

An Ensemble-Based Three-Dimensional Variational Assimilation Method for Land Data Assimilation

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Received 22 February 2009; revised 16 April 2009; accepted 16 April 2009; published 16 May 2009

Abstract Land surface models are often highly nonlinear with model physics that contain parameterized discontinuities. These model attributes severely limit the application of advanced variational data assimilation methods into land data assimilation. The ensemble Kalman filter (EnKF) has been widely employed for land data assimilation because of its simple conceptual formulation and relative ease of implementation. An updated ensemble-based three-dimensional variational assimilation (En3-DVar) method is proposed for land data assimilation. This new method incorporates Monte Carlo sampling strategies into the 3-D variational data assimilation framework. The proper orthogonal decomposition (POD) technique is used to efficiently approximate a forecast ensemble produced by the Monte Carlo method in a 3-D space that uses a set of base vectors that span the ensemble. The data assimilation process is thus significantly simplified. Our assimilation experiments indicate that this new En3-DVar method considerably outperforms the EnKF method by increasing assimilation precision. Furthermore, computational costs for the new En3-DVar method are much lower than for the EnKF method.

Keywords: land data assimilation, En3-DVar, POD, EnKF

Citation: Tian, X.-J., and Z.-H. Xie, 2009: An ensemble-based three-dimensional variational assimilation method for land data assimilation, *Atmos. Oceanic Sci. Lett.*, **2**, 125–129.

1 Introduction

Numerical weather or climate prediction in meteorology uses the power of computers to make weather or climate forecasts. Data assimilation provides a framework for merging observational and meteorological model estimates to improve weather and climate predictions. Many simple data assimilation methods, such as the polynomial fitting method (Panofsky, 1949), the successive-correction method (SCM) (Bergthorsson et al., 1955; Cressman, 1959) and optimal interpolation (OI) (Gandin, 1963), have been proposed since numerical weather predictions were first introduced. In recent years, many advanced data assimilation methods, such as the four-dimensional variational assimilation (4-DVar) method (Courtier, 1997; Zheng, 2003; Kalnay, 2005; Tian et al., 2008a; Wang and Li, 2009), the extended Kalman filter (EKF) (Miller et al.,

1994; Zheng, 2003; Kalnay, 2005) and the ensemble Kalman filter (EnKF) (Evensen, 1994; Kalnay, 2005), have been developed and applied to data assimilation in the atmospheric and oceanographic sciences. In contrast, data assimilation in the land surface and hydrological sciences was not established as a distinct field until the mid-1990s. Since that time, land data assimilation has become an increasingly active field with pioneering studies. Assimilating microwave remote sensing data with “off-line” land surface models has become the predominant characteristic of land surface data assimilation. Based on the assumption that land surface observational techniques and analytical methods are sufficiently advanced, an accurate description of land surface states and fluxes can be produced by assimilating remote sensing data or *in situ* observations in a data assimilation framework. For land surface data assimilations, the EnKF method is probably the most frequently used optimization algorithms because of its simple conceptual formulation and relative ease of use (Evensen, 2003, 2007; Tian and Xie, 2008; Tian et al., 2008b; De Lannoy et al., 2007). There are also variational assimilation methods (Yang et al., 2007) that have been tested in land surface data assimilation. It is well known that land surface models are usually highly nonlinear and that model physics also contain parameterized discontinuities, which limits their application (Mu and Wang, 2003).

In this study, an updated ensemble-based three-dimensional variational assimilation (En3-DVar) method is proposed that merges Monte Carlo methods and proper orthogonal decomposition (POD) techniques into the traditional 3-DVar method to simplify data assimilation. This method is similar to Tian et al. (2008a), but is reduced to the 3-D case for the purpose of land surface data assimilation. The ensemble members in Tian et al. (2008a) are constructed by forecast states at selected time points over the assimilation time window, while they are obtained only at a single time point in the current method. The basic idea of the POD technique is to start with an ensemble of data, called snapshots, collected from an experiment or a numerical procedure of a physical system. The POD technique is then used to produce a set of base vectors, which span the snapshot collection. The goal of the technique is to represent the ensemble of the data in terms of an optimal coordinate system. That is, the snapshots can be generated by the smallest possible set of base vectors. We conducted several numerical experiments using one-dimensional (1-D) soil water equations and synthetic

observations to evaluate our method in land surface data assimilation. Comparisons were also made between our method and the EnKF method. We found that our new En3-DVar method outperformed the EnKF method by increasing the assimilation precision and reducing computational costs.

