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Inverse three-dimensional variational data assimilation for an advection-diffusion problem: Impact of diffusion and hybrid application

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[1] In this study, the performance of inverse three-dimensional variational assimilation (I3D-Var) is investigated in terms of dissipation process for an advection-diffusion problem. The performance of I3D-Var becomes poorer with larger diffusion coefficients. However, even for strong dissipation, the cost function during early iterations in the I3D-Var decreases still much faster than it does in the standard four-dimensional variational assimilation (4D-Var). Based on this observation a hybrid approach that combines the I3D-Var and the 4D-Var is suggested to accelerate the performance of 4D-Var. Application of this hybrid method demonstrates that the I3D-Var can serve as a preconditioner for carrying minimization in the full 4D-Var framework. Using the initial conditions obtained through the I3D-Var, the 4D-Var showed much faster convergence in minimizing the cost function. *INDEX TERMS:* 3337 Meteorology and Atmospheric Dynamics: Numerical modeling and data assimilation; 3367 Meteorology and Atmospheric Dynamics: Theoretical modeling; 3332 Meteorology and Atmospheric Dynamics: Mesospheric dynamics. **Citation:** Park, S. K., and E. Kalnay (2004), Inverse three-dimensional variational data assimilation for an advection-diffusion problem: Impact of diffusion and hybrid application, *Geophys. Res. Lett.*, *31*, L04102, doi:10.1029/2003GL018830.

1. Introduction

[2] The four-dimensional variational data assimilation (4D-Var) is considered as a promising tool for fitting model solutions to observations (see a review by *Talagrand* [1997]). In the 4D-Var, a cost function, which is defined as the weighted square distance between model solutions and observations, is minimized via iterative processes.

[3] The 4D-Var requires to run both the adjoint model and the minimization algorithm at each iteration. There exist several minimization algorithms for solving large-scale unconstrained optimization [see *Polak*, 1997], which require the gradient information provided by the adjoint integration. When applied to meteorological 4D-Var problems, these algorithms mostly require several tens of iterations to reach a local minimum of the cost function.

[4] Some considerable efforts have been made for operational implementation of the 4D-Var during the last decade [e.g., *Županski*, 1993; *Courtier et al.*, 1994]. However, due to a large computational cost, implementing the complete 4D-Var scheme into the operational system is practically infeasible without] major simplifications [e.g., *Rabier et al.*, 2000].

[5] Recently, *Kalnay et al.* [2000] developed an efficient variational assimilation scheme called the ''Inverse 3D-Var'' (I3D-Var) based on the *quasi-inverse* model integration. In the I3D-Var, the observational increment at initial time is obtained by a backward integration of the tangent linear model (TLM), in which the sign of time step is changed (i.e., *inverse*). Here, the sign of dissipative term is also changed (i.e., *quasi-inverse*) in order to avoid computational blow-up. They demonstrated that the I3D-Var solves the minimization problem close to the 4D-Var at much less computational cost.

[6] *Wang et al.* [1997] employed the quasi-inverse approach to obtain the Newton descent direction and developed a new optimization method called the adjoint Newton algorithm, which showed faster convergence of the cost function toward its minimum compared to the conventional 4D-Var scheme using the limited-memory BFGS (LBFGS) algorithm [*Liu and Nocedal*, 1989]. More recently, *Leslie et al.* [2000] compared the performance of the full 4D-Var and the I3D-Var for 40 cases of hurricane forecast showing that the I3D-Var is faster than the full 4D-Var by a factor of 8 with comparable accuracy in forecasting hurricane tracks.

[7] In the I3D-Var, solutions are smoothed in both forward and inverse runs [*Kalnay et al.*, 2000]; thus the I3D-Var results are considered to be reasonably correct for processes with small diffusion. However, explicit comparison of the performances by the I3D-Var and the standard 4D-Var in the context of diffusion process has never been made.

[8] In this study, we first investigate the effect of diffusion magnitude on the performance of I3D-Var, especially in comparison with the 4D-Var. Then a hybrid approach, which combines the I3D-Var and the 4D-Var, is applied to complement shortcomings arising from independent application of each method. In this approach, the 4D-Var is preconditioned by the I3D-Var.

