT, 1997). First, the cross section latitude in Fig. 1b of SKT (45 S) was accidentally omitted from the legend. And second, on page 206, SKT used the wrong phrase "sign" for distinguishing among the different phases of the leading LLV. At most other places, however, we believe that EL's criticisms are unjustified for 3 reasons. First, at several places *EL erroneously attribute statements to us that we have not made* in any of our papers. Second, EL make statements, or form conclusions that, based on independent research, are incorrect or very questionable. Finally, at other places, EL make statements that are confusing. We believe that most of the misdirected, incorrect or confusing statements could have been avoided either by reading some of the published references, especially the TK97 paper mentioned above, or by informal discussions. For the sake of brevity, we address only the most relevant issues below, grouped by topic areas.

1. Lyapunov vectors

EL state in Section 2 of their comments that "The definition ... of LLVs presented in SKT and their references (is) not clear in many respects", but they fail to point out anything unclear, inconsistent or contradictory in the definitions used by SKT and others. SKT adopted the well-established definitions of the Lyapunov vectors introduced earlier into the meteorological literature by Lorenz (1984, 1996), Buizza and Palmer (1995), Trevisan and Legnani (1995), and Vannitsem and Nicolis (1997). Following Trevisan and Legnani (1995) (who defined only the first LLV), SKT also used the word "local" to emphasize the LVs' dependence on phase space location. In later studies, Legras and Vautard (1996) called the same vectors

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"backward Lyapunov vectors", while Smith and Gilmour (1998) called them "global" Lyapunov vectors (to emphasize that their definition is given in the limit of infinite time).

In Section 2, EL state that orthogonalization is needed to define a set of LLVs, suggesting that the spectrum of LLVs is norm dependent. While orthogonalization, and hence the use of a norm is essential for estimating the spectrum of LLVs (apart from the leading LLV) as defined in SKT, the subspace of any number of the leading LLVs is *norm independent* (as pointed out also by EL at another place). It is important to note that for a broad class of chaotic systems a complete norm-independent set of non-orthogonal and generally unique LLVs can also be defined (Trevisan and Pancotti, 1998).

EL suggest in Section 2, and assert in Section 7, that SKT "misstate" certain properties of the LLVs: "When orthogonalization of a set of vectors is required to achieve independence, a particular norm must be selected. Furthermore, instantaneous growth rates are necessarily norm dependent." We never said either in SKT or in any other paper that the *full spectrum* of LLVs, as defined in SKT, or instantaneous growth rates associated with any of the LLVs are norm independent. Instead, SKT (p. 201, right col.) states, in agreement with EL, that: "Unlike optimal vectors (i.e., SVs), the leading Lyapunov vector (but not a full spectrum of vectors) is independent of the choice of norms or time intervals, indicating that it is more general in nature."

In Section 2, EL suggest that we over-generalized the role of LLVs. They say that SKT "claimed that the LLV describes the perturbation behavior in the nonlinear model." We have never indicated that nonlinear perturbations would necessarily evolve like LLVs. See, for example, the last sentence of SKT's abstract: "... the leading LLV is the vector toward which all random perturbations, including the optimal vectors (i.e., SVs), are attracted, which gives the LLV a unique role in *linear* (emphasis added) perturbation development." We would also like to draw EL's attention to another paper in which we specifically point out how misleading the use of strictly linear concepts and methods can be in a nonlinear environment (TK97, p. 3302, middle part of left column). Lorenz (1996), and Legras and Vautard (1996) also discuss similar issues.

2. Bred vectors

In Section 3, EL state that the "method of generating LLVs ... is critically different from the BGV breeding method ... for reasons to be made clear in the remainder of this paper." Though the two methods are similar, we never said they are identical (see discussion offered by SKT on p. 208; further details can be found in TK97). As Toth and Kalnay (1993, TK93) suggested, nonlinearity is the critical difference between the breeding method and the generation of LLVs using a linear tangent model. Fast growing but energetically irrelevant modes such as individual convective instabilities become nonlinearly saturated in the BVs when the amplitude is chosen to be in the range of analysis uncertainty, but they can dominate the LLVs or other linear estimates of instability, such as SVs. This phenomena were later studied by Lorenz (1996) and Boffetta et al. (1998) who performed experiments with models that coupled two systems with motions of different time scales. They conclude that the predictability properties of complex flows associated with finite size initial uncertainty cannot be described by the traditional Lyapunov exponents (LE). As pointed out by TK97, the breeding method offers an extension or generalization of the linear Lyapunov characteristics concept into the nonlinear perturbation domain. A formal definition of "Finite Size Lyapunov Exponent" (FSLE) was given by Aurell et al. (1997).

