

OPERATIONAL IMPLEMENTATION OF VARIATIONAL DATA ASSIMILATION

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1. Introduction

Over the last few years, the variational form of statistical estimation has been implemented at many operational centres. The motivation originated from the difficulties associated with the assimilation of satellite data such as TOVS (TIROS-N Operational Vertical Sounders) radiances. Lorenc (1986) showed that the statistical estimation problem could be cast in a variational form (3D-Var) which is just a different way of solving the problem that the so-called *optimal interpolation* attempts to solve directly. Eyre (1989) showed, in a 1D-Var context, that a variational formulation leads to a more natural framework for the direct assimilation of radiances instead of *retrieved* temperature and humidity profiles. This is also true for any indirect measurement of the state of the atmosphere. Talagrand and Courtier (1987) showed that the use of the adjoint of a numerical model makes it possible to determine the initial conditions leading to a forecast that would best fit data available over a finite time interval. These two formulations can be combined to yield what is now called the 4D variational formulation of the statistical estimation problem or *4D-Var*.

The first implementation of 3D-Var was done at NCEP (Parrish and Derber, 1992) and later on at ECMWF (Courtier *et al.*, 1998). Other centres like the Canadian Meteorological Centre (Gauthier *et al.*, 1999) and the Met Office (Lorenc *et al.*, 2000) also implemented operationally a 3D-Var scheme. Courtier (1997) noted that there exists a dual formulation of 3D-Var on which is based the assimilation of NASA's Data Assimilation Office (Cohn *et al.*, 1998) and of the US Naval Research Laboratory (Daley and Barker, 2000). In 1997, ECMWF implemented 4D-Var (Rabier *et al.*, 2000) and so did Météo-France in 2000 (Gauthier and Thépaut, 2001). A considerable amount of research was necessary to achieve these operational implementations. Courtier *et al.* (1994) pointed out that a direct implementation of 4D-Var requires a computational time exceeding the capacity of even the most powerful computers. The incremental formulation of 4D-Var was proposed in which a simplified model is used to perform inner iterations followed by an integration of the full model based on the updated initial conditions. This *outer iteration* provides an updated evaluation of the innovations and of the reference trajectory required to define the simplified tangent linear model. In this context, an operational implementation of 4D-Var is possible. In recent years, experimentation with now operational 4D-Var systems indicates that it is necessary to

make the simplified model to agree more closely with the complete high-resolution model both for its dynamics and physical parameterizations. This question is the object of current research regarding the nature of the simplified physical parameterizations that need to be used (Janisková *et al.*, 1999; Mahfouf, 1999).

In the context of the data assimilation cycles, the background error statistics should reflect the information gained from past observations, which is implicitly contained in the background state. Fisher and Andersson (2001) report recent results of experiments with a reduced rank Kalman filter, used to provide flow dependent background error covariances to 4D-Var. Their results did not show substantial improvements in the forecasts. This topic is being investigated using different types of simplified Kalman filters.

In this paper, the focus will be on the variational formulation of the data assimilation problem. In section 2, the incremental formulation will be presented and discussed first in the context of 3D-Var. Section 3 presents the incremental form of 4D-Var. Results with a simple barotropic model are presented to illustrate the capabilities and limitations of the approach. Section 4 reviews some recent results obtained from experimentations by several groups (e.g., ECMWF, Météo-France). Section 5 discusses some avenues being explored in current research. This includes the ensemble Kalman filter (Evensen, 1997; Houtekamer and Mitchell, 2001) or representer algorithms (Bennett and Thorburn, 1982; Xu and Daley, 2002).