[9] For a detailed discussion on theoretical background on the I3D-Var, which is omitted here, readers are referred

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to *Kalnay et al.* [2000]. Section 2 provides a brief description of the nonlinear model and its forward and quasi-inverse TLMs, and the experimental design as well. Section 3 discusses the performance of I3D-Var in terms of diffusion magnitude and the potential of I3D-Var using the hybrid approach. Conclusions are given in section 4.

2. Model Description and Experiment Design

[10] We apply the I3D-Var to a simple advection-diffusion problem including a passive scalar transport. This can be well described by the nonlinear viscous Burgers' equation [*Burgers*, 1948]. Despite of its simplicity, the model based on this equation has been used in many assimilation studies because it can handle a variety of important aspects in data assimilation problems, especially when new assimilation schemes were developed and tested [e.g., *Menard*, 1994; *Uboldi and Kamachi*, 2000; *Xu and Daley*, 2000].

[11] An advection velocity (u) is the basic variable in the Burgers' equation. In this study, an additional equation is also considered to represent the advection of a passive scalar (q). For a detailed description of the governing equations and derivation of corresponding forward and inverse TLMs, readers are referred to *Kalnay et al.* [2000]. Here, the exact-inverse TLM is formulated by changing the sign of time step from the forward TLM (see *Kalnay et al.* [2000, equation 17] for u). In the quasi-inverse TLM, the sign of diffusion term is also changed to avoid numerical instability.

[12] A discrete nonlinear model (NLM) of the viscous Burgers' equation is constructed using the leapfrog scheme for advection and the DuFort-Frankel scheme for diffusion [see *Anderson et al.*, 1984]. It is described for u as:

$$\frac{U_j^{n+1} - U_j^{n-1}}{2\Delta t} = -U_j^n \frac{U_{j+1}^n - U_{j-1}^n}{2\Delta x} + \nu \frac{U_{j+1}^n - U_j^{n+1} - U_j^{n-1} + U_{j-1}^n}{(\Delta x)^2} \quad (1)$$

It should be noted that a numerical scheme which includes implicit dissipative property, such as the Lax scheme, is not feasible for the I3D-Var [*Kalnay et al.*, 2000]. The forward and inverse TLMs and the adjoint model (ADJM) are developed directly from the discrete NLM. Since the Burgers' equation may have a shock jump, time integration is limited to N = 121. Adjoint solution of this system is described by *Mohammadi and Pironneau* [2001].

[13] Model parameters for the control experiment are: the grid size Δx = 1 m; the number of grids NX = 101; the domain length X = 100 m; the time step Δt = 0.1 s; the number of time levels N = 81 or 121; and the diffusion coefficient $\nu = 1 \times 10^{-4}$ m^{2}s^{-1}. The computational domain is set to [$-X/2$, $X/2$]. In large scale atmospheric flows, the diffusion process is almost negligible. Thus the choice of the ν value here is reasonable for describing weakly diffusive flows.

[14] The initial conditions are given by

$$u_0 = u(x,0) = \sin\left(\frac{2\pi x}{L}\right), \qquad q_0 = q(x,0) = -\sin\left(\frac{2\pi x}{L}\right) \quad (2)$$

where L is wavelength of the domain, which is set to the same as the domain length, X, and the boundaries are fixed to zero.

[15] The observational fields (u_{obs}, q_{obs}) are obtained through an NLM simulation with model parameters and initial conditions as specified above (i.e., *simulated* observation). The nonlinear basic fields ($\overline{u}$, $\overline{v}$) are generated from an NLM run with an initial condition in which a systematic error is added to the observational fields (i.e., for a 10% error, $\overline{u}_0 = (1 + 0.1)u_{obs}$ and similarly for q_0).

