

# A 4DVar-based Ensemble Four-Dimensional Variational (En4DVar) Hybrid Data Assimilation System for Global NWP: System Description and Primary Tests

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## Abstract

This study developed an ensemble four-dimensional variational (En4DVar) hybrid data assimilation (DA) system. Different from most of the available En4DVar systems that adopted ensemble Kalman Filter class or ensemble DA approaches to produce ensemble covariances for their hybrid background error covariances (BECs), it used a four-dimensional ensemble-variational (4DVar) system to obtain the ensemble covariance. The localization scheme for 4DVar applied orthogonal functions to decompose the correlation matrix so that it was implemented easily and rapidly. In terms of analysis quality and forecast skill, the En4DVar system was evaluated in the single-point observation experiments and observing system simulation experiments (OSSEs) with sounding and cloud-derived wind observations, using its standalone four-dimensional variational (4DVar) and 4DVar components as references. The single-point observation experiments visually verified the explicit flow-dependent characteristic of the BEC due to the introduction of the ensemble covariance from the 4DVar system. The OSSE-based sensitivity experiments revealed different contributions of the weight for the ensemble covariance in the En4DVar system to the forecasts in the Northern and Southern Extratropics and Tropics. A much higher weight for the ensemble covariance in a properly inflated hybrid covariance helped En4DVar produce the most reasonable analysis. The forecast initialized by En4DVar is overall better than by 4DVar and 4DVar, although the quality of En4DVar analysis is between those of 4DVar and 4DVar ensemble mean analyses. It indicates that the flow-dependent ensemble covariance provided by 4DVar dominantly contributes to the improvements in the En4DVar-initialized forecast, with certain but necessary constraint from the balanced climatological covariance.



# **A 4DVar-based Ensemble Four-Dimensional Variational (En4DVar) Hybrid Data Assimilation System for Global NWP: System Description and Primary Tests**

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## **Key Points:**

- An En4DVar data assimilation system with a hybrid background error covariance was developed for global numerical weather predictions
- The hybrid covariance is realized by linearly combining the climatological covariance of 4DVar and the ensemble covariance of 4DVar
- The En4DVar-initialized forecast is improved relative to 4DVar- and 4DVar-initialized forecasts



## Abstract

This study developed an ensemble four-dimensional variational (En4DVar) hybrid data assimilation (DA) system. Different from most of the available En4DVar systems that adopted ensemble Kalman Filter class or ensemble DA approaches to produce ensemble covariances for their hybrid background error covariances (BECs), it used a four-dimensional ensemble-variational (4DEnVar) system to obtain the ensemble covariance. The localization scheme for 4DEnVar applied orthogonal functions to decompose the correlation matrix so that it was implemented easily and rapidly. In terms of analysis quality and forecast skill, the En4DVar system was evaluated in the single-point observation experiments and observing system simulation experiments (OSSEs) with sounding and cloud-derived wind observations, using its standalone four-dimensional variational (4DVar) and 4DEnVar components as references. The single-point observation experiments visually verified the explicit flow-dependent characteristic of the BEC due to the introduction of the ensemble covariance from the 4DEnVar system. The OSSE-based sensitivity experiments revealed different contributions of the weight for the ensemble covariance in the En4DVar system to the forecasts in the Northern and Southern Extratropics and Tropics. A much higher weight for the ensemble covariance in a properly inflated hybrid covariance helped En4DVar produce the most reasonable analysis. The forecast initialized by En4DVar is overall better than by 4DVar and 4DEnVar, although the quality of En4DVar analysis is between those of 4DVar and 4DEnVar ensemble mean analyses. It indicates that the flow-dependent ensemble covariance provided by 4DEnVar dominantly contributes to the improvements in the En4DVar-initialized forecast, with certain but necessary constraint from the balanced climatological covariance.

## Plain Language Summary

The balance constraint and flow dependence characteristic of the background error covariance (BEC) are two key factors to affect the analysis quality of a data assimilation (DA) system. The balanced BEC used in the four-dimensional variational (4DVar) DA approach has no explicit flow dependence, while the flow-dependent BEC estimated by an ensemble-based DA method rarely keeps balanced. The hybrid of the 4DVar approach and an ensemble class DA method can achieve these two important characteristics of BEC. In this study, a hybrid DA system



called ensemble 4DVar (En4DVar) system was developed. It has two unique features. First, it used a four-dimensional ensemble-variational (4DEnVar) system to dynamically provide the ensemble covariance, which differs from most of the available En4DVar systems that estimate their dynamic covariances with the ensemble Kalman Filter class approaches or ensemble of 4DVars method. Second, the ensemble covariance was localized in the sample space using a limited number of leading eigenvectors of the correlation function. In the single-point observation experiments and observing system simulation experiments, the new En4DVar system exhibited obvious flow-dependent characteristic and higher forecast skill than both the 4DVar and 4DEnVar systems although its analysis error is between those of the latter two.



## 1 Introduction

Data assimilation (DA) can provide the optimal analysis of the atmospheric state for the numerical weather prediction (NWP) model combining the background forecasts and observations. The quality of the analysis relies on proper estimates of the background and observation error covariances. In recent decades, several advanced research centers have adopted the four-dimensional variational (4DVar) DA approach for the global NWP model (Rabier et al., 2000; Gauthier & Thépaut, 2001; Kadowaki, 2005; Rawlins et al., 2007; Gauthier et al., 2007; Zhang et al., 2019). 4DVar can include the constraints of both the dynamics and physics to the analysis (Rabier et al., 2000; Wang et al., 2010a), but its background error covariance (BEC) is a highly parameterized model based on the homogeneous and isotropic assumptions (Walsak and Cullen, 2014). Although the flow dependence of the BEC is implicitly realized within the assimilation window by the tangent linear model (TLM) and the adjoint model (ADM), this information cannot be developed into the next assimilation window (Lorenc, 2003). Therefore, the static climatological covariance model used by 4DVar is difficult to match with the time-variant atmospheric state (Buehner et al., 2010a). In parallel with the development of the variational approach, the ensemble Kalman filter (EnKF) approach, which estimates the BEC using ensemble forecasts, has also been noted for its timesaving and the ability to provide the explicit flow-dependent BEC spanning the assimilation windows (Evensen, 1994). This approach has been applied to many models (Whitaker et al., 2008, 2009; Buehner et al., 2010a, 2010b), but the sampling error and the underestimation of the BEC during the assimilation cycle limit its performance.