2. The incremental formulation of variational assimilation

The variational assimilation problem is expressed here as

$$J(\mathbf{X}) = \frac{1}{2}(\mathbf{X} - \mathbf{X}_b)^T \mathbf{B}^{-1}(\mathbf{X} - \mathbf{X}_b) + \frac{1}{2}(\mathbf{H}(\mathbf{X}) - \mathbf{y})^T \mathbf{R}^{-1}(\mathbf{H}(\mathbf{X}) - \mathbf{y}) \quad (2.1)$$

where \mathbf{X} is the model state, \mathbf{X}_b is the background state, \mathbf{B} represents the background-error covariances, \mathbf{y} is the observation vector, \mathbf{H} , the observation operator while \mathbf{R} represents the observation error covariances. To precondition the minimization, the

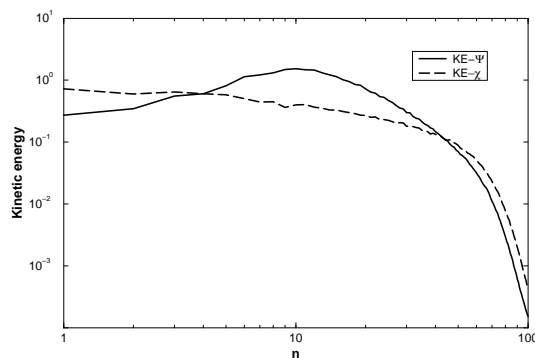


Figure 1. Kinetic energy spectra for the rotational and divergent component for the autocorrelation of background-error statistics at 500 hPa.

control variable $\xi = \mathbf{B}^{-1/2}(\mathbf{X} - \mathbf{X}_b)$ is introduced so that $\mathbf{X} \equiv \mathbf{X}(\xi) = \mathbf{X}_b + \mathbf{B}^{1/2}\xi$ and (2.1) can be rewritten as

$$J(\xi) = \frac{1}{2}\xi^T \xi + \frac{1}{2}(\mathbf{H}(\mathbf{X}(\xi)) - \mathbf{y})^T \mathbf{R}^{-1}(\mathbf{H}(\mathbf{X}(\xi)) - \mathbf{y}). \quad (2.2)$$

In 3D-Var, the analysis increment $\delta\mathbf{x} = \mathbf{B}^{1/2}\xi$ has an effective lower resolution that is dictated by the background-error covariances. For example, Fig.1 shows the spectrum of the rotational and divergent kinetic energy of correlations. The use of such covariances will lead to an analysis increment with a resolution that cannot exceed 200 km.

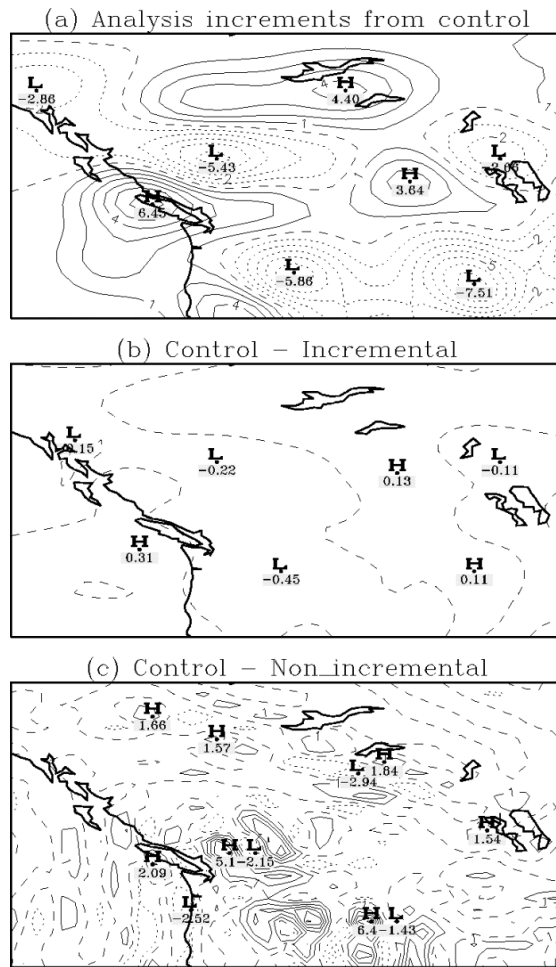


Figure 2. a) Analysis increments of dew point depression at 700 hPa from the control experiment valid at 1200 UTC 24 September 1997. b) Analysis increment of a) minus that of the incremental experiment. c). Analysis increments shown in a) minus that of the non-incremental experiment (from Laroche *et al.*, 1999)

