A New Approach to Data Assimilation*

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ABSTRACT

A significant attempt to design a timesaving and efficient four-dimensional variational data assimilation (4DVar) has been made in this paper, and a new approach to data assimilation, which is noted as 'three-dimensional variational data assimilation of mapped observation (3DVM)' is proposed, based on the new concept of mapped observation and the new idea of backward 4DVar. Like the available 4DVar, 3DVM produces an optimal initial condition (IC) that is consistent with the prediction model due to the inclusion of model constraints and best fits the observations in the assimilation window through the model solution trajectory. Different from the 4DVar, the IC derived from 3DVM is located at the end of the assimilation window rather than at the beginning conventionally. This change greatly reduces the computing cost for the new approach, which is almost the same as that of the three-dimensional variational data assimilation (3DVar). Especially, such a change is able to improve assimilation accuracy because it does not need the tangential linear and adjoint approximations to calculate the gradient of cost function. Therefore, in numerical test, the new approach produces better IC than 4DVar does for 72-h simulation of TY9914 (Dan), by assimilating the three-dimensional fields of temperature and wind retrieved from the Advanced Microwave Sounding Unit-A (AMSU-A) observations. Meanwhile, it takes only 1/7 of the computing cost that the 4DVar requires for the same initialization with the same retrieved data.

Key words: mapped observation, variational data assimilation, timesaving, backward 4DVar

1. Introduction

Variational data assimilation is one of the most efficient methods to initialize a prediction model in the numerical weather prediction (NWP) (Bouttier and Rabier, 1997; Courtier et al., 1994; Daley, 1991; Navon et al., 1992; Wang et al., 2000; Zhang et al., 2002, 2003; Thepaut et al., 1993; Zou et al., 1995; Zou and Xiao, 1999; Zupanski, 1993). The three-dimensional variation (3DVar) and four-dimensional variation (4DVar) are the two typical representatives of this kind of methods, which have been playing more and more important roles in the NWP since the 1980s when the variational principle (Derber, 1989; Le Dimet and Talagrand, 1986; Lewis and Derber, 1985) was introduced in data assimilation. They produce the best estimation of model initial state by incorporating observations into the assimilation window with background in an optimal way. Especially, the 3DVar has become a popular tool of initialization in many prediction centers and research institutions in the world at present, because it is much more timesaving than the 4DVar. In this method, however, there are also some limitations derived from the approximation of unchangeable weather state in the assimilation window $[t_0\text{-}3\ \text{h},\ t_0\text{+}3\ \text{h}]$ and lack of model constraints. This approximation actually treats all observations at different times in the window as the data at the same time t_0, and mostly leads to extra errors to reduce the quality and accuracy of assimilation. On the other hand, lack of model constraints results in inability to ensure the consistence between the prediction model and the initial condition (IC) from the assimilation, and in particular, it can not globally adjust the three-dimensional structure of the IC in the case of sparse observations. Some constraints of simple balance equations can too hardly replace the function of full model constraints, although they may partly act as some dynamical constraints of model. The 4DVar should be the best choice of initialization tool to avoid

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the limitations of 3DVar, because it includes the model constraints for producing an IC consistent with the prediction model and thus replaces the unchangeable weather state by the model weather state for best fitting the observations at different times in the window through model trajectory. Inclusion of the model constraints, however, brings calculation of the cost function gradients tough problem. The adjoint technique gives the best solution to this problem, but the cost of computing gradient is still huge. It may also seriously affect convergence and accuracy of the assimilation due to inexistence of tangential linear approximation when dealing with on-off (or discrete) processes of physical parameterization schemes in the prediction model. Furthermore, establishment of the adjoint model is a tough work and cannot be completed in a short time, and thus greatly reduces the efficiency of implementing the 4DVar. That is why it is not so popular as the 3DVar in the world. The European Center for Medium-range Weather Forecast (ECMWF) is one of a few centers in the world to use the 4DVar to initialize their operational NWPs. Limited by the huge computation of the adjoint model, the ECMWF can only use coarser resolutions in the 4DVar system, whose increments are interpolated to the fine grid of the high-resolution prediction model for producing the optimal IC. Obviously, the huge cost required for running the adjoint model has been the bottleneck slowing down development and application of the 4DVar. How to greatly reduce the huge computational cost of the 4DVar has become a significant issue expected to be resolved urgently.