To overcome the limitation of using static covariance model in 4DVar, attempts have been made to incorporate the flow-dependent information extracted from the ensemble forecasts into the standard variational framework. This is typically realized by linearly combining the climatological covariance and the ensemble covariance (Hamill & Snyder, 2000), or using the control variables preconditioned by the square root of the ensemble covariance to extend the variational control variables (Lorenc, 2003), or using ensemble information to estimate the parameters of the covariance model (Bonavita et al., 2012). Upon these advances, the hybrid DA system including ensemble information is gradually replacing the standard 4DVar system (Raynaud et al., 2011; Bonavita et al., 2012; Clayton et al., 2013; Lorenc et al., 2015; Wang et al., 2013; Kleist & Ide, 2015a, 2015b). The European Centre for Medium-range Weather Forecasts



(ECMWF) and Météo-France used the ensemble of 4DVars to provide the dynamic BECs for the hybrid DA system and achieve higher forecast skills (Bonavita et al., 2012; Raynaud et al., 2011). The Met Office combined the climatological covariance and the ensemble covariance obtained by the ensemble transformed Kalman filter (ETKF) method to construct hybrid DA system (Clayton et al., 2013). The use of the TLM and ADM is retained in the aforementioned hybrid DA systems, which is referred to as the En4DVar method. Another method called 4DEnVar, which avoids the use of the ADM, has also been implemented in some prediction centers. The National Centers for Environmental Prediction (NCEP), and the Met Office utilized the ensemble covariance obtained from the ensemble Kalman filter (EnKF) class methods, namely the ensemble square root filter (EnSRF) method, and the ensemble transform Kalman Filter (ETKF) method to construct the hybrid 4DEnVar system, respectively (Kleist & Ide, 2015b; Bowler et al., 2017a).

Recently, there have been interests in using the 4DEnVar system to estimate the ensemble covariance for hybrid DA systems. The Met Office verified that the hybrid DA system can be benefited from using the En-4DEnVar system instead of using the ETKF system (Bowler et al., 2017a). Some 4DEnVar methods that can reduce the dimension of the optimization problem from the model space to a subspace composed by a set of basis vectors and can avoid the ADM have been proposed (Qiu et al., 2007; Tian et al., 2008; Wang et al., 2010a). The dimension-reduced projection 4DVar (DRP-4DVar) method is one of the representative 4DEnVar methods. In contrast to the extensive and successful applications of the DRP-4DVar method in regional meso-scale weather forecasts (Wang et al., 2010a; Zhao & Wang, 2010; Liu & Wang, 2011; Zhao et al., 2012) and global decadal climate predictions (He et al., 2017, 2020a, 2020b; Li et al., 2021a, 2021b; Shi et al., 2021a, 2021b), its applications in global medium-range weather forecasts are very lacking except an early primary tests on it based on a three-dimensional variational (3DVar) DA system (Shen et al., 2015) and a very recent effort under a 4DVar framework (Zhu et al., 2022).

Using the original ensemble covariance directly may result in sampling error and rank deficiency problems, and localization techniques can alleviate these problem (Hamill et al., 2001). The localization of the ensemble covariance in hybrid DA systems is usually implemented upon unbalanced variables in model space using the transformations copied from the variational system (Clayton et al., 2013; Lorenc, 2015). In addition to this implementation of localization (e.g., spectral filtering transformation), ensemble-sample-based subspace localization approaches using



orthogonal functions to decompose the correlation function were developed (Liu et al., 2009; Buehner et al., 2010a, 2010b; Bishop et al., 2011; Kuhl et al., 2013; Wang et al., 2010b, 2018).

This study focuses on developing an En4DVar hybrid DA system for the global NWP model. It has two unusual aspects compared with other hybrid DA systems. On one hand, a 4DEnVar system based on the DRP-4DVar method, which uses the statistical relationship between the model space and the observation space to avoid the use of ADM, was utilized to estimate the ensemble covariance for the En4DVar system. On the other hand, a limited number of leading eigenvectors of the correlation function was employed to localize the ensemble covariance instead of localization transformations from the climatological covariance model.

The purpose of this study is to provide a mathematical derivation and system introduction to the En4DVar hybrid DA system. The performance of this system was also evaluated with single-point observation experiments and observing system simulation experiments (OSSEs), using its standalone 4DVar and 4DEnVar components with identical settings as references. The theoretical basis of the En4DVar system is presented in Section 2. The designs of the system and experiments are introduced in Section 3. The results are analyzed in Section 4. Finally, the conclusions and discussions are given in the last section.

## 2 Methodology

### 2.1 Climatological covariance

The global 4DVar system (Zhang et al., 2019) used in this study minimizes the following incremental formulation (Courtier, 2004) defined within the DA window  $[t_0, t_n]$  by introducing  $\delta x = x - x^g$ , and obtained the optimal analysis increment at the initial time  $t_0$ :

$$J[\delta x(t_0)] = \frac{1}{2} \{ \delta x(t_0) - [x^b(t_0) - x^g(t_0)] \}^T B_0^{-1} \{ \delta x(t_0) - [x^b(t_0) - x^g(t_0)] \} + \frac{1}{2} \sum_{i=0}^n [\mathbf{H}_i \delta x(t_i) - d_i]^T R_i^{-1} [\mathbf{H}_i \delta x(t_i) - d_i]. \quad (1)$$

Here,  $x$  and  $\delta x$  represent the state vector and its increment, respectively;  $x^b$  and  $x^g$  denote the state vectors of background and first guess, separately;  $B$  and  $R$  are severally the BEC matrix (B-matrix) and observation error covariance matrix, respectively;  $d_i = y_i^o - H_i[x^g(t_i)]$  and  $y_i^o$  represent the observation innovation and observation itself at time  $t_i$ , separately;  $H_i$  and  $\mathbf{H}_i$  are the nonlinear observation operator and its tangent linear operator at time  $t_i$ ,



correspondingly;  $M_i$  and  $\mathbf{M}_i$  mean the nonlinear forecast model and its tangent linear model that integrate from the analysis time to time  $t_i$ , severally; and  $\delta x(t_i) = \mathbf{M}_i \delta x(t_0)$  it indicates the forecast state vector at time  $t_i$  initialized from the increment state.

Introducing the preconditioning transformation  $\delta x = Uv$ , the condition number of the Hessian matrix of Eq. (1) can be improved. Thus, the background term of Eq. (1) can be simplified as  $\frac{1}{2} [v(t_0)]^T [v(t_0)]$ . Here,  $U$  is the square root of the climatological B-matrix  $B$ , and  $v$  is the preconditioned state variable vector.

The BEC utilized in the standard 4DVar system is a highly parameterized model:

$$B_c = UU^T. \quad (2)$$

$U$  includes multiple transformation processes:

$$U = U_p s^u U_h U_v. \quad (3)$$

Here,  $U_h$  and  $U_v$  represent the horizontal and vertical transformations of the background error correlation transformation matrix, respectively.  $s^u$  denotes the diagonal matrix consisting of the background root mean square error of the approximately uncorrelated variables (e.g., stream function, unbalanced velocity potential, unbalanced non-dimensional pressure and specific humidity), which is usually obtained by the National Meteorological Center (NMC) method and zonally averaging.  $U_p$  is the physical transformation operator that converts the approximately uncorrelated variables into the model variables (Zhang et al., 2019).

Although the standard 4DVar system realizes the implicit flow-dependent characteristic of the BEC within the assimilation window using the TLM and ADM, this characteristic cannot carry over to the next assimilation window. Thus, the abovementioned climatological covariance model can only simply describes the mean state of BEC, but cannot represent the evolution of BEC with the weather state in detail.

## 2.2 Ensemble covariance

Unlike the static climatological covariance, the ensemble covariance can realize the explicit flow-dependence of the BEC using the ensemble forecasts initialized from different initial conditions (ICs).