However, it is beneficial to compute the innovations $\mathbf{y}' = \mathbf{y} - \mathbf{H}(\mathbf{X}_b)$ using the background state at its full resolution. Following Courtier *et al.* (1994), we approximate $\mathbf{H}(\mathbf{X}) \cong \mathbf{H}(\mathbf{X}_b) + (\partial\mathbf{H}/\partial\mathbf{X})(\mathbf{X}_b) \delta\mathbf{x} \equiv \mathbf{H}(\mathbf{X}_b) + \mathbf{H}'(\mathbf{X}_b) \delta\mathbf{x}$ so that (2.2) is now approximated by

$$J_L(\xi) = \frac{1}{2} \xi^T \xi + \frac{1}{2} (\mathbf{H}'(\mathbf{X}_b) \delta\mathbf{x}(\xi) - \mathbf{y}')^T \mathbf{R}^{-1} (\mathbf{H}'(\mathbf{X}_b) \delta\mathbf{x}(\xi) - \mathbf{y}') \quad (2.3)$$

with $\delta\mathbf{x}(\xi) = \mathbf{B}^{1/2} \xi$. As pointed out in Courtier *et al.* (1994), J_L has a form very similar to the original problem except that the observation operator has been linearized around \mathbf{X}_b and the resulting Jacobian, $\mathbf{H}'(\mathbf{X}_b)$, is used instead of the nonlinear form of the observation operator. Fig.2 from Laroche *et al.* (1999) shows the analysis increment obtained by using the original cost function at the full resolution of the model and differences between this analysis increment and that obtained by using (2.3) (Fig.2b). The differences indicate that the analyses are virtually identical. Fig.2c however shows the difference between the reference analysis increment and that obtained by solving (2.1) but at a lower resolution. The differences are significant and stress the importance of computing the innovations with respect to the full resolution of the background field.

This approach has been used at the Canadian Meteorological Centre (Laroche *et al.*, 1999) and Météo-France (Desroziers *et al.*, 2003) to produce regional analyses for a variable resolution model while the analysis increment remains global and at a coarser resolution. The small scales features found in the analysis are therefore produced by the model itself in response to changes brought by the analysis to the large-scale components.

3. The incremental form of 4D-Var

The reasons why low-resolution increments are sufficient in 4D-Var are different than those presented above for 3D-Var. In Thépaut and Courtier (1991) and later on in Tanguay *et al.* (1995) and Laroche and Gauthier (1999), it is shown that for the large-scale dynamics, 4D-Var adjusts the more energetic large-scale components first. To determine the analysis increments of 4D-Var within the inner loop, Courtier *et al.* (1994) then proposed to use the tangent linear model (TLM) and its adjoint (Adj) at a coarser resolution with simplified physical parameterizations. However, as for the 3D-Var case, the innovations must be computed with respect to a high-resolution trajectory generated by the high-resolution model with its complete set of physical parameterizations. Outer loops are however needed to update the reference trajectory that defines the TLM and Adj.

Two questions are then raised. First, is it sufficient for the minimization to consider only the large-scale components of the gradient of the cost function and, second, can the evolution of these large scale components be correctly predicted by a simplified model? Fig.3 from Laroche and Gauthier (1999) summarizes results from several experiments carried out with a simple barotropic model on a β -plane. The experiments were cast as identical twins with observations generated from a reference trajectory provided by the assimilating model and random noise representative of observation error was added to those *synthetic* observations. No background term is included. Fig. 3 shows the correla-