2 Methodology

In principle, the traditional 3-DVar analysis x_a is obtained by minimizing a cost function, J , that measures the misfit between model trajectory, $H(x)$, and the observation, y , as follows:

$$J(x) = (x - x_b)^T \mathbf{B}^{-1} (x - x_b) + (y - H(x))^T \mathbf{R}^{-1} (y - H(x)), \quad (1)$$

with the forecast model M imposed as a strong constraint, and defined as:

$$x(t_k) = M(t_{k-1}), \quad (2)$$

where t is the time, the superscript, T , stands for a transposed, and b , as a background value. H is the observational operator and the matrices, \mathbf{B} and \mathbf{R} , are the covariances of background and observational error, respectively.

Briefly, application of the updated method requires generating N random perturbation fields using a Monte-Carlo method and adding each perturbation to the initial background field at a time level $t = t_0$ before the assimilation time step to produce N initial fields, $x_n(t_0)$, $n = 1, 2, \dots, N$. Additional steps involved in the method involve integrating the forecast model $x_n = M(x_n(t_0))$ to obtain the ensemble state, x_n . When the ensemble size, N , is increased by adding random samples, the ensemble space may cover the analysis vector, x_a . That is, x_a is approximately assumed to be embedded in the linear space,

$\Omega(\overbrace{x_1, x_2, \dots, x_N})$ that comprises the ensemble members, x_n ($1 \leq n \leq N$). The analysis vector, x_a , can then be expressed by the linear combinations of one set of base vectors of $\Omega(\overbrace{x_1, x_2, \dots, x_N})$ since it is contained in this space.

The final task involves obtaining appropriate base vectors. We found that the POD technique was a good method for obtaining the appropriate base vectors. It can produce a set of base vectors spanning the ensemble of data in terms of least squares optimization (Ly and Tran, 2001, 2002). We then applied the POD technique to the forecast ensemble so that the orthogonal base vectors could capture the ensemble state spatial structure, while at the same time reflecting its temporal evolution. After the model status is expressed with a truncated expansion of the base vectors, the data assimilation process becomes significantly simplified.

The average of the ensemble of snapshots is given by:

$$\bar{x} = \frac{1}{N} \sum_{n=1}^N x_n. \quad (3)$$

A new ensemble is formed by:

$$\delta x_n = x_n - \bar{x} \quad (1 \leq n \leq N), \quad (4)$$

which forms the matrix \mathbf{A} ($M \times N$), where $M = M_g \times M_v$ and M_g , M_v are the number of model spatial grid points and the number of model variables, respectively. PODs for \mathbf{A} can produce the POD modes ϕ_k ($1 \leq k \leq N$). The truncated reconstruction of the analysis variable in the 3-D space, x_a , is then given by:

$$x_a = \bar{x} + \sum_{i=1}^r \alpha_i \phi_i, \quad (5)$$

where r is the rank of \mathbf{A} and $\alpha = (\alpha_1, \dots, \alpha_r)$ are the expansion coefficients. The 3-D background error covariance is modeled approximately by:

$$\mathbf{B} = \frac{\mathbf{A}\mathbf{A}^T}{N-1} \approx (N-1)\lambda^{-1}\alpha\alpha^T, \quad (6)$$

where λ are the nonzero eigenvalues. By substituting Eqs. (5)–(6) into Eq. (1), the control variable becomes $\alpha = (\alpha_1, \dots, \alpha_r)$ instead of x . The cost function is further transformed as follows:

$$J(\alpha) = (N-1)\lambda^{-1}\alpha\alpha^T + (y - H\bar{x} - H\Phi\alpha)^T \mathbf{R}^{-1} (y - H\bar{x} - H\Phi\alpha), \quad (7)$$

where H is the tangent linear observation operator. The covariance for the observation error, \mathbf{R} , is always diagonal and $\Phi = (\phi_1, \phi_2, \dots, \phi_r)$. Since \mathbf{R} is symmetrical, the gradient of the cost function is obtained through the following simplified calculation:

$$\nabla J(\alpha) = 2(N-1)\lambda^{-1}\alpha - 2(H\Phi)^T \mathbf{R}^{-1} (y - H\bar{x} - H\Phi\alpha). \quad (8)$$