The ICs to initialize the ensemble forecasts are provided by the 4DEnVar system (Zhu et al., 2022). This system was developed using the DRP-4DVar method that solves the optimization problem on the subspace composed of a limited number of ensemble samples (Wang et al., 2010a). The 4DEnVar system uses a set of IC perturbation samples in model space  $\delta X = [\delta x_1, \delta x_2, \dots, \delta x_K]$  ( $K$  is the ensemble size), and the corresponding observational perturbation samples  $\delta Y = [\delta y_1, \delta y_2, \dots, \delta y_K]$  calculated by  $\delta X$  to define the projection matrices:

$$\begin{cases} p_x = \frac{1}{\sqrt{K-1}} [\delta x_1 - \overline{\delta x}, \delta x_2 - \overline{\delta x}, \dots, \delta x_K - \overline{\delta x}] \\ p_y = \frac{1}{\sqrt{K-1}} [\delta y_1 - \overline{\delta y}, \delta y_2 - \overline{\delta y}, \dots, \delta y_K - \overline{\delta y}] \end{cases} \quad (4)$$

Here,  $\overline{\delta x}$  and  $\overline{\delta y}$  are the ensemble means of the IC perturbation samples in model space and observational perturbation samples in observation space, respectively.  $\delta y_k$  is calculated using the TLM and tangent linear observation operators.  $\delta x$  and  $\mathbf{H}_i \delta x(t_i)$  can be projected onto the subspace composed of the aforementioned projection matrices as the following:

$$\begin{cases} \delta x = p_x \alpha \\ \mathbf{H}_i \delta x(t_i) = p_y(t_i) \alpha \end{cases} \quad (5)$$

where  $\alpha = \alpha(t_0) = (\alpha_1(t_0), \alpha_2(t_0), \dots, \alpha_N(t_0))^T$  is the vector composed of the linear combination coefficients.

Substituting Eq. (5) into Eq. (1), a new cost function defined in the subspace is obtained:

$$J[\alpha] = \frac{1}{2} [\alpha]^T [\alpha] + \frac{1}{2} \sum_{i=0}^n [p_y(t_i) \alpha - d_i]^T R_i^{-1} [p_y(t_i) \alpha - d_i]. \quad (6)$$

The optimal analysis can be obtained by minimizing Eq. (6) and using the first transformation in Eq. (5).

The ensemble covariance can be estimated using the ensemble forecasts initialized from the previous ensemble analyses produced by the 4DEnVar system:

$$B_e = p_x p_x^T. \quad (7)$$

The limited ensemble size, which is much smaller than the dimension of the model space may easily result in the spurious correlation and rank deficiency problems in the BEC. Thus, a localization technique should be conducted upon the ensemble covariance (Hamill et al., 2001).



195 The localized ensemble BEC can be implemented as the Schür product between the ensemble BEC  
 196 and the localization correlation matrix  $C$ :

$$B_e = (p_x p_x^T) \circ C, \quad (8)$$

197 where  $\circ$  represents the Schür (element-by-element) product of two matrices with the same  
 198 dimension. The localization correlation matrix  $C$  is designed to reduce the spurious correlation in  
 199 the ensemble covariance and as a result to increase the rank of BEC.

200 In implementation, the zonal (meridional) correlation model is defined adopting the GC  
 201 correlation function (Gaspari & Cohn, 1999) with respect to the dimensionless distance  $r$  in zonal  
 202 (meridional) direction:

$$C(r) = \begin{cases} -\frac{1}{4}r^5 + \frac{1}{2}r^4 + \frac{5}{8}r^3 - \frac{5}{3}r^2 + 1, & 0 \leq r \leq 1 \\ \frac{1}{12}r^5 - \frac{1}{2}r^4 + \frac{5}{8}r^3 + \frac{5}{3}r^2 - 5r + 4 - \frac{2}{3}r^{-1}, & 1 < r \leq 2 \\ 0, & 2 < r \end{cases} \quad (9)$$

203 and the vertical correlation model is defined using the following correlation function with respect  
 204 to the non-dimensional logarithmic pressure distance  $r$ :

$$C(r) = \frac{1}{1.0 + K_p r^2}. \quad (10)$$

205 Due to using the localized ensemble covariance in Eq. (8) directly may lead to lots of  
 206 computational costs, the localization correlation matrix  $C$  is usually decomposed into  
 207 transformations that can be copied from the variational system (Clayton et al., 2013; Lorenc, 2015).  
 208 The localization of the ensemble covariance may lead to the reduction of sampling errors through  
 209 producing extended ensemble samples based on the Schür products between the ensemble  
 210 forecasts with small ensemble size and a number of leading eigenvectors of  $C$ , without a lot of  
 211 extra complex modeling. Therefore, the localization can be implemented in an extended-ensemble-  
 212 sample-based subspace. Through approximately decomposing the correlation matrix into a number  
 213 of leading eigenvectors and ignoring their time-variation, the extended IC perturbation samples in  
 214 model space and the corresponding observational perturbation samples are obtained:

$$\begin{cases} Ep_x = [(p_{x,1} \circ \rho_{x,1}, \dots, p_{x,1} \circ \rho_{x,L}), \dots, (p_{x,N} \circ \rho_{x,1}, \dots, p_{x,N} \circ \rho_{x,L})] \\ Ep_y = [(p_{y,1} \circ \rho_{y,1}, \dots, p_{y,1} \circ \rho_{y,L}), \dots, (p_{y,N} \circ \rho_{y,1}, \dots, p_{y,N} \circ \rho_{y,L})] \end{cases} \quad (11)$$



where  $\boldsymbol{\rho}_{x,j}$  and  $\boldsymbol{\rho}_{y,j}$  ( $j = 1, 2, \dots, L$ ) are the selected leading eigenvectors in model and observation spaces according to the cumulative contribution of variance, respectively. The leading eigenvectors can be further decomposed into zonal, meridional and vertical components.

The leading eigenvectors are obtained using the empirical orthogonal function (EOF) in the zonal and vertical directions, and the sine function in the meridional direction:

$$\begin{cases} \boldsymbol{\rho}_{x,j} = \mathbf{E}_{x,j}(\lambda_{x,j})^{1/2} \\ \boldsymbol{\rho}_{y,j} = \mathbf{E}_{y,j}(\lambda_{y,j})^{1/2} \end{cases} \quad (12)$$

Here,  $\mathbf{E}_{x,j}$  and  $\mathbf{E}_{y,j}$  are the eigenvectors of the correlation functions in the model space and observation space, and  $\lambda_{x,j}$  and  $\lambda_{y,j}$  are the corresponding eigenvalues, respectively.

Redefining an  $K \times L$ -dimensional vector  $\boldsymbol{\beta} = \boldsymbol{\beta}(t_0)$  that consists of the combination coefficients of the extended ensemble samples, a newer cost function is defined in the extended subspace composed of the extended ensemble samples:

$$J[\boldsymbol{\beta}] = \frac{1}{2} [\boldsymbol{\beta}]^T [\boldsymbol{\beta}] + \frac{1}{2} \sum_{i=0}^n [Ep_y(t_i)\boldsymbol{\beta} - d_i]^T R_i^{-1} [Ep_y(t_i)\boldsymbol{\beta} - d_i]. \quad (13)$$

The optimal analysis can be obtained by minimizing Eq. (13) and using the transformation  $\delta\mathbf{x} = Ep_x\boldsymbol{\beta}$ . Moreover, the localized ensemble BEC can be expressed as:

$$B_e = Ep_x Ep_x^T. \quad (14)$$

### 2.3 Hybrid covariance

The hybrid covariance can be obtained by a linear combination of the climatological covariance and the ensemble covariance:

$$B = \gamma_c B_c + \gamma_e B_e. \quad (15)$$

Here,  $\gamma_c$  and  $\gamma_e$  denote the scalar weights of the climatological and ensemble covariances, respectively. Both the climatological and ensemble covariances of the En4DVar system have a time-variant feature inside the assimilation window, but the way to achieve the time-variant feature is different. The climatological (ensemble) covariance realizes the implicit flow dependence through the TLM and ADM (the statistical relationship between the model space and the observation space). However, they greatly differ in the inclusion of balance constraint and characteristic of explicit flow dependence spanning the assimilation windows. The climatological



covariance includes the balance constraint but fails to store and use its implicit evolution information for the next assimilation window, while the ensemble covariance explicitly evolves with state from one window to the next but includes little balance constraint. Therefore, a hybrid of these covariances may be an efficient way to keep the balance and characteristic of explicit flow dependence in the BEC.

To achieve a hybrid BEC, we use the extended control variable approach (Lorenc, 2003), which is mathematically equivalent to directly combining the covariances linearly (Wang et al., 2007). The climatological and ensemble contributions to the increment  $\delta x$  are multiplied by  $\sqrt{\gamma_c}$  and  $\sqrt{\gamma_e}$ , respectively:

$$\delta x = \sqrt{\gamma_c} \delta x_c + \sqrt{\gamma_e} \delta x_e, \quad (16)$$

where  $\delta x_c = Uv$ ,  $\delta x_e = Ep_x\beta$ .

Then, the new cost function can be obtained:

$$J[v(t_0), \beta(t_0)] = \frac{1}{2} [v(t_0)]^T [v(t_0)] + \frac{1}{2} [\beta(t_0)]^T [\beta(t_0)] + \frac{1}{2} \sum_{i=0}^n [\mathbf{H}_i \mathbf{M}_i \delta x(t_0) - d_i]^T R_i^{-1} [\mathbf{H}_i \mathbf{M}_i \delta x(t_0) - d_i]. \quad (17)$$

To minimize Eq. (13),  $v(t_0)$  and  $\alpha(t_0)$  needs to satisfy  $\begin{cases} \left[ \frac{\partial J}{\partial v(t_0)} \right]^T = 0 \\ \left[ \frac{\partial J}{\partial \beta(t_0)} \right]^T = 0 \end{cases}$ . The calculation of the gradient for the variational component in Eq. (17) requires the use of the ADM, while that for the ensemble component can avoid the use of the ADM by adopting the transformation  $\mathbf{H}_i \delta x(t_i) = Ep_y(t_i)\beta$ :

$$\left[ \frac{\partial J}{\partial \beta(t_0)} \right]^T = \beta(t_0) + \sqrt{\gamma_e} \sum_{i=0}^n [Ep_y(t_i)]^T R_i^{-1} [\mathbf{H}_i \mathbf{M}_i \delta x(t_0) - d_i]. \quad (18)$$

### 3 Experimental design

#### 3.1 Configuration of En4DVar system

The En4DVar system developed in this study realized the hybrid BEC by a linear combination of the static climatological covariance from the standard 4DVar system and the flow-dependent ensemble covariance from the 4DEnVar system. The ensemble covariance in the



En4DVar system is estimated by the low-resolution ensemble samples, which is produced by previously running 60-member 4DEnVar system. The 4DVar and 4DEnVar systems all adopt a dual-resolution framework with  $0.5^\circ \times 0.5^\circ$  for the outer loop and  $1.0^\circ \times 1.0^\circ$  for the inner loop. The flowchart of the En4DVar system is given in Figure 1.

Unlike the ensemble prediction systems that use singular vectors as initial perturbations without including any observations, the 4DEnVar system itself produces the initial perturbations that considers both the model constraints and observational information. The IC samples of the 4DEnVar system in the first assimilation window are generated by the “randomcv” method (Baker, 2005), which generates an ensemble of reasonable and balanced samples by the control variable transformation  $\delta x = Uv$ . To alleviate the problems of sampling error and underestimation in BEC during the assimilation cycle, localization, inflation, and observation and SST perturbation techniques are employed. Flow-dependent ensemble samples are generated by assimilating perturbed observations at every 6-hour assimilation window during the assimilation cycle (Figure 1a).

In the En4DVar system, 4DVar uses the same 6-hour assimilation window, and the analysis time is located at the beginning of the assimilation window as 4DEnVar does. Therefore, at the beginning of each assimilation window of 4DVar, the flow-dependent ensemble samples in model space and the corresponding observational ensemble samples at different time slots can be extracted from the 4DEnVar system to estimate the ensemble covariance for the En4DVar system (Figure 1b). A localization scheme with a filter radius of  $7^\circ$  in the horizontal directions and a filter parameter  $K_p$  of 3 in the vertical direction is designed based on the theoretical basis introduced in Section 2.2, which is utilized to remove the spurious remote correlations in the ensemble covariance. The optimal problem of the ensemble component of the En4DVar is solved in a subspace consisting of extended samples obtained by the Schür product between the ensemble samples and the leading eigenvectors of the localization correlation function (Figure 1a).

### 3.2 Experiment design

To verify the impact of introducing the ensemble covariance into the 4DVar system, six sets of experiments were conducted based on the En4DVar, standard 4DVar and 4DEnVar systems using identical settings, respectively, including three sets of assimilation cycle experiments and three sets of deterministic 10-day forecast experiments. The experiments based on the latter two



DA systems were used as the references for comparisons and evaluations. The analyses from the 4DVar system used the ensemble means of its 60 analysis samples.

All experiments were conducted and evaluated based on an OSSE. The forecast model used in these experiments are the GRAPES-GFS model version V3.0 with three different horizontal resolutions (i.e.,  $0.25^\circ \times 0.25^\circ$ ,  $0.5^\circ \times 0.5^\circ$  and  $1.0^\circ \times 1.0^\circ$ ) and the same 87 vertical levels (Su et al., 2020). The 4DVar system of the GRAPES-GFS model was in use in operational global forecasts, which was demonstrated to outperform the operational 3DVar system in terms of both the analysis error and medium-range forecast skill (Zhang et al., 2019). OSSE allows an objective evaluation of DA system (Wang et al., 2008; Wang et al., 2010a; Kleist & Ide, 2015a, 2015b). Here, the GRAPES-GFS version with the resolution of  $0.25^\circ \times 0.25^\circ$  was used to generate an uninterrupted free run from 0600 UTC 10 September to 1200 UTC 22 October, 2016, initialized from the ERA-5 reanalysis, and the results of this run starting from the second day were used as the “truth” state of the OSSE. The run for the first day was adopted to eliminate the effects of spin-up, and the simulated geopotential height and precipitation of the run for the first 8 days were verified using the ERA-Interim reanalysis. The “observations” were the “truth” state transformed from the model space to the observation space by the observation operators of the sounding and cloud-derived wind superimposed with normal distribution random perturbations of which the expectations equal zero and the standard deviations adopt the observation errors. In addition, the 15-hour forecast by the GRAPES-GFS version with the resolution of  $0.5^\circ \times 0.5^\circ$  initialized from the 6-hour forecast of the ERA-Interim dataset was used as the background field of three sets of assimilation cycle experiments for the first assimilation window. For the 4DVar systems in the first assimilation window, 60 ensemble background fields were produced using the aforesaid background plus 60 random perturbations whose ensemble mean is equal to zero. The results of the experiments for the first 2 days were used for spin-up, and those from day 3 onwards for about one month covering the period from 0900 UTC 13 September 2016 to 0900 UTC 11 October 2016 were analyzed. To facilitate comparisons with the reanalysis data, the analyses at the middle of each assimilation window were produced with 3-h forecasts initialized from the corresponding analyses at the beginning of the window for the evaluations and comparisons. Restarted from these analyses, three sets of 10-day deterministic forecast experiments were carried out and the forecast skills were evaluated and compared.



Moreover, in order to visually verify the performances and flow-dependent characteristics of the DA systems, the results of the single-point observation experiments in the assimilation window (0900 UTC 13 September 2016 to 1500 UTC 13 September 2016) on the third day of the OSSE were used. Three single-point observation experiments based on the En4DVar system with three linear combinations of the variational and ensemble components adopted the same background, single-point observation, observation error ( $0.95^\circ\text{K}$ ) and horizontal filter radius ( $15^\circ$ ) of localization. The three combinations included  $\gamma_c = 0.8$  and  $\gamma_e = 0.2$ ,  $\gamma_c = 0.5$  and  $\gamma_e = 0.5$  and  $\gamma_c = 0.2$  and  $\gamma_e = 0.8$  in Eq. (16), respectively. The background used the ensemble mean of the background samples of the 4DEnVar system at the beginning of this assimilation window. The single-point observation was selected from the sounding temperature observations in the OSSE valid at 1200 UTC 13 September 2016, located upstream of the top of the short-wave ridge ( $60.77^\circ\text{S}$ ,  $161.83^\circ\text{W}$ ) in the middle troposphere (500hPa), with an observation innovation of -1.53K.

## 4 Results

### 4.1 Single-point observation experiments

To demonstrate the impact of introducing the ensemble covariance provided by the 4DEnVar system, three experiments assimilating the same single-point observation by the En4DVar system with different linear combinations for its hybrid covariance were conducted. The analysis increments produced in these experiments are shown in Figure 2. All the experiments show maximum negative temperature increments near the observation at the beginning of the assimilation window resulting from assimilating the single-point observation, implying lower temperatures in three analysis fields than in the background field. There are also clear cyclonic wind responses around the maximum negative temperature increments, which indicates that the BEC of all experiments satisfy certain balance constraints. In addition, it is satisfactory that no significant spurious correlations are exhibited in the experiments due to the localization of the ensemble BEC (Figure 2a-2c).

In addition to examining the basic assimilation capability, the single-point observation experiments can also visualize the flow-dependent characteristic of the BEC. On one hand, by visualizing the evolution of the increments over time, we can find that the center of the maximum



negative value of all experiments moves to the southeast of the observation. At the end of the assimilation window, the movement of the center of the maximum negative value and the extension of the increment along the gradient of the geopotential height are most obvious. This is reasonable considering that the background field in the vicinity of the observation is the northwest flow, and indicates that the BECs in all the experiments have flow-dependent characteristics. On the other hand, the analysis increments in the experiments with higher weight to the ensemble covariance extend more strongly along the gradient of the geopotential height and show more obvious asymmetric distributions. This highly weighted ensemble covariance helps the En4DVar system acquire a more obvious flow-dependent characteristic than the lowly weighted one.

## 4.2 Observing system simulation experiments

### 4.2.1 Evaluation metric

To evaluate the performance of the En4DVar system, its analysis quality and forecast skill were measured by comparing the analysis and forecast against the “truth” state. The root mean square error (RMSE) is usually utilized to measure the analyses and forecast errors. Here, we adopted a metric called anomaly root mean square error (ARMSE; He et al., 2021a) instead of RMSE to exclude the systematic bias and only measure the random error that cannot be corrected like the systematic bias. This metric is defined as:

$$ARMSE = \sqrt{\frac{\sum_{n=1}^N w_{(n)} \times (M_{(n)} - truth_{(n)} - bias)^2}{\sum_{n=1}^N w_{(n)}}}, \quad (19)$$

where  $w_{(n)}$  is the weighted coefficients at the  $n$ -th grid point,  $N$  is the grid size,  $M_{(n)}$  and  $truth_{(n)}$  denote the forecast (or analysis) and the “truth” state at the  $n$ -th grid point,  $bias$  represents the mean error ( $bias = \frac{\sum_{n=1}^N w_{(n)} \times (M_{(n)} - truth_{(n)})}{\sum_{n=1}^N w_{(n)}}$ ). We use the anomaly correlation coefficient (ACC) metric to assess the similarity between the anomalies of the forecast (or analysis) and the “truth” state. The statistically significant results of the differences of the metrics between different experiments were given by the paired t-test. In addition, to facilitate comparisons of the abovementioned metrics, we divided the globe into three regions including the Northern Extratropics (20°N~90°N, 180°W~180°E; NH-X), Southern Extratropics (20°S~90°S, 180°W~180°E; SH-X) and Tropics (20°S~20°N, 180°W~180°E; TR).



#### 4.2.2 Weights of climatological and ensemble covariances in the hybrid covariance

In this subsection, the weight coefficients of the climatological and ensemble covariances in the hybrid covariance were determined based on two sets of sensitivity experiments. These sensitivity experiments aim to investigate the effect of different linear combinations of two covariances in the hybrid covariance with and without inflation on the analysis quality of the En4DVar system, respectively. Without inflation, the sum of the weight coefficients of two covariances is equal to 1, i.e.,  $\gamma_c + \gamma_e = 1$ . In this case, the first set of sensitivity experiments were conducted using a small, a medium and a large weight coefficients of the ensemble covariance, i.e.,  $(\gamma_c = 0.8, \gamma_e = 0.2)$ ,  $(\gamma_c = 0.5, \gamma_e = 0.5)$  and  $(\gamma_c = 0.2, \gamma_e = 0.8)$ , respectively. The scorecards of the ACC and ARMSE for the forecasts initialized by the En4DVar system with the aforesaid three linear combinations against the 4DVar-initialized forecast are shown in Figure 3. The En4DVar system with these three combinations shows significant improvements on the first 4 lead forecast days and comparable performances on the last 5 lead days in the Northern Extratropics compared with the 4DVar system. In Tropics, its improvements extend to almost all the lead forecast days. In the Southern Extratropics, however, performance degradations occurs in the lead days 2-5. In summary, introducing the ensemble covariance from the 4DVar system into the 4DVar system benefits the short-term forecasts in the Northern Extratropics and the forecasts on almost all lead days in Tropics, although it degrades the short-term forecasts in the Southern Extratropics. Without inflation, the En4DVar system with the same weight for both the climatological and ensemble covariances performs best, indicating equal importance of the balance constraint and flow dependence in assimilation analysis.

Moreover, four inflated linear combinations in which the sum of weight coefficients of two covariances is larger than 1 were used in the En4DVar system to seek further improvements of the forecasts, especially in the Southern Extratropics. They include  $(\gamma_c = 0.8, \gamma_e = 0.25)$ ,  $(\gamma_c = 0.6, \gamma_e = 0.5)$ ,  $(\gamma_c = 0.5, \gamma_e = 0.6)$  and  $(\gamma_c = 0.25, \gamma_e = 0.8)$ . Figure 4 displays the scorecards of the ACC and ARMSE for the En4DVar-initialized forecasts with the above combinations against the 4DVar-initialized forecasts, from which it is found that the En4DVar system with all combinations except  $(\gamma_c = 0.5, \gamma_e = 0.6)$  in the Southern Extratropics outperforms the 4DVar system in the globe. It is suggested that linear combinations with proper inflations perform better than those without any inflations (Figures 3 and 4). In particular, some of the inflated combinations



shows improvements in the Southern Extratropics. This is probably due to the underestimation of the hybrid covariance without inflation although the ensemble covariance has already been inflated in the 4DVar system, and therefore proper inflations are required to allow more observational information to be incorporated into ICs for better forecast skills.

Finally, the inflated combination in which the ensemble covariance is dominant, i.e., ( $\gamma_c = 0.25, \gamma_e = 0.8$ ), was chosen as the optimal combination to construct the hybrid covariance of the En4DVar system. The reasons include three aspects. Firstly, the combinations without inflation have worse performances than those with inflation in the Southern Extratropics (Figures 3 and 4) and thus they are impossible the optimal choice. Secondly, among the four inflated combinations, the combination ( $\gamma_c = 0.5, \gamma_e = 0.6$ ) can be excluded, because it performs worst in the Southern Extratropics although it has comparable performance to the others in the Northern Extratropics and Tropics (Figure 4). Thirdly, the combinations ( $\gamma_c = 0.6, \gamma_e = 0.5$ ) and ( $\gamma_c = 0.25, \gamma_e = 0.8$ ) are better than ( $\gamma_c = 0.8, \gamma_e = 0.25$ ) except some degradations in their initialized short-term forecasts in the Southern Extratropics (Figures 5a-5b). At last, the combination ( $\gamma_c = 0.25, \gamma_e = 0.8$ ) basically outperforms ( $\gamma_c = 0.6, \gamma_e = 0.5$ ), although it degrades the short-term forecasts in the Southern Extratropics compared with the latter (Figure 5c). In addition, it slightly improves the medium-range forecasts compared with the 4DVar system (Figure 4d).

The dominant role of the ensemble covariance in the hybrid BEC of the En4Var system in this study quite differs from those in the available En4DVar systems in which the climatological covariances are usually dominant (Clayton et al., 2013; Lorenc et al., 2015), indicating the high quality of the initial perturbations generated by the 4DVar system that allows increasing the weighting of the ensemble covariance in an En4DVar system (Clayton et al., 2013; Bowler et al., 2017a).

#### 4.2.3 Analysis quality

After the weight coefficients of the climatological and ensemble covariances were determined, the En4DVar system was completed and came into evaluations in terms of analysis quality. The analysis errors of the En4DVar, 4DVar and 4DVar systems verified against the “truth” state were compared and evaluated to investigate whether the En4DVar system further improved the analysis quality on the basis of both 4DVar and 4DVar systems.



First, the vertical profiles of the ARMSE differences of the analysis and background between the En4DVar and 4DVar systems and between the En4DVar and 4DEnVar systems are provided in Figure 6. In general, the ARMSE differences between the En4DVar and 4DVar analyses and backgrounds keep negative for zonal wind, temperature and specific humidity in the globe on almost all vertical layers. It is indicated that En4DVar fully outperforms 4DVar in terms of both analysis and background errors except the degraded performances in zonal wind and temperature at the vertical layers above 100hPa in the Southern Extratropics, with more significant improvements in the analysis than in the background (Figures 6d-6l). For geopotential height, En4DVar performs slightly better than 4DVar in the Northern Extratropics and on the middle and upper layers in the Tropics, and slightly (significantly) worse on the middle (upper) layers in the Southern Extratropics and on the lower layers in the Tropics (Figures 6a-6c). In contrast, the ARMSE differences between the En4DVar and 4DEnVar ensemble mean analysis and background errors have various signs for different variables at different vertical layers. The analysis and background of geopotential height in En4DVar outperform the 4DEnVar ensemble mean, especially on the upper layers in the Southern Extratropics (Figure 6a-6c). The error differences of zonal wind are positive on the layers below 400hPa (200hPa) in the Northern and Southern Extratropics (Tropics), indicating less observational information incorporated by the En4DVar than by the 4DEnVar ensemble mean on these layers (Figures 6d-6f). For temperature, the En4DVar performs worse than the 4DEnVar ensemble mean on the lower layers except the layers near surface in the Northern and Southern Extratropics and on the layers above 200hPa in the Northern Extratropics and Tropics, but better on the layers between 500hPa and 200hPa (above 500hPa) in the Northern Extratropics and Tropics (Southern Extratropics) (Figures 6g-6i). The analysis and background of specific humidity in En4DVar are inferior to those in 4DEnVar ensemble mean (Figures 6j-6l). In conclusion, the analysis and background of En4DVar draw closer to the observations than those of 4DVar during the assimilation cycle by introducing flow-dependent information produced by 4DEnVar although they are not as close to the observations as those of 4DEnVar ensemble mean.

The pressure-latitude distributions of the ARMSEs in the analysis fields of geopotential height, zonal wind, temperature and specific humidity were further analyzed (Figure 7). The error maxima in the En4DVar analyses of geopotential height occur in the stratosphere near 60°S (Figure 7a). The error maxima in the zonal wind analyses related to jets are mainly concentrated



in the stratosphere and middle and upper troposphere near 60°S, which extend toward lower troposphere (Figure 7d). The error maxima in the temperature analyses occur near the surface from the poles to the equator and extend to the middle and upper troposphere and stratosphere near 60°S (Figure 7g). In addition, the error structure of the specific humidity analyses showed a semicircular region with large values at low and middle latitudes in the lower and middle troposphere (Figure 7j). The ARMSE differences between the En4DVar and 4DVar analyses of geopotential height, zonal wind, temperature and specific humidity are shown in the middle column of Figure 7. The differences are negative on almost all vertical layers at all latitudes for all four variables except the stratosphere at high latitudes in the Southern Hemisphere for geopotential height, zonal wind and temperature, which indicate the almost all decrease of the errors in the En4DVar analyses of the four variables compared with 4DVar. However, from the right column of Figure 7 that displays the ARMSE differences between the En4DVar and 4DEnVar analyses of the aforesaid four variables, it can be observed that the En4DVar analyses of zonal wind and specific humidity are not as close to the observations as the 4DEnVar ensemble mean analyses in general, except the improvements in the zonal wind analyses at the upper troposphere and stratosphere in the Southern Hemisphere and at high latitudes in the Northern Hemisphere. The En4DVar system improves the temperature analyses near the poles and at the middle troposphere near the equator, but degrades them above the upper troposphere and at the low troposphere near the equator, compared with 4DEnVar ensemble mean. Overall, among the aforesaid three kinds of analyses, the 4DEnVar ensemble mean analyses of all the variables except geopotential height are the closest to the observations, which may possibly benefit from the flow dependence of the ensemble covariance, while the 4DVar analyses are the farthest from the observations, which may probably result from the balance constraint included in the climatological covariance. The En4DVar analyses of all the variables except geopotential height are between the above two kinds of analyses, which may be attributed to the use of the hybrid covariance with both the flow dependence and balance constraint. In addition, the En4DVar analyses of geopotential height are closer to the observations than the 4DEnVar ensemble mean analyses in most regions, indicating that the hybrid covariance allows larger improvements in the analyses of geopotential height than in those of other variables (Figure 7c). Given the roles of the flow dependence and balance constraint in the analysis quality, their impacts on the forecast skill are more concerned.



#### 4.2.4 Forecast skill

A good fit of the analysis to the observations does not necessarily lead to an improved forecast. Therefore, we measured the forecast error to verify the impact of improved or degraded analysis on the forecast skill.

Figure 8 shows the comparison results of the ACC metric for the 500hPa potential height forecast. The forecast initialized by En4DVar performs better than (comparable to) that initialized by 4DVar after (within) two (four) days in the Northern (Southern) Extratropics (Figures 8a-8b), and significantly better on all the lead days in the Tropics (Figure 8c). As for the 4DEnVar-initialized forecast, its improvements against the 4DVar-initialized forecast are only sighted on part of the lead days, including the lead days 5-8 (7-10) in the Northern (Southern) Extratropics and the lead days 6-10 in the Tropics. Significant (slight) degradations are found on the lead days 2-4 (5-6) in the Southern Extratropics and on the lead days 1-3 (4-5) in the Tropics. The 9- and 10-day forecasts in the Northern Extratropics also become worse. Moreover, Figure 8 also indicates that the En4DVar-initialized forecast outperforms the 4DEnVar-initialized forecast in general except the lead days 7, 8 and 10 in the Southern Extratropics. It is concluded that En4DVar is overall better than both 4DVar and 4DEnVar in terms of the ACC-based forecast skill. This conclusion is also true when the forecast skill is measured by ARMSE (Figure 9), except the obvious degradations of En4DVar relative to 4DVar (4DEnVar) before the lead day 5 (on the lead days 7-8) in the Southern (Northern) Extratropics. The most likely reason for the improvements in the forecast of 500hPa geopotential height initialized by En4DVar against those initialized by both 4DVar and 4DEnVar is its alleviation of excessively or insufficiently incorporating observations into the IC analysis through the hybrid covariance that combines the flow-dependent ensemble covariance from 4DEnVar and the climatological covariance with balance constraint from 4DVar.

The En4DVar system can also improve the geopotential height forecasts on other vertical levels. Large ARMSEs in the En4DVar-initialized forecast are mainly distributed in the stratosphere and upper troposphere in the Northern and Southern Extratropics and increase with the lead time (Figures 10a and 10d ), which are consistent with the analysis error distribution. These forecast errors are significantly reduced for most lead forecast days compared with those in the 4DVar-initialized forecast, although they seriously increase in the upper stratosphere on all the lead days and extend to the lower troposphere on the first 3 lead days in the Southern Extratropics



(Figures 10e). This is consistent with the increased analysis errors located on the upper layers (Figures 6b and 7b). The errors also decrease compared with those in the 4DVar-initialized forecast, except the slight (large) increase at the layers between 800hPa and 500hPa on the lead days 6-9 in the Northern Extratropics and in the middle and lower troposphere (stratosphere) on the lead days 7-10 in the Southern Extratropics (Figures 10c and 10f). Significant improvements can be found in the stratosphere in both the Northern and Southern Extratropics on the lead days 1-9 and 1-6, respectively, and in the upper and middle troposphere in the Southern Extratropics on the lead days 4-6. In the Tropics, the errors of the En4DVar-initialized forecast are much smaller than in the Northern and Southern Extratropics, and En4DVar slightly outperforms or performs comparably to both 4DVar and 4DEnVar (Figures 10g-10i).

The error structure of the En4DVar-initialized zonal wind forecast is similar to that of the geopotential height forecast, with large errors in the stratosphere and upper troposphere in the Northern and Southern Extratropics and increasing with the lead time (Figures 11a and 11d). The performance of En4DVar for the zonal wind forecast is similar to that for the geopotential height forecast, with significantly reduced errors on most lead forecast days compared with both 4DVar and 4DEnVar (the middle and right column of Figure 11). Compared with the forecast errors in the En4DVar-initialized geopotential height on the first lead day in the Southern Extratropics and Tropics that are not reduced against the 4DVar-initialized one, the forecast errors in zonal wind are decreased (Figures 11e and 11h). This is consistent with the reduced analysis errors of zonal wind by En4DVar relative to those by 4DVar in contrast with the undiminished analysis errors of geopotential height (Figure 6e).

The error structure of the En4DVar-initialized temperature forecast is slightly different from those of the geopotential height and zonal wind forecasts. There are large ARMSEs in both the stratosphere and the lower and middle troposphere in the Northern and Southern Extratropics, which increase with the lead time (Figure 12a and 12d). These errors are reduced in the Northern Extratropics on all lead days compared with those in the 4DVar- and 4DEnVar-initialized forecasts, except the last two lead days when the errors are slightly larger than those in the 4DVar-initialized forecast (Figures 12b-12c). In the Southern Extratropics, the En4DVar-initialized forecast is better (worse) than the 4DVar-initialized forecast mainly on the last 4 lead days below (above) 200hPa (Figure 12e), and is better than the deterministic forecast initialized from the 4DEnVar ensemble mean analysis at all vertical layers on all the lead days except the upper and low troposphere on



the last 3 lead days (Figure 12f). The significant improvements by En4DVar are located at the vertical layers between 900hPa and 100hPa on the lead days 4-6 compared with 4DEnVar. In the Tropics, the performance of En4DVar for the temperature forecast is similar to those for the geopotential height and zonal wind forecasts, with much smaller AMSEs than in the Northern and Southern Extratropics and slightly smaller AMSEs than in both the 4DVar- and 4DEnVar-initialized forecasts overall (Figures 12g-12i).

The error structure of the En4DVar-initialized specific humidity forecast is slightly different from those of other variables. There are large errors at the layers between 900hPa and 700hPa, which increase with lead time (Figures 13a, 13d and 13g). On one hand, the En4DVar-initialized forecast is better than the 4DVar-initialized forecast, except the last 2 lead days at the layers near surface in the Northern Extratropics. On the other hand, the En4DVar-initialized forecast outperforms the 4DEnVar-initialized forecast except in the first few hours due to the larger analysis errors of En4DVar than that of 4DEnVar. The significant improvements by En4DVar are located in the lower troposphere compared with both 4DVar and 4DEnVar.

Overall, the change from 4DVar to En4DVar significantly (slightly) improves the (medium-range) forecasts in the Tropics and Northern Extratropics (Southern Extratropics) (Figure 4d). In particular, it leads to a sustained improvement in the middle troposphere in the Tropics and the differences of ACC and ARMSE are statistically significant on almost all the lead days. This is similar to the findings in Kleist et al. (2015a) on the change from 3DVar to 3D Hybrid. Similarly, the change from 4DEnVar to En4DVar also significantly improves the forecasts at all vertical levels in the Tropics on almost all the lead days (Figure 14). Significant improvements can also be found in the short-term forecasts in the Northern Extratropics. In addition, the improvements in the Southern Hemisphere are basically more significant than in the Northern Hemisphere.

## 5 Summary and discussion

In this study, a new En4DVar hybrid DA system for the GRAPES-GFS model was proposed and implemented using the extended control variable method based on the original 4DVar system. Most operational centers in the world have chosen to use an ensemble of 4DVars or EnKF or something like this to estimate the ensemble covariance for En4DVar hybrid DA systems. Bowler et al. (2017a, 2017b) also used the En-4DEnVar system instead of the ETKF



system to provide ensemble forecasts to the hybrid DA systems and obtained encouraging results, but there are fewer related studies. Here, a 4D<sub>En</sub>Var system was adopted to estimate the ensemble covariance for the new En4DVar system. This system gave a dominant weight to the ensemble covariance and a small weight to the balanced climatological covariance of 4DVar. The weight coefficients of two covariances were determined based on the sensitivity experiments. In addition, we applied an ensemble-sample-based subspace localization scheme, which is different from the localization transformations in the climatological covariance, to reduce the spurious remote correlations in the ensemble covariance. This scheme is not only easy to implement, but also allows rapid generation of expanded samples thus improving the quality of the ensemble covariance and benefiting the optimal analysis.

We conducted single-point observation experiments and OSSE-based one-month DA cycle experiments and batch forecast experiments to systematically evaluate the analysis quality and forecast skill of the new system using the 4DVar and 4D<sub>En</sub>Var systems as references. Single-point observation experiments show that introducing the ensemble covariance can help the En4DVar system acquire the explicit flow-dependent characteristic. We also investigated the roles of the ensemble and climatological covariances in the improvements of the En4DVar-initialized forecast. The results show that a properly inflated hybrid covariance with a dominant weight to the ensemble covariance leads to the optimal improvements in the forecast, indicating a more important role of the flow dependence included in the ensemble covariance than that of the balance constraint incorporated in the climatological covariance. According to the above investigation, the weight coefficients of the climatological and ensemble covariances in the hybrid covariance of the En4DVar system were finally determined, which were 0.25 and 0.8, respectively.

Using the optimal hybrid covariance, the performance of En4DVar on the analysis was evaluated. The analysis error of the En4DVar system is smaller than that of the 4DVar system, but basically larger than that of the 4D<sub>En</sub>Var system. It is encouraging that the 500hPa geopotential height forecast initialized from the En4DVar analysis overall outperforms those initialized from both the 4DVar analysis and 4D<sub>En</sub>Var ensemble mean analysis in terms of the ACC-based and ARMSE-based forecast skills. The En4DVar system performs similarly for the geopotential height forecast on other vertical layers. It also improves the forecasts of other variables in general relative to both 4DVar and 4D<sub>En</sub>Var. Overall, on one hand, the upgrade from 4DVar to En4DVar significantly improves the forecasts in the Tropics and Northern Extratropics, and also slightly



ameliorates the medium-range forecasts in the Southern Extratropics. On the other hand, although the ICs from the En4DVar analysis are as not close to the observations as those from the 4DEnVar ensemble mean analysis, the En4DVar-initialized forecast generally performs better than the 4DEnVar-initialized forecast, significantly in the middle and upper troposphere in the Tropics and in the short-term forecasts in the Northern and Southern Extratropics. It is suggested that a much more accurate IC may not lead to a farther improvement of forecast unless the generation of this IC includes some balance constraint.

Future improvements of the En4DVar system will depend on the increase of the quality of the ensemble covariance and the use of more observations. To increase the quality of the ensemble covariance, the 4DEnVar system needs further development and updating. For example, the observational ensemble samples can be generated using nonlinear forecast models instead of TLMs, which can both improve the qualities of the ensemble samples and save time in model integration. The inclusion of the balance constraint into the 4DEnVar system may also ameliorate the ensemble covariance, which may be implemented through an advanced localization technique upon the separated unbalanced variables. In addition, the assimilation of satellite observations may also effectively improve the ensemble covariance and the En4DVar analysis.

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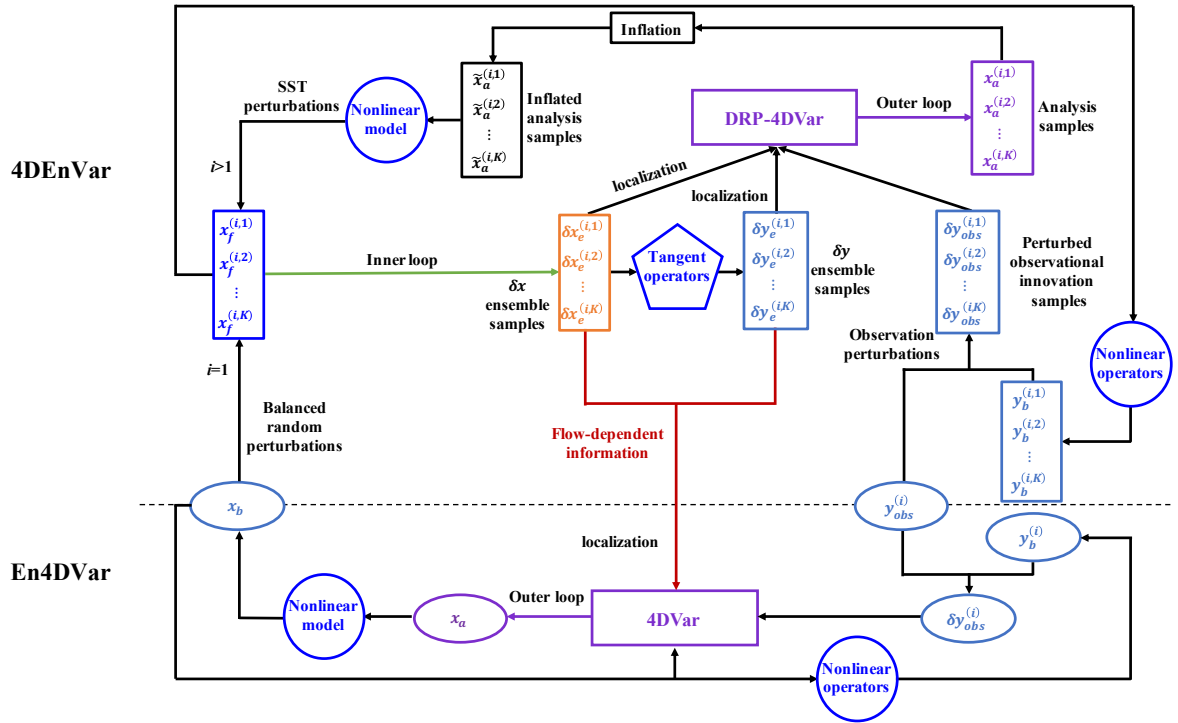
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