In Section 3, EL write: "What makes the breeding described here (with a very small perturbation) most unlike BGV at NCEP, is their application of what they call a 'mask' in place of the rescaling of all the fields by a single scalar." This sentence is very confusing. The confusion is due to a lack of distinction between theoretical and practical issues. Note that by "breeding", without specifiers, we always mean the procedure described by EL, with a single rescaling applied to all variables. This is also the definition used by SKT and by many other studies. This procedure was in fact used operationally at NCEP (then NMC) prior to May 1994 for generating initial ensemble perturbations (see TK93). Instead of using infinitesimal perturbations, however, the hemispherically averaged perturbation amplitude was finite (about the size of the estimated analysis uncertainty). This constitutes both the link (use of the same algorithm) and the difference (use of finite perturbation amplitude) between the breeding method (TK93) and the algorithm for generation of LLVs described in the literature (Shimada and Nagashima, 1979; Benettin et al., 1980). Additional details about this relationship can be found in Legras and Vautard (1996). For practical applications such as ensemble forecasting, however, one needs to modify the BVs to reflect the fact that analysis uncertainty is smaller near data rich regions. To attain this, a variant of breeding, with regional rescaling, was developed strictly for practical applications in operational ensemble forecasting (TK97). The regionally rescaled bred vectors are, by design, different from LLVs (or BVs without regional rescaling), but regional rescaling impacts mainly the continental scales, introducing no major changes in the smaller scale and vertical structure of the perturbations.

In Section 3, EL say: "The degree to which bred modes begun from different randomly perturbed initial conditions still appear dissimilar after a forecast period indicates a lack of convergence to the leading LLV." As discussed in TK97, one *should not expect* a full global convergence of bred modes. There are several reasons for this. First, the distribution of growth rates associated with the fastest growing nonlinear perturbations for a given amplitude may be flat. In a complex system like the atmosphere, instabilities that are only loosely coupled or independent of each other may coexist in time at geographically distant locations, giving rise to different superpositions of these localized perturbations, and leading to globally similar growth rates. In addition, the continuous stochastic forcing by smaller scale processes such as convection, and nonlinear interactions may also prohibit full convergence. Therefore we can only expect a loose convergence in a global geographical sense*, but convergence can be much stronger regionally (Fig. 4 and related discussion in TK97). As indicated by TK97, the lack of global convergence of bred perturbations is an advantage of breeding for ensemble applications, where one needs to capture a combination of fast developing structures (Molteni et al,1996).

* As SKT noted, the question of whether full convergence of perturbations to the leading LLV is to be expected even in a linear framework for complex systems like the atmosphere is not settled yet.

3. Analysis errors and SVs, LVs and BVs

In Section 4, EL state that "SVs of short enough time period can tell us something about possible analysis errors ..." Then they add that this can happen only if the analysis errors are known at a previous time. We agree with EL that the SVs would be the right tool to evaluate how analysis errors would evolve in time *if all their flow-dependent statistical properties were known*, and their time evolution was strictly linear (Ehrendorfer and Tribbia, 1997). However, we find it misleading to suggest that the SVs have information about the analysis errors. It is the other way around: when computing SVs for certain applications, it should be done with a norm that properly accounts for the properties of analysis errors and not with an arbitrary norm (Barkmeijer, 1998).

In Section 4, EL state that "LLVs ... should not be expected to describe analysis errors produced by an assimilation system, even approximately." In Section 7, EL write: "Model LLVs do not describe analysis errors because such errors are constrained by observations, unlike model LLVs." In the same section, EL state that "No credible theoretical reason why BGVs should resemble analysis errors has been offered." These statements contradict the theoretical and experimental results of several important studies on the nature of analysis errors, using systems of different complexity, starting from 3-variable systems through complex observed physical systems (Pires et al., 1996; Swanson et al., 1998; Smith and Gilmour, 1998): As shown in the first two of these papers, an ideal analysis system based on noisy observations would have errors *mainly along the leading LLVs* or bred vectors: "As suggested by the work of Pires et al. (1996), our results show that when long (4DVAR) assimilation periods are used, assimilation errors are mostly concentrated on the unstable manifold of the model, or alternatively, along the leading LVs." (Swanson et al., 1998). In a more realistic setup, Smith and Gilmour (1998, Fig. 10) studied an imperfect computer model to predict a chaotic physical system, a rotating annulus. They found that BVs project onto analysis errors consistently better than either SVs or LLVs. These studies clearly confirm the conjecture of TK93: analysis errors, due to the use of dynamical forecasts as background fields, necessarily "accumulate" in the subspace of the leading BVs (or LLVs, depending on the size of the errors). Of course, to the extent an analysis system is not ideal, errors will also project on directions that are not dynamically conditioned but result from stochastic components in the analysis (random observational and approximation errors, etc.), but these will also evolve into the subspace of the leading LLVs or BVs.