In this paper, a careful study on this issue was carried out, and a significant attempt to construct the new approach to data assimilation was made, including the suggestion of the concept of the backward 4DVar in Section 2, followed by the proposal of the new approach called 'three-dimensional variational data assimilation of mapped observation (3DVM)' in Section 3, and introduction of the mapping method from real observations to model grid values in Section 4, and finally the numerical tests in Section 5.

2. The concept of backward 4DVar

The 4DVar produces an optimal IC x_a^0 by minimizing the cost function:

$$J(x_a^0) = \min_x J(x). \tag{1}$$

Similar to available theoretical studies on the 4DVar, it might be assumed here as well that all variables at the model degrees of freedom are measured, and thus the cost function is defined as

$$\begin{aligned} J(x) = & \frac{1}{2}(x - x_b^0)^{\mathrm{T}} \boldsymbol{B}_0^{-1}(x - x_b^0) \\ & + \frac{1}{2}\sum_{i=1}^{N}(M_{t_0\to t_i}(x,\tau) - x_i^{\mathrm{obs}})^{\mathrm{T}} \boldsymbol{O}_i^{-1} \\ & \cdot (M_{t_0\to t_i}(x,\tau) - x_i^{\mathrm{obs}}), \end{aligned} \tag{2}$$

where x_b^0 is the background or the first guess at the time t_0, $\boldsymbol{B}_0$ is the covariance matrix of background error at t_0, $x_i^{\mathrm{obs}}(i = 1, 2, \cdots, N)$ is the observation at t_i in the assimilation window $[t_0, t_N]$ ($t_N - t_0 \leqslant 6$ h), $\boldsymbol{O}_i$ is the covariance matrix of observation error of x_i^{obs}, $M_{t_0\to t_i}(x,\tau)$ is a mapping from t_0 to t_i by the model integration starting from the initial state x with the time step τ. As mentioned in Section 1, there were some difficulties in the 4DVar, which slow down development and application of the 4DVar. Therefore, it is necessary to improve the available 4DVar methods or propose new approaches. For this purpose, it is essential to know what causes these difficulties of 4Dvar, then try to find the answer from a careful analysis on the principle of the 4DVar.

From Eqs.(1)-(2), it was clearly known that the optimal IC x_a^0 produced by the 4DVar was located at the time t_0. Compared with the time location of x_a^0, the observations in the window $[t_0, t_N]$ were all located at the future time, except those at t_0. The feedback of the observations to the beginning of the window, however, may have to apply some kind of backward integration of the prediction model. It is the adjoint model that played the role in implementing the backward integration and thereby caused the aforesaid difficulties. Obviously, the 'improper' time location of the optimal IC produced by the 4DVar may be the key factor to lead to its major difficulties. Hence, change of the time location of the optimal IC in the assimilation window may be a good way to find a new approach to overcome the difficulties of 4DVar.

Here, we try to move the optimal IC of 4DVar from the beginning to the end of the assimilation window so that the adjoint model is not needed anymore, because the observations are not at the future time but at the past time of the optimal IC in this case. A new concept called the backward 4DVar was derived from the above attempt that got information from the observations just in an inverse way of 4DVar. For the subsequent reasonable definition of inverse 4DVar, the cost function of the old 4DVar may be expressed in incremental form firstly:

$$J(x') = \frac{1}{2}(x')^{\mathrm{T}}\boldsymbol{B}_0^{-1}x' + \frac{1}{2}\sum_{i=1}^{N}(L_{t_0\to t_i}x' - y_i')^{\mathrm{T}} \cdot \boldsymbol{O}_i^{-1}(L_{t_0\to t_i}x' - y_i'). \tag{3}$$