One can solve the optimization problem as follows:

$$\nabla J(\alpha) = 0, \quad (9)$$

and

$$\begin{aligned} & \left[(N-1)\lambda^{-1} + (H\Phi)^T \mathbf{R}^{-1} (H\Phi) \right] \alpha \\ & = (H\Phi)^T \mathbf{R}^{-1} (y - H\bar{x}). \end{aligned} \quad (10)$$

Eq. (10) can be solved directly and without an iterative procedure as follows:

$$\alpha = \left[(N-1)\lambda^{-1} + (H\Phi)^T \mathbf{R}^{-1} (H\Phi) \right]^{-1} (H\Phi)^T \mathbf{R}^{-1} (y - H\bar{x}). \quad (11)$$

Monte Carlo-based methods are also used to produce the ensemble in En3-DVar. However, unlike EnKF, the analysis procedure in En3-DVar is conducted when observational data are available.

3 Numerical experiments

This section describes the results of tests to apply this new updated methodology to land data assimilation. Several assimilation experiments were undertaken with a simple 1-D soil-water equation model. In addition, comparisons of the En3-DVar and EnKF methods were performed.

3.1 Experimental design

The conservation of water mass, (θ) , for 1-D vertical

water flow in a soil column in the Community Land Model (CLM) (Bonan et al., 2002) is expressed as:

$$\frac{\partial \theta}{\partial t} = -\frac{\partial q}{\partial z} - E - R_{\text{fm}}, \quad (12)$$

where q is the vertical soil water flux (mm s^{-1}) (note: the model assumes no horizontal water movement), E is the evapotranspiration rate, R_{fm} is the melting (negative) or freezing (positive) rate, and z is the soil depth from the surface. Both q and z are positive downward.

The soil water flux, q , is described by Darcy's law:

$$q = -k \frac{\partial(\varphi + z)}{\partial z}, \quad (13)$$

where k is the hydraulic conductivity (mm s^{-1}), and φ is the soil matrix potential (mm). The CLM computes soil water content in 10 soil layers (Table 1) by Eqs. (12)–(13).

$$k = k_s \left(\frac{\theta}{\theta_s} \right)^{2b+3}, \quad \varphi = \varphi_s \left(\frac{\theta}{\theta_s} \right)^{-b}, \quad (14)$$

where k_s is the saturated hydraulic conductivity (mm s^{-1}), θ_s is the saturated moisture, φ_s is the saturated soil matrix potential (mm), and b is the soil matrix constant (Table 2). The time step (Δt) is 1800 sec.

In our experiments, the soil water equation model forced by “perfect” infiltration represents the perfect model, whereas the soil water equation model forced by the “imperfect” infiltration represents an imperfect model (Fig. 1). The “true” state is produced by integrating the “perfect” model with the “perfect” initial soil moisture (Fig. 2) for 365 days. The “imperfect” state is produced by integrating the “imperfect” model with the “imperfect” initial soil moisture. This means that the source of forecast model error is not only associated with noise from the initial field but also from uncertainties in the forecast model. One assimilating observation frequency every 12

hours was adopted for the group of experiments. An ensemble size of 40 was used in experiments examining both assimilation methods. The “observations” were generated by adding 3% random error perturbations to the time series of the “perfect” state (i.e., “observation” = $(1 + \varepsilon) \times \text{“perfect”}$, where ε is a real random number varying from -3% – 3%). These “observations” were assimilated with both methods for the purpose of our experiments, but not in the forecast experiments. In particular,

only the skin layer soil moisture observation is used in our experiments.

3.2 Experimental results

We use the following root mean square error (RMSE) calculation of assimilated soil moisture ($\text{m}^3 \text{m}^{-3}$) to evaluate our method:

$$\text{RMSE} = \sqrt{\frac{1}{10} \sum_{i=1}^{10} (\theta_{\text{ass}}(i) - \theta_{\text{tru}}(i))^2}, \quad (15)$$

where the subscript, ass, denotes the assimilated value, and the subscript, tru, stands for the true value. Fig. 3a shows the time series of daily RMSE values for the En3-DVar assimilated soil moisture ($\text{m}^3 \text{m}^{-3}$) with the 12-hour sample observation frequency. The RMSE values for the En-3DVar is significantly lower than the EnKF values, especially from days 1–180. This indicates that the En3-DVar method performed much better than the EnKF. With the observations being assimilated, there is so much observation information merged into the analyzed soil moisture calculation that the error values for the En3-DVar became very low (Fig. 3a). On the contrary, the errors of the EnKF are not reduced as so much as the En3-DVar's. Most of the observed En3DVar error is $< 0.01 \text{ m}^3 \text{m}^{-3}$ from days 81–180, whereas some of the EnKF error values approach $0.0218 \text{ m}^3 \text{m}^{-3}$. Similarly, the

Table 1 Thickness of 10 soil layers.