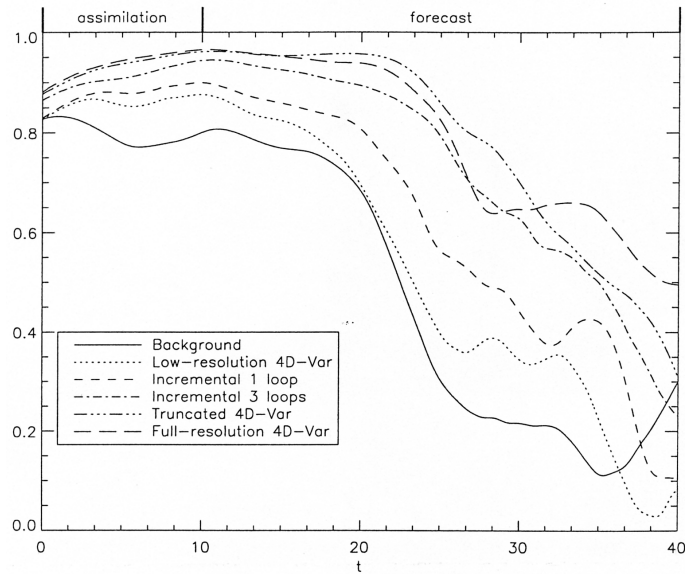


Figure 3. Correlation between the reference vorticity field and those obtained from various variational formulations. The synthetic observations are at low resolution and random noise has been added (from Laroche and Gauthier, 1999).

tion between the reference trajectory (or *nature run*) and the results from several experiments. The assimilation takes place over the first 10 nondimensional time units and forecasts at full resolution are made up to $t = 40$. The full resolution 4D-Var shows the best that can be obtained from the low-resolution observations. Given the limit of predictability, a reasonable forecast can be obtained up to $t \approx 30$. The truncated 4D-Var experiment is one in which the adjoint model is used at the full resolution but the resulting gradient is truncated at a lower resolution (reduced by a factor of 4). In this case, Fig.3 shows that the truncated 4D-Var compares to the results obtained with the full resolution 4D-Var.

The low-resolution 4D-Var experiment is a complete 4D-Var based on the model at low-resolution. Fig.3 indicates that it only marginally improves the fit to the reference trajectory compared to what is obtained from the starting point of the minimization. Finally, the incremental form of 4D-Var shows that with only one outer loop, the results are only slightly improved compared to the low-resolution 4D-Var. However, if three outer loops are considered, then the incremental formulation yields to a reasonable approximation of the truncated 4D-Var. These results show the crucial role of updating the trajectory by performing outer iterations of 4D-Var.

Another question raised by 4D-Var is the impact of model error. It is implicitly assumed that any misfit to the observations is the result of error in the initial conditions. Experience shows that bad forecasts are often caused by errors in the model itself. An example is presented in the context of the barotropic model used in the experiments presented above. To mimic phase errors that occur with numerical weather prediction models that do not displace meteorological systems at the correct phase speed, synthetic

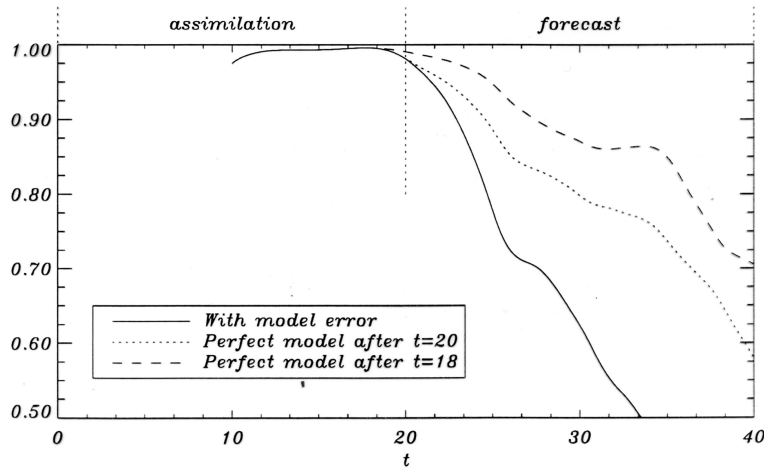


Figure 4. Solid line shows the correlation between the nature run obtained by using $\beta = 0.5$ and the assimilation/forecast of a full 4D-Var based on a model using $\beta = 0.4$. Using the perfect model to perform the forecast, the dashed (dotted) line show the correlation obtained when using the initial conditions at $t = 18$ ($t = 20$).

observations were generated from a nature run obtained with $\beta = 0.5$ while β was set to 0.4 in the model used in the assimilation. Fig.4 shows the correlation between the true state and the assimilation/forecast based on the erroneous model: the assimilation window here is $10 < t < 20$. It shows that the best solution is obtained not at the end of the assimilation window but at some earlier time. To test the quality of the analysis, the true model ($\beta = 0.5$) was used to make the forecast using the 4D-Var analysis at $t = 20$ (dotted line) and at $t = 18$ (dashed line) where the maximal correlation to the true state was obtained. It shows that the latter case yields to a substantially better forecast. So, even though these experiments used perfect observations at all grid points and at all times, the presence of model error cannot translate the information from the observations into a better forecast.