This expression is directly deduced from Eq.(2) after the tangential linear approximation, where $L_{t_0\to t_i}x'$ is the tangential linear model of the prediction model $M_{t_0\to t_i}(x,\tau)$ and

$$\begin{cases} x' = x - x_b^0 \\ y_i' = x_i^{\mathrm{obs}} - x_i^0, \end{cases} \tag{4}$$

where

$$x_i^0 = M_{t_0\to t_i}(x_b^0,\tau). \tag{5}$$

According to the feature of model integration, it is easy to prove that the tangential linear operator $L_{t_0\to t_i}$ can be formulated as the following:

$$L_{t_0\to t_i} = I + \tau D(M_{t_0\to t_i}(x_b^0,\tau)), \tag{6}$$

where I is the unit operator, $D(M_{t_0\to t_i}(x_b^0,\tau))$ the tangent linear tendency operator with respect to the basic state, independent from the increment x'. Based on the inequality $t_i - t_0 \leqslant t_N - t_0 \leqslant 6$ h, it is true that the term $\tau D(M_{t_0\to t_i}(x_b^0,\tau))$ in Eq.(6) is very small when the time step τ is limited in some range, i.e.,

$$\| \tau D(M_{t_0\to t_i}(x_b^0,\tau)) \| << \| I \| . \tag{7}$$

Clearly, there exists $L^{-1}_{t_0\leftarrow t_i}$, the inverse operator of $L_{t_0\to t_i}$, which can be expressed as:

$$L^{-1}_{t_0\leftarrow t_i} = I - \tau D(M_{t_0\to t_i}(x_b^0,\tau)) + \boldsymbol{O}(\tau^2). \tag{8}$$

Using the inverse operator of $L_{t_0\to t_i}$, we can similarly define the cost function of the backward 4DVar:

$$\tilde{J}(\tilde{x}') = \frac{1}{2}(\tilde{x}')^{\mathrm{T}}\boldsymbol{B}_N^{-1}\tilde{x}' + \frac{1}{2}\sum_{i=1}^{N}(L^{-1}_{t_i\leftarrow t_N}\tilde{x}' - \tilde{y}_i')^{\mathrm{T}} \cdot \boldsymbol{O}_i^{-1}(L^{-1}_{t_i\leftarrow t_N}\tilde{x}' - \tilde{y}_i'), \tag{9}$$

where x_b^N is the background or first guess at t_N, $\boldsymbol{B}_N$ the covariance matrix of background error at t_N, $\tilde{x}'$, and $\tilde{y}'$ may be defined as

$$\begin{cases} \tilde{x}' = x - x_b^N \\ \tilde{y}_i' = x_i^{\mathrm{obs}} - x_i^N, \end{cases} \tag{10}$$

where x_i^N satisfies

$$M_{t_i\to t_N}(x_i^N,\tau) = x_b^N. \tag{11}$$

The introduction of the inverse operator of the tangential linear operator in Eq.(9), however, makes the new cost function more complicated than the old one in Eq.(3) in form. Furthermore, unlike x_i^0 in Eq.(5), x_i^N cannot be explicitly obtained from Eq.(11), or there may even exist no solution or non-unique solution x_i^N in Eq.(11) due to the nonlinearity of the prediction model. This is the most serious problem in the backward 4DVar, which may be the key reason why this scheme has never been considered before. If this problem is removed, the scheme may be a good approach of data assimilation. An attempt to find a solution to the problem is made in the next section.

3. The three-dimensional variational data assimilation of mapped observation (3DVM)

Here, we introduce a new concept: mapped observation, to overcome the difficulty of the backward 4DVar. The mapped observation is a kind of data derived from a transform or mapping of observation. The transform or mapping may be a unit operator, a linear interpolation, a model mapping, a tangential linear model mapping or its inverse mapping, observation operator, or a composite mapping and so on. In this paper, the mapping we will use is the model mapping, and the mapped observations x_i^{mo} are located at t_N, produced by mapping the observations x_i^{obs} at t_i to the end of the window:

$$M_{t_i\to t_N}(x_i^{\mathrm{obs}},\tau) = x_i^{\mathrm{mo}}. \tag{12}$$

The tangential linear approximation is applied into the expression derived from subtracting Eq.(11) from Eq. (12), and the following equation may be obtained:

$$L_{t_i \to t_N}(x_i^{\mathrm{obs}} - x_i^N) = x_i^{\mathrm{mo}} - x_b^N. \tag{13}$$