4. Regionally rescaled BVs

In Section 7, EL state that "If there is any resemblance of BGV results to analysis errors, it must be built in by the 'masking' applied." This is clearly an incorrect statement. We just refer to the study by Smith and Gilmour (1998) who did not use any masking and in many cases found that the BVs strongly project on analysis errors. Similar results are presented in Iyengar et al. (ITKW, 1996), just a paragraph below the place rephrased by EL earlier in their comments. For example, without using any constraint in the vertical, the BVs explain more than 50% of the variance in the vertical distribution of analysis uncertainty.

In Section 4, EL state that the claim of ITKW that the BVs are representative of analysis uncertainties "is partly based on the fact that the (geographically dependent) masking coefficients applied to the BGVs are determined from analysis error statistics ..." We note that this point is made very clear in ITKW and no credit is claimed for representativeness of BVs in terms of analysis uncertainty in the *horizontal* domain: the size "of the perturbations is set to a fixed value at 500 hPa (which is given in a geographical mask ...) Therefore the horizontal distribution of the rms magnitude of bred vectors follows that of the analysis uncertainty ..." (ITKW).

In Section 4, EL state that "the NCEP bred modes do not at all resemble differences among analyses produced at different centers. The BGV structures have extremely large horizontal scale and large variance. In the northern hemisphere, they tend to be dominant northward of the storm tracks, rather than within them." We do not want to suggest that the regionally rescaled BVs used operationally as initial ensemble perturbations at NCEP are optimized in all respects. In fact, until a recent correction of a bug, the perturbation amplitudes were larger than the estimated analysis uncertainty at high latitudes. Nevertheless, *all features criticized by EL are consistent with estimates of analysis errors and with theoretical expectations.* First, the BVs have no strong projection on small scales because they attempt to sample the subspace of fast growing possible finite size analysis errors, disregarding the errors due to observational and other stochastically driven uncertainties, which contribute to smaller scale errors. Second, the perturbation size is of the order of estimated analysis uncertainty. For example, independent observational data collected in the NORPEX-98 field experiment (Langland et al., 1999) by I.Sz. and Z.T., in close collaboration with Dr. Rolf Langland, indicate that the average initial ensemble spread over the northeast Pacific ocean is within 10% of the size of the average analysis residuals there (difference between observations and the analysis). Third, the largest uncertainties in atmospheric analyses occur, on average, at high latitudes, and not along the westerly jet axis. This can be readily seen from Fig. 1 of the present note where the long term average of rms difference between NCEP and ECMWF reanalysis fields is shown. The largest uncertainty (30 m in the 500 hPa height fields), on average, is clearly at high latitudes, and not around the jet areas. This should be expected given the fact that the density of radiosonde observations is roughly four times lower north of 70 N than elsewhere in the northern extratropics. The maximum local amplitudes of 60–70 m differences in Fig. 1 of EL over small areas at high latitudes are also consistent with those found between separate analysis cycles run in an ensemble mode (P. Houtekamer, personal communication). BVs with global rescaling would have larger amplitudes near the midlatitude jets but due to the regionally dependent rescaling, the NCEP initial ensemble perturbations reflect the generally larger analysis uncertainty at high latitudes.

Near the end of Section 4, EL claim that "in ITKW, analysis error is mistaken for other kinds of errors." ITKW never confuse analysis errors (which exist but are unknown to us) with estimates of analysis uncertainty.