In operational systems, model error is often associated with weaknesses in the numerous physical parameterizations used in the model. The incremental formulation of 4D-Var introduces a simplified set of physical parameterizations that should be consistent with those of the complete model. The development of a simplified set of physical parameterizations (deep convection, stratiform precipitation, surface and gravity-wave drag, vertical diffusion and radiation) is presented in Janisková *et al.* (1999) and Mahfouf (1999). As discussed in Mahfouf and Rabier (2000), this translated in a better fit to the observations within the inner loop of the 4D-Var. In Barkmeijer *et al.* (2001) and Puri *et al.* (2001), it is shown that the inclusion of a simplified physics in the TLM/Adj for the computation of the singular vectors used in their ensemble prediction system, has a significant impact on the spread of the resulting ensemble of forecasts.

Finally, it is important to stress that the 4D-Var analysis and forecast are better balanced with respect to the internal balance of the model. Fig.5 shows the average precipitation rates (over 24-h) as a function of forecast time. It clearly shows that,

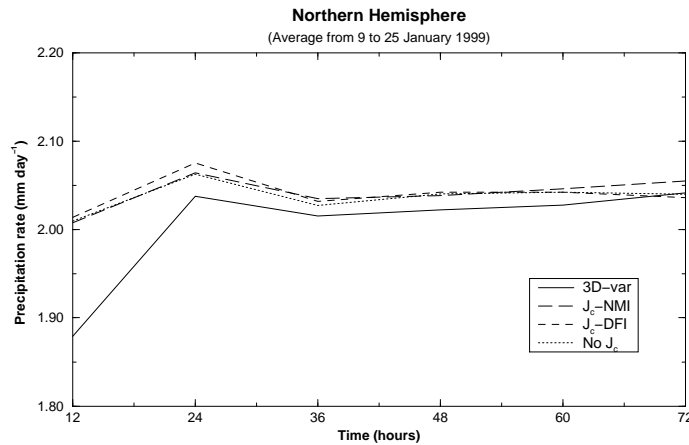


Figure 5. Average precipitation rates (in mm/day) as a function of forecast time. Those have been averaged over the Northern hemisphere for the two-week period extending from 9 to 25 January 1999. (see Gauthier and Thépaut, 2001 for details)

compared to 3D-Var, the 4D-Var analyses do not show a significant imbalance in the first hours of the forecast. This *spin-up* process is often associated with the presence of spurious gravity waves that need to be removed by an initialization process such as nonlinear normal mode initialization or a digital filter. The experiments of Gauthier and Thépaut (2001) show that even without any constraint to suppress these fast oscillations (No J_c experiment), the 4D-Var analysis does not lead to an appreciable precipitation spin-up at the initial time.

4. Experimentation with 4D-Var

The introduction of the time dimension in the assimilation allows information to be extracted from a time series of observations. For instance, the 4D-Var assimilation of measurements related to passive tracers provides information about the winds (Andersson *et al.*, 1994). Moreover, the 4D-Var analysis increments have a baroclinic structure that can be related to the fastest growing perturbations (Thépaut *et al.*, 1996). Based on the extensive experimentation carried out at ECMWF in preparation for the implementation of 4D-Var, Rabier *et al.* (1998, 2000) report that the main differences between the 3D-Var and 4D-Var analysis increments were observed in those regions identified as the most sensitive to perturbations in the initial conditions. The sensitive regions were determined from the singular vectors. Their results also indicate that the gain obtained with 4D-Var lies in reducing the number of missed forecasts due to rapid cyclogenesis. This indicates that 4D-Var is able to determine the changes to the initial conditions that will trigger or not the development of synoptic systems.