[16] The cost function (J) for standard 4D-Var is defined as

$$J = \frac{1}{2}\left(\mathbf{x}_0^a - \mathbf{x}_0^b\right)^T B^{-1}\left(\mathbf{x}_0^a - \mathbf{x}_0^b\right) + \sum_{t=1}^{n} \frac{1}{2}\left[H\left(\mathbf{x}_t^b\right) - \mathbf{y}_t^o\right]^T \cdot R^{-1}\left[H\left(\mathbf{x}_t^b\right) - \mathbf{y}_t^o\right], \quad (3)$$

where $\mathbf{x}_0^a$ and $\mathbf{x}_0^b$ are the analysis and first guess, respectively, at the beginning of the interval, $\mathbf{x}_t^b$ is the first guess at time t, and H is the operator which converts the model first guess into first guess observations. B is the background error covariance and R is the observational error covariance. Although the cost function in I3D-Var is defined in terms of increments as by *Kalnay et al.* [2000, equation 7], it is computed for nonlinear solutions based on equation (3) for fair comparison between 4D-Var and I3D-Var. In the identical twin framework, as in this study, the background error term is neglected and then observation becomes a vector of model variables defined on grid points [*Li et al.*, 2000]. In addition, with this framework, the cost function values for 4D-Var and I3D-Var are identical in the condition that observation is available only at the end of the assimilation interval.

[17] For the standard 4D-Var, the ADJM is run backward from the final condition $\partial J/\partial \mathbf{x}_N$, where $\mathbf{x}_N = (u_N, q_N)^T$ stands for the model state at the final time (i.e., at time level N). For the I3D-Var, the quasi-inverse TLM (Q-ILM) is run from the final condition $(\delta u_N, \delta q_N)^T$ where

$$\delta u_N = \overline{u}_N - (u_{obs})_N, \qquad \delta q_N = \overline{q}_N - (q_{obs})_N. \quad (4)$$

The Q-ILM is integrated backward in time by changing the signs of time step and diffusion term.

[18] The observational data being assimilated are generated through the model using the initial conditions given in equation (2). The diffusion coefficients are set to the same in generating both observations and model solutions. For the 4D-Var experiments, we have employed the LBFGS algorithm [*Liu and Nocedal*, 1989] for minimization. Such minimization process is not required in the I3D-Var [*Kalnay et al.*, 2000].

3. Results

[19] The standard 4D-Var can incorporate all observations available during the assimilation interval whereas the I3D-Var can take one observation at the end of the assimilation interval. *Kalnay et al.* [2000] have demonstrated that the I3D-Var with one observation at the end outperforms the 4D-Var with observations at all time steps in both accuracy and computing time. They also discussed computational

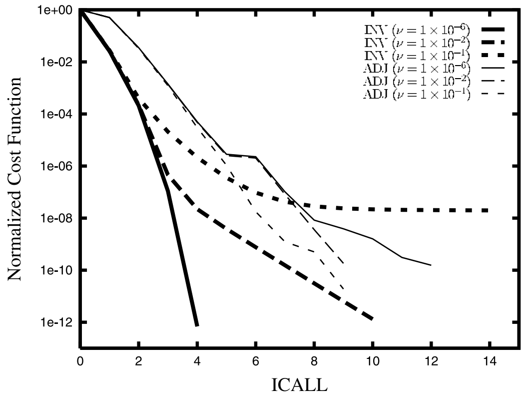

Figure 1. Evolution of normalized cost function in terms of the number of function calls (ICALL) for different diffusion coefficients using the I3D-Var (INV: thick lines) and the adjoint 4D-Var (ADJ: thin lines). The assimilation length is $N = 81$ and a systematic error of 50% is introduced to initial u.

issue in incorporating several observations in assimilation interval while performing I3D-Var. Thus we avoid discussions on these aspects here. Experiments are performed with one observation at the end for both 4D-Var and I3D-Var, unless otherwise mentioned.

3.1. Impact of Diffusion

[20] It is known that the Q-ILM solutions describe the forward TLM well when the magnitude of diffusion is sufficiently small [*Kalnay et al.*, 2000]. Here we investigate the actual impact of diffusion on the performance of I3D-Var for various diffusion magnitudes and compare it with that of 4D-Var.