5. Total energy SVs

In Section 5 (and in a related statement in Section 7), EL state that "SKT misinterpret the

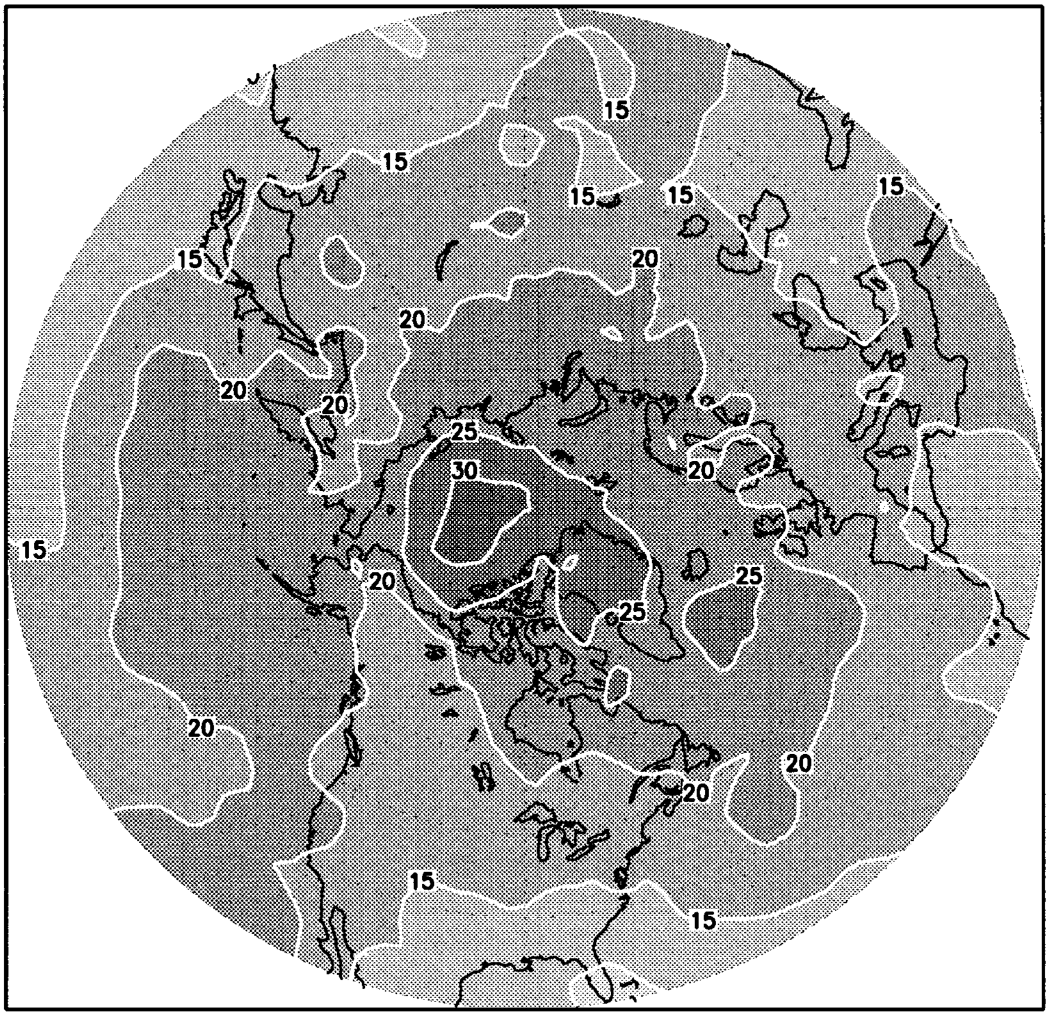

Fig. 1. Average of daily rms difference fields between 500 hPa height NCEP and ECMWF reanalysis fields for the years 1988–1994.

results of Ehrendorfer and Errico, 1995." In reality, SKT give no interpretation of EE's results. Ehrendorfer and Errico's (1995) results are quoted as they were published because their SVs showed geostrophic adjustments similar to those found by SKT. It is EL, not SKT, who present a re-interpretation of results from Ehrendorfer and Errico (1995), pointing out that after a careful subsequent study, a bug and a formulation error were found in their original study. SKT suggested an interpretation of their own results.

In Section 7, EL state that "The re-interpretation by Szunyogh et al. (1997) of the geostrophic adjustment problem described by Ehrendorfer and Errico (1995) is erroneous, as a great wealth of studies indicate. The large growth rates reported for SVs in the literature ... are not due to initial geostrophic imbalances in the SVs (the result reported by EE is an exception) ... these SVs are devoid of imbalances that project onto fast gravity waves." First, there is no "great wealth" of information on SVs and geostrophic imbalances in the literature. As Thorpe (1998) points out, it has been generally "assumed that they satisfy such a balance condition". Second, it is not true that total energy norm based SVs satisfy the geostrophic balance condition. In a careful study of TE SVs generated at ECMWF, Thorpe (1998) says that "An initial calculation of the balance condition suggests that the curvature terms, included in non-linear balance, are small, and furthermore that the linear or geostrophic balance is *only satisfied at around 60% level* (emphasis added). The thermal component in the thermal wind balance is larger than the vorticity component." This result is in qualitative agreement with that presented by SKT.