The advantage of 4D-Var over 3D-Var is that it makes it possible to assimilate data at the observation time, which results in an increase of the volume of data that can be

assimilated. Moreover, information contained in the temporal variation can also be extracted. However, Järvinen *et al.* (1999) present some difficulties, encountered in the assimilation of surface pressure data from stations reporting every hour. In regions where the real orography differs from that of the model, a bias can be introduced in the surface pressure data. When all hourly reports are assimilated, this results in a significant negative impact. This problem is more acute for isolated stations since there are no surrounding data to weigh against this biased estimate. Removing the effect of this bias from the data can be addressed in different ways and Järvinen *et al.* (1999) introduced a time-correlation in the observation error that manages to alleviate the problem. The net effect is to focus the analysis more on the *variation* of surface pressure than on the mean value of surface pressure. It is the surface pressure tendency that is more closely linked to developing baroclinic systems (Bengtsson, 1980).

5. Conclusion

Any variational problem raises the issue of the convergence of the minimization. One iteration of the minimization being particularly expensive in 4D-Var, its practical implementation has to limit the number of iterations to a rather low number, typically less than a hundred. Fisher and Andersson (2001) proposed a preconditioning of the minimization by approximating the Hessian of the 4D-Var cost function and this significantly improved the convergence. Problems in the conditioning could also explain a case of poor convergence in a 4D-Var experiment reported by Andersson *et al.* (2000). Convergence of the minimization is therefore still an issue and given the nonlinear nature of the model, so is the existence of multiple minima (Tanguay *et al.*, 1995).

Currently, a lot of research is going on to address the importance of model error in 4D-Var and data assimilation in general. In particular, in the context of 4D-Var, the model is assumed to be perfect and even more, in the incremental formulation, the simplified model should be a good approximation of the more accurate high-resolution model with sophisticated physical parameterizations. As discussed in Bouttier (2001), extending the assimilation window to 12-h has accentuated the importance of these differences that could be diagnosed from the differences between observation departures computed with respect to the simplified and high-resolution models. Extending 4D-Var to longer assimilation windows may be more difficult than was thought initially due to the importance of model errors.

It was mentioned briefly that cycling 4D-Var requires that the background-error covariances reflect their flow-dependent nature. Results presented by Fisher and Andersson (2001) indicate that there is a long way from theory to practice. The reduced-rank Kalman filter used in their experiments provided a flow-dependent estimate of the covariances but this only had a marginal impact on the resulting forecasts.

Other avenues are being explored in 4D data assimilation. In particular, the ensemble Kalman filter (EnKF) (Evensen, 1997; Houtekamer and Mitchell, 2000) has been proposed recently to obtain a practical way of implementing a Kalman filter for complex models without having to develop the adjoint of a numerical model. The

Monte-Carlo approach that supports the EnKF then raises some questions about the required size of the ensemble. Up to now, the direct estimate is often noisy and some assumptions must be introduced to address the rank deficiency problem. It also makes it more difficult to introduce non-Gaussian error statistics for errors, and to maintain dynamical balance in the analysis increments.

The 4D-Var algorithm imposes the model as a strong constraint, which has some limitations. Bennett and Thorburn (1992) introduced the weak constraint formulation in which the model is imposed only as a weak constraint. Because it uses the complete model trajectory and not only the initial conditions, this approach is much more demanding than 4D-Var. Recently, Xu and Daley (2002) introduced the *accelerated representer algorithm* which is referred to as *4D-PSAS* in Courtier (1997). It corresponds to the dual formulation of 4D-Var and can be built from the same basic operators (e.g., model integrations, observation operators, and their tangent linear and adjoint, covariance models). In Lagarde *et al.* (2001), a graphical representation has been introduced to represent a wide class of assimilation algorithms altogether with their dual representations. Their analysis show that if some care is taken in developing a data assimilation system, it would be possible to reuse the same basic *building blocks* to obtain new algorithms. This would be an advantage for operational centres that must adapt quickly to new advances in a rapidly evolving field.

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