Setting

$$\tilde{x}_i' = x_i^{\mathrm{mo}} - x_b^N. \tag{14}$$

It is easy to get the solution of Eq.(13):

$$\tilde{y}_i' = L_{t_i \leftarrow t_N}^{-1} \tilde{x}_i', \tag{15}$$

where $\tilde{y}_i'$ is defined in Eq.(10). Substituting it into Eq.(9), a new expression for the cost function of the backward 4DVar is deduced:

$$\tilde{J}(\tilde{x}') = \frac{1}{2}(\tilde{x}')^{\mathrm{T}} \boldsymbol{B}_N^{-1} \tilde{x}' + \frac{1}{2}\sum_{i=1}^{N}(\tilde{x}' - \tilde{x}_i')^{\mathrm{T}} \widetilde{\boldsymbol{O}}_i^{-1} \cdot (\tilde{x}' - \tilde{x}_i'), \tag{16}$$

where

$$\widetilde{\boldsymbol{O}}_i = L_{t_i \to t_N} \boldsymbol{O}_i L_{t_i \to t_N}^{\mathrm{T}}. \tag{17}$$

Equation (16) may also be written into the non-increment form:

$$\tilde{J}(x) = \frac{1}{2}(x - x_b^N)^{\mathrm{T}} \boldsymbol{B}_N^{-1}(x - x_b^N) + \frac{1}{2}\sum_{i=1}^{N}(x - x_i^{\mathrm{mo}})^{\mathrm{T}} \widetilde{\boldsymbol{O}}_i^{-1}(x - x_i^{\mathrm{mo}}). \tag{18}$$

Unlike the cost function of 4DVar Eq.(2), we are surprised to find that the model state variable x was no longer expressed implicitly, but simply and explicitly in the cost function of the backward 4DVar defined by Eq.(18), just as expected. In this way, the approach of backward 4DVar became a 3DVar scheme without any constraints. Especially, the assimilation objects were no longer the real observations other than the mapped observations by the prediction model. Therefore, this approach is named as 'three-dimensional variational data assimilation of mapped observation (3DVM)'. It is not difficult to find that there were two major differences between the 3DVM and 3DVar. Firstly, the assimilation data used in the 3DVM were mapped observations that were all located at the end of the window, while those used in the 3DVar were real observations distributing at different times in the assimilation window. Secondly, the 3DVM had model constraints contributed by the model information contained in mapped observations, and thereby its optimal IC was consistent with the prediction model as well as best fit the observations through the model trajectory, which indicated its same performance as the 4DVar, while the 3DVar included no model information because real observations were completely independent of the prediction model, and thus its optimal IC lacked harmony with the prediction model. As a compensation of this defect of 3DVar, some constraints of simple balance relations were added to its cost function or considered in its covariance matrix of background error, but they were far away from replacing the functions of model constraints.

There were also two significant differences between the 4DVar and 3DVM. The optimal ICs at different time, which were obtained from the same observations, were the marked difference of the two approaches. The 4DVar produced the optimal IC at the beginning of the assimilation window, in contrast to the 3DVM at the end of the window. When these two ICs were used to predict the state of atmosphere at the time $t_p (t_p \gg t_N)$, the cost of the model integration starting from the IC of 3DVM will be t_N-t_0 less than that starting from the IC of 4DVar. It meant that the initialization by 3DVM not only saved model integration time, but also reduced accumulated model error to some extent. The second remarkable difference between the two approaches was their necessary or unnecessary requirement of adjoint technique. The 4DVar must use the adjoint model to calculate the gradient of cost function, which caused its huge computing cost and even led to on-off problem when dealing with discontinuous physical processes, while the 3DVM needed no adjoint technique and greatly saved computing time as its cost was comparable to the 3DVar's. This will be verified in numerical tests which will be described later. The next issue was how to determine the error covariance matrix of mapped observation. There were two ways to do it. The first was to determine the matrix according to Eq.(17). To avoid the use of tangential linear model, the prediction model was applied to replace the tangential linear model in Eq.(17).