[21] In Figure 1, evolution of normalized cost functions for variational data assimilation using adjoint and quasi-inverse method is shown for different diffusion coefficients. For the 4D-Var, the gradient norms of cost function showed monotonic decrease (not shown). As diffusion increases the performance of I3D-Var becomes poor – more iterations to reach the minimum of the same cost function. For the given range of diffusion, convergence of cost function in the 4D-Var shows smaller variation than that in the I3D-Var.

[22] It should be noted that such result does not necessarily mean that the 4D-Var performance has no problem with diffusion processes. *Li and Droegemeier* [1993] showed that the 4D-Var performance is sensitive to the magnitude of diffusion coefficients. Our result implies that the performance of 4D-Var is relatively less sensitive than that of I3D-Var to variations of diffusion magnitude. As shown, the performance of I3D-Var becomes poorer with larger diffusion coefficients; thus the I3D-Var should be applied with caution in flows with strong diffusion. However, it is notable that the decrease rate of cost function in the I3D-Var during early iterations is still much higher than that in the 4D-Var even for a strong diffusion case. This leaves a possibility of applying the hybrid method as will be discussed in the next section.

3.2. Hybrid Application: I3D-Var as a Preconditioner of 4D-Var

[23] In this section, we investigate the possibility of combining the I3D-Var and the 4D-Var for the purpose of efficient performance in minimization. Although the I3D-Var may not replace the full adjoint 4D-Var due to problems with diffusion, it may serve as a preconditioner when carrying minimization in the framework of the 4D-Var. That is, the first few iterations can be made through the I3D-Var, then the 4D-Var can start from the initial conditions obtained by the I3D-Var. This is based on the observation that, even in the large diffusion case, the I3D-Var showed sharp decrease in the cost function during early iterations (see Figure 1). To test this idea, a preliminary experiment is performed.

[24] In Figure 2, the case of preconditioning with one iteration of the I3D-Var is compared to the full 4D-Var. In both I3D-Var and 4D-Var, two observations (at $N = 61$ and 121) within an assimilation period of $N = 121$ are incorporated. For doing this, an ensemble I3D-Var strategy is employed as by *Kalnay et al.* [2000]. With preconditioning by the I3D-Var, the 4D-Var showed much better performance in minimizing the cost function. The preconditioned minimization saturates after about 30 iterations while minimization without preconditioning does so after about 100 iterations. This may be related to differences in random errors in observation and systematic errors in initial conditions. It is also notable that the 4D-Var results, both with and without preconditioning, converge at the same minimum. Figure 3 represents evolution of the gradient norms of cost function in the 4D-Var for cases with and without preconditioning, which shows almost monotonic decrease in both cases. Thus the minimizations are performed appropriately.

[25] Noting that the I3D-Var may not be feasible for physical processes that are irreversible, our result shows a possibility of using the I3D-Var as a preconditioner of the 4D-Var that includes full physics. That is, the I3D-Var (with no physics or simplified physics) can be applied before the effect of diffusion and/or microphysical processes become significant, after which the 4D-Var can take over the

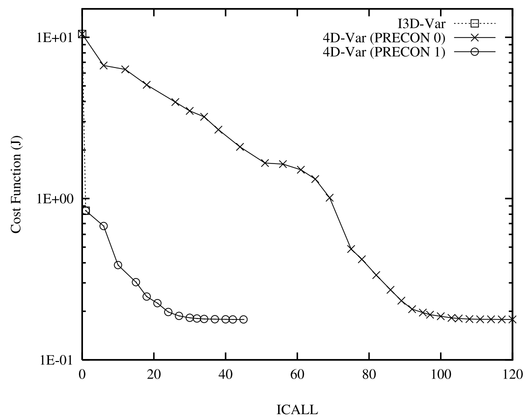

Figure 2. Variations in the cost function from the I3D-Var and the 4D-Var starting from "no preconditioning" (PRECON 0) and from preconditioning using one iteration of the I3D-Var (PRECON 1). The assimilation period is $N = 121$ and the diffusion coefficient is $\nu = 10^{-3}$ m^2s^{-1}. The initial error magnitude is 40% in u and each observation includes random errors with maximum magnitude of 10%. Observations are provided at $N = 61$ and 121.