EL might be right in their statement in Section 7 that "the dynamic imbalances obtained by SKT in their SV determinations are likely due to either an energy-inconsistent formulation of vertical finite-difference equations in their model or due to an inconsistent computation of the energy". SKT used a standard approximation of the total energy consistent with that of many other authors (Molteni et al., 1996; Langland et al., 1999), but the strong sensitivity of the SVs to subtle details of the norm definition pointed out by EL does not change the main results, conclusions and conjectures of SKT, which have been fully confirmed by other studies since then, as follows.

(a) The SVs represent transient behavior, during which the initial SVs rotate toward leading LLVs. As Trevisan and Pancotti (1998) say: "Transient error growth is thus related to the evolution of … singular vectors toward their asymptotes" (which are the Lyapunov vectors). In particular, when a fast decaying LLV, that has a negative projection onto a fast growing LLV, is combined with the growing LLV, it can, depending on the norm, "hide" the true projection of the combined vector onto the growing LLV at initial time. And because the decaying LLV becomes irrelevant by final time, "it appears that there is faster than exponential growth" (i.e., super-Lyapunov growth associated with the leading SVs), as Frederiksen (1997) observed it in the context of time-dependent normal modes. This phenomenon has also been well documented by others for steady basic states (Zhang, 1988; Frederiksen and Bell, 1990; Buizza and Palmer, 1995) where the LVs are the traditional normal modes, and for time dependent systems (Legras and Vautard, 1996).

(b) The SVs, and "the nature of (their) rapid rotation (toward leading LLVs) depends on the length of the optimization period and the norm chosen" (SKT). SKT also note that geostrophic adjustment is only one of many processes that can possibly contribute to transient behavior, depending on the norm chosen. The fact that SVs can strongly depend on the norm and optimization time period used in their definition is well documented in the literature (Buizza, 1994; Molteni et al, 1996; Hartmann et al., 1995; Barkmeijer, 1998). The critical sensitivity of the SVs to the choice of norm is highlighted by EL's findings: as they report, minor changes in model/norm formulation had a profound impact on the SVs in terms of geostrophic balance.

(c) The initial SVs are generally off the attractor. Independent research has since confirmed this conjecture of SKT. As Trevisan and Pancotti (1998) state, "The leading Lyapunov vectors … are tangent to the attractor, while the leading initial singular vectors, in general, point away from it." Similar results are presented by Legras and Vautard (1996). As Frederiksen (1997) showed, the presence of fast decaying vectors in initial SVs cannot be explained by linear dynamics in the case of several commonly used norms (TE SVs). The use of these norms is justified only if the very specific, dynamically fast vanishing part of the SVs can be explained by external forcing, such as analysis errors or nonlinear processes. Frederiksen (1997) states that "structures like adjoint mode and maximum sensitivity perturbation errors (defined with commonly used norms) must be specially prepared by some previous instability mechanism or nonlinear effect or by the data assimilation scheme to have their initial specific structures." The fact that initial SV perturbations are typically not realizable in dynamical systems may explain why so little is known about the transition processes that bring these "alien" or "non-physical" structures close to the attractor (or "reality"). This is a mainly uncharted territory in atmospheric sciences, though several aspects of this transition process, related to TE SVs, are "currently being investigated" (Thorpe, 1998). It is interesting to note that most of the peculiar properties and transition processes associated with total energy based initial SVs disappear when the SVs are computed using a norm consistent with known statistical properties of analysis errors (Barkmeijer et al., 1998).

6. Conclusions

We fully agree with EL's statement in Section 7: "In conclusion, anyone using BGVs should carefully investigate how they were produced and what their structures and magnitudes are before using them in any application". However, given their more sensitive nature, the use of SVs should warrant at least as much attention as that of the BVs. For each application, one needs to carefully consider the practical advantages and disadvantages of using either methods. Using a combination of the two methods, as discussed by Toth et al. (1996), and Swanson et al. (1998), is yet another possibility. The debate on the usefulness of the two methods in ensemble forecasting and data assimilation likely will not end with this exchange of opinions. Nevertheless we are grateful to EL for raising these important issues, and to Tellus for allowing us to respond.

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