According to the definition of observation error covariance, the matrix can be decomposed into the following form:

$$\begin{cases} \boldsymbol{Q}_i = \boldsymbol{E}_i \boldsymbol{E}_i^{\mathrm{T}} \\ \boldsymbol{E}_i = (e_{i,1}, e_{i,2}, \ldots, e_{i,j_0}), \end{cases} \tag{19}$$

where $e_{i,j}$ is the jth error anomaly sample and j_0 the total number of sample. Using the above formulae, Eq.(17) may be expressed as:

$$\widetilde{\boldsymbol{Q}}_i = \widetilde{\boldsymbol{E}}_i \widetilde{\boldsymbol{E}}_i^{\mathrm{T}}, \tag{20}$$

where

$$\begin{aligned} \widetilde{\boldsymbol{E}}_i &= (L_{t_i \to t_N} e_{i,1}, L_{t_i \to t_N} e_{i,2}, \ldots, L_{t_i \to t_N} e_{i,j_0}) \\ &= [M_{t_i \to t_N}(x_i^{\mathrm{obs}} + e_{i,1}) - x_i^{\mathrm{mo}}, \\ &\quad M_{t_i \to t_N}(x_i^{\mathrm{obs}} + e_{i,2}) - x_i^{\mathrm{mo}}, \ldots, \\ &\quad M_{t_i \to t_N}(x_i^{\mathrm{obs}} + e_{i,j_0}) - x_i^{\mathrm{mo}}]. \end{aligned} \tag{21}$$

If there were a great deal of samples, the computing cost to produce the error covariance matrix of mapped observation according to Eqs.(20)-(21) would be much large, thus this method was not viable and not recommended in this paper. Here, the second method was suggested to calculate the matrix $\widetilde{\boldsymbol{O}}_i$ by directly estimating the observation error of x_i^{mo} using the statistical method similar to that for the estimation of the observation error of x_i^{obs}. The advantage of this method was consideration of influence of the model errors in $\widetilde{\boldsymbol{O}}_i$, which may lead to better assimilation effect than the 4Dvar, while not increase the extra computing cost, comparing with that for calculation of the matrix $\boldsymbol{O}_i$.

4. Mapping from real observations to model grid values

The new assimilation approach was theoretically studied in Sections 2 and 3 under the assumption that all variables at the model degrees of freedom were measured. Once it was applied to initializations for real operational predictions and numerical modeling, however, the above assumption was not true in general. Usually, there were different kinds of observations with various and irregular distributions in space and time, some were sparse, some dense. How to assimilate these real observations using the 3DVM became the key point to evaluate viability of the new approach. According to the basic principle of the 3DVM, the first thing that has to be done was to map these irregularly distributed observations into the regular model grid.

In stead of the ideal observations x_i^{obs} in the aforesaid discussion, N real observations y_i^{obs} were irregularly distributed in the assimilation window $[t_0, t_N]$, with respect to the model state variables by an observation operator H_i. If there existed a model state variable x_i^H, satisfying the following equation:

$$H_i(x_i^H) = y_i^{\mathrm{obs}}. \tag{22}$$

then x_i^H may be called a mapping of the observation y_i^{obs} into the model grid. Generally, the solution to Eq.(22) is an undetermined problem because the dimension of the observation is much smaller than that of the model degrees of freedom. Here, the 3DVar without any constraints was applied to get the optimal solution x_i^H of Eq.(22) using the first guess or background field x_b^i:

$$\begin{cases} J_{\mathrm{3DV}}(x_i^H) = \min\limits_x J_{\mathrm{3DV}}(x) \\ J_{\mathrm{3DV}}(x) = \dfrac{1}{2}(x - x_b^i)^{\mathrm{T}} \boldsymbol{B}_i^{-1}(x - x_b^i) \\ \qquad + \dfrac{1}{2}[H_i(x) - y_i^{\mathrm{obs}}]^{\mathrm{T}} \boldsymbol{O}_i^{-1} \\ \qquad \cdot [H_i(x) - y_i^{\mathrm{obs}}]. \end{cases} \tag{23}$$