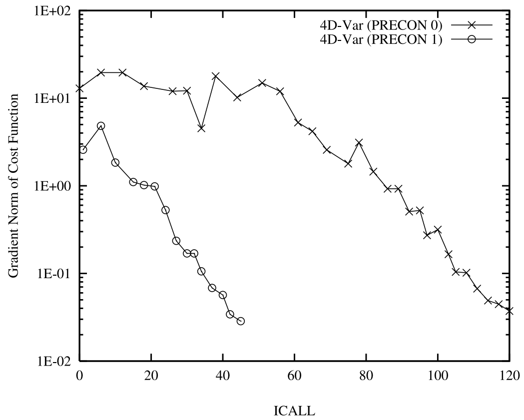

Figure 3. Evolution of the gradient norms of cost function in terms of ICALL for cases of PRECON 0 and PRECON 1 as in Figure 2.

minimization process from the point where the I3D-Var stopped.

[26] The use of I3D-Var may deal efficiently with the part of the spectrum of the Hessian of the cost function related to the dynamics part of the model. This will allow the minimization to focus only on the nonlinearities associated with the physics and result in a large computational saving (I. M. Navon, personal communication, 1999).

[27] This approach is called the *hybrid* assimilation method [see *Park and Županski*, 2003] in the sense that two different algorithms are combined in one minimization problem. *Li et al.* [2000] also employed the hybrid method which involves an iterative procedure involving inner iterations with incremental model [see *Courtier et al.*, 1994], with no physics in the adjoint, and outer iterations with full physics model in several cycles.

[28] It would be more practical to perform data assimilation experiments in a cycled mode, that is, assimilated results from previous assimilation cycle are used in current cycle. We have performed such experiments using three assimilation cycles within an assimilation period of N = 121, that is, each cycle having 40 time steps. However, since the model employed here is very simple and the assimilation and forecast periods are quite short to prevent a shock jump, the 4D-Var/I3D-Var solutions have converged to the minimum very quickly even at the very first cycle. Therefore, it is not feasible to do the cycling experiments with current model system.

4. Conclusions

[29] In this study, the inverse 3D-Var (I3D-Var), which employs the quasi-inverse method, is applied to an advection-diffusion problem. The performance of I3D-Var is compared with that of standard 4D-Var, which is based on the adjoint method, for various magnitudes of dissipation. A hybrid method is also suggested to use the I3D-Var as a preconditioner of the standard 4D-Var for cases with strong diffusion and full physics.

[30] The performance of I3D-Var becomes poor as diffusion increases. For given range of diffusion coefficients, the convergence rate of cost function in the I3D-Var shows much larger variation than that in the 4D-Var, which implies that the I3D-Var performance is very sensitive to the magnitude of diffusion.

[31] Although the I3D-Var may not replace the full 4D-Var, it is demonstrated that it can serve as a preconditioner, using a hybrid approach, for carrying minimization in the 4D-Var framework. Using the initial conditions obtained through the I3D-Var, the 4D-Var showed much faster convergence in minimizing the cost function.

[32] Overall, for this simple advection-diffusion problem, the I3D-Var showed better performance in both convergence rate and accuracy than the standard 4D-Var except for the case with strong diffusion. For strong diffusion cases, we may expect better performance in the I3D-Var by neglecting the diffusion process (i.e., set the diffusion coefficient to zero) in both forward and inverse runs. However, this may result in completely different model solutions especially when diffusion processes are very important. It can be alleviated by neglecting diffusion only in the inverse run. Further studies are needed in applying the I3D-Var to realistic meteorological models which includes physical processes.

[33] It should be also noted that our experiments were performed for the use of observations in all available grid points with disregard to the background term. For more realistic experiments, we may need to consider situations where only a subset of observations are available and thus background term is necessary. We also need to develop methods to include all available intermediate observations within the assimilation period in the I3D-Var. These issues are planned to be investigated in the future study.

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