Soil layer	1st	2nd	3rd	4th	5th	6th	7th	8th	9th	10th
Thicknesses (m)	1.75×10^{-2}	2.75×10^{-2}	4.54×10^{-2}	7.49×10^{-2}	0.12	0.20	0.34	0.55	0.91	1.14

Table 2 Parameters used in the soil water equation model.

θ_s	k_s	b	φ_s
0.46	$2.07263 \times 10^{-6} \text{ m s}^{-1}$	8.634	-3.6779 m

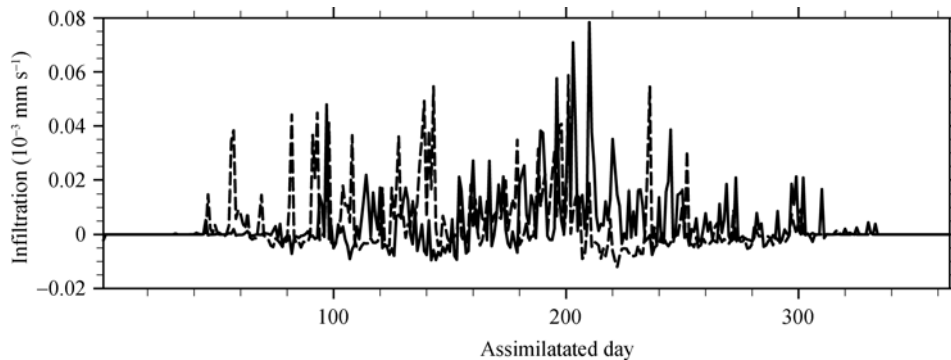


Figure 1 The “perfect” (solid line) and “imperfect” (dashed line) infiltration time series used in the assimilation experiments.

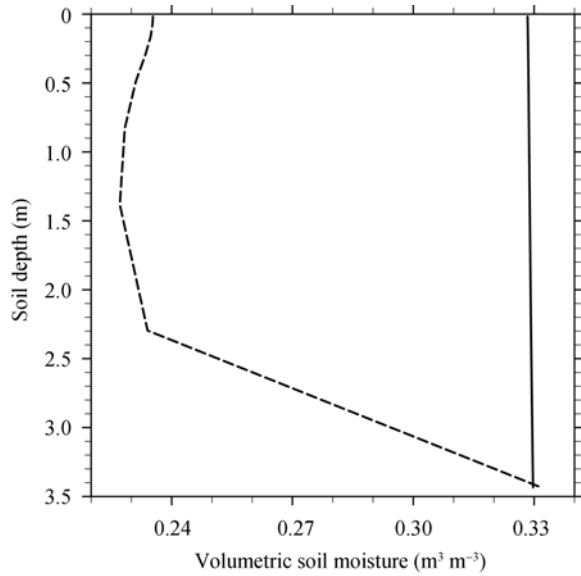


Figure 2 The “perfect” (solid line) and “imperfect” (dashed line) initial soil moisture profiles used in the assimilation experiments.

time series of daily observed and assimilated (En3-DVar and EnKF) volumetric soil moisture ($\text{m}^3 \text{m}^{-3}$) shown in Figs. 3b–c illustrates that the En3-DVar assimilated curve can be adjusted to approach the true curve more rapidly than in the EnKF method.

The ratio of computational costs for the En3-DVar and EnKF methods was about 1:5 for the group of experiments undertaken. High computational costs in the EnKF method were mainly due to the fact that the analysis process, which consists of sizable matrices, has to be conducted repeatedly during the assimilation process. Conversely, for the En3-DVar method, the computation is performed only when there are observations. Of course, this conclusion is case-dependent because the minimization of cost functions may significantly vary within different numerical models. Nevertheless, our results show that the computational costs of the En3-DVar method should be relatively low.