In order to keep the consistency between the first guesses or the background fields at different times in the assimilation window, an available analysis x_a^0 at the beginning of the window was chosen to be the first guess x_b^0 at this time, and then the other first guesses x_b^i and x_b^N were produced from the model predictions starting from the beginning of the window and using x_a^0 as the IC. This method may meet the requirement of the 3DVM, of which analysis or optimal IC was at the end of the window. We used the following formulae to describe the production of the consistent first guesses:

$$\begin{cases} x_b^0 = x_a^0 \\ x_b^i = M_{t_0 \to t_i}(x_a^0, \tau) \\ x_b^N = M_{t_0 \to t_N}(x_a^0, \tau). \end{cases} \tag{24}$$

After mapping the observations into the model gird, another important thing is to supply the lacked information at some model grid points, because weak or non-observation information may be obtained from the mapping at these grid points due to the sparseness of observations.

The lack of observation information at some model grid points meant the values of increment $x'_{\rm obs} = x_i^H - x_b^i$ obtained from Eq.(23) at these points were zero. The method to supply the values at data-void grid points was simply to make 20- to 50-step forward integration by the prediction model with the IC x_i^H. At each step, the values of the predicted model state variables were replaced by the values of x_i^H at the model grid points where the values of $x'_{\rm obs}$ were not zero. In this way, the observation information was reflected to those model grid points without observation information through the dynamical and physical constraints of the prediction model. After the above process, all variables at the model degrees of freedom at t_i were 'measured', and a complete 'observation' $x_i^{\rm obs}$ was obtained, which satisfied the assumption of the 3DVM. Therefore, we can finally produce an optimal IC by the 3DVM.

5. Numerical tests and discussion

In order to test the viability of the 3DVM, three numerical experiments were designed for 72-h predictions of track and intensity of the TY9914 (Dan). The experiments had different ICs and aimed at comparison of the performances and computing costs between the 3DVM and the 4DVar. The first was the control experiment, noted as 'CTRL', which directly used the background field from NCEP/NCAR reanalysis as the IC. The second was the experiment of which the IC was produced by the 3DVM assimilation. The third was the experiment initialized by the 4DVar assimilation. The observations used in the two assimilation experiments were three-dimensional fields of temperature and wind retrieved from the Advanced Microwave Sounding Unit-A (AMSU-A). The MM5 was used as the prediction model in the three experiments, and the adjoint model of the MM5 was applied into the 4DVar assimilation experiment. Because the observation data were available only at one time point, they are extended from one time to 11 time points equally distributed in the window $[t_0 - 10m, t_0]$ with the same values, as in the paper (Zhang et al., 2003). To fairly compare the two assimilation experiments, same extension was made for the 4DVar assimilation experiment in the time window $[t_0, t_0 + 10m]$.

Figure 1 shows the typhoon tracks from the three experiments and observation of the TY9914 (Dan). Obviously, the simulated typhoon tracks by both the 3DVM and the 4DVar experiments were improved comparing with the results of CTRL. In particular, the track produced from the experiment with the 3DVM was the closest to the observation. It was also found

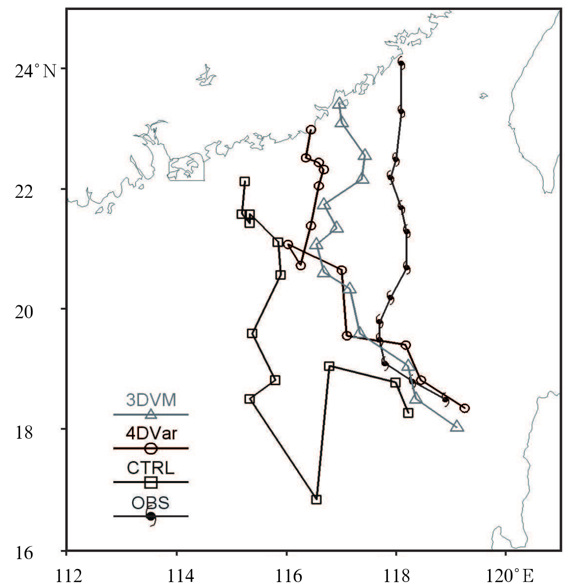

Fig.1. 72-h (00UTC 6-00UTC 9 October 1999) prediction of track of the typhoon Dan (the time interval is 6 h).