4 Summary and concluding remarks

Land surface models are usually highly nonlinear with

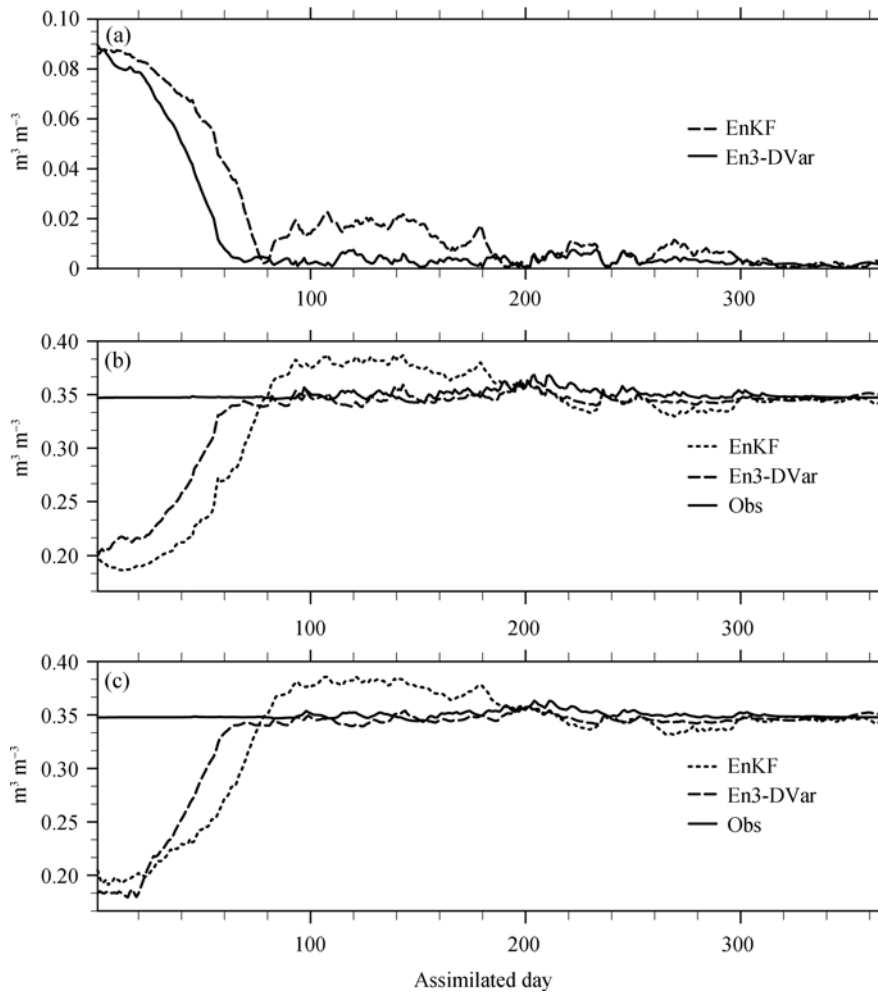


Figure 3 (a) Time series of RMSE ($\text{m}^3 \text{m}^{-3}$) for the En3-DVar and EnKF models of assimilated soil moisture; (b) Time series of the 1st layer observed and assimilated (En3-DVar and EnKF) for volumetric soil moisture ($\text{m}^3 \text{m}^{-3}$); (c) Time series of the 7th layer observed and assimilated (En3-DVar and EnKF) for volumetric soil moisture ($\text{m}^3 \text{m}^{-3}$) with a 12-hour observation frequency.

model physics that contain parameterized discontinuities. These model attributes severely limit the application of advanced variational data assimilation methods in land surface data assimilation. A new En3-DVar method for land data assimilation introduces a Monte Carlo sampling strategy into the typical 3-DVar model framework. A POD technique is used to efficiently approximate a forecast ensemble produced by the Monte Carlo method in 3-D space using a set of base vectors that span the ensemble. The data assimilation process is thus significantly simplified. Several numerical experiments performed with a simple 1-D soil water equation show that the new En3DVar method performed much better than the EnKF method. Assimilation errors using the new En3-DVar method were reduced to a fraction of those observed using the EnKF method. These results show that this updated En3-DVar method provides a promising new tool for land surface data assimilation.

Acknowledgments. We would like to thank two anonymous reviewers for their helpful comments. This work was supported by the National Natural Science Foundation of China (Grant No. 40705035) and the National High Technology Research and Development Program of China (863 Program) (Grant Nos. 2009AA12Z129 and 2007AA12Z144).

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