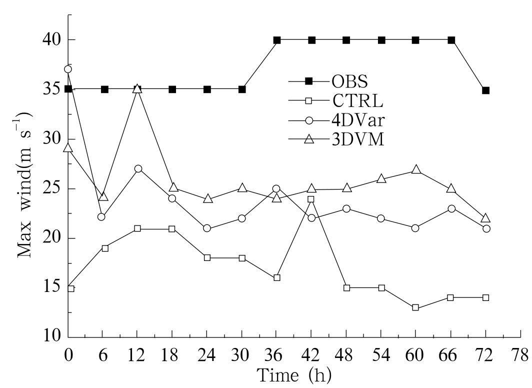

Fig.2. 72-h prediction of intensity of the typhoon Dan (unit: m s^{-1}; time interval: 6 h).

Table 1. Comparison of computing costs between the 3DVM and the 4DVar

Items to evaluate computational cost	Assimilation schemes	
	3DVM	4DVar
Time step for forward or adjoint integration (in minute)	1	1
Length of assimilation window (in minute)	10	10
Number of iteration for assimilation	1	34
Number of steps for forward integration by prediction model	30+10=40	10×34=340
Number of steps for inverse integration by adjoint model	0	10×34=340
Number of interpolations from observation location to model grid	35	10×34=340
Number of adjoint interpolations from model grid to observation location	35	10×34=340
CPU time on a single processor (in minute)	44	325

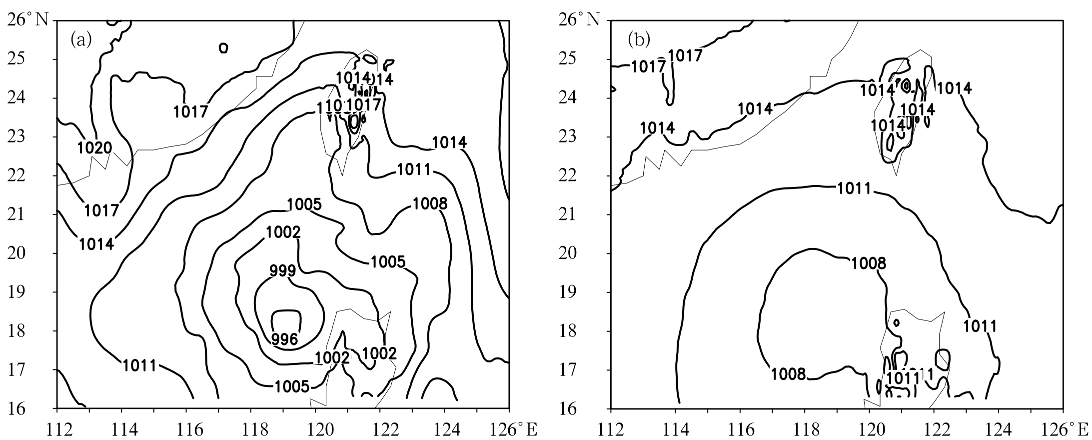

Fig.3. Horizontal distribution of sea level pressure at initial time (contour interval: 5 hPa). (a) 3DVM, (b) 4DVar.

in Fig.2 that both the 3DVM and 4DVar experiments produced evolutions of intensity better than the CTRL did, and the experiment with the 3DVM produced the best simulation of typhoon intensity. The better performance of the 3DVM in modeling typhoon track and intensity than that of the 4DVar may be benefited from its stronger potential in simulation of vortex structure, because the 3DVM experiment produced a lower central pressure and a clearer vortex structure in the field of sea-level pressure than the 4DVar experiment did (see Fig.3).

Meanwhile, the 3DVM approach required much less computing cost than 4DVar did. The CPU time of the 3DVM was only about 1/7 of that of 4DVar. Please refer to Table 1 for details about the costs of both the assimilation approaches.

The much timesaving property and very good performance of the 3DVM in the numerical modeling of the typhoon Dan indicated its great potential in future operational NWP and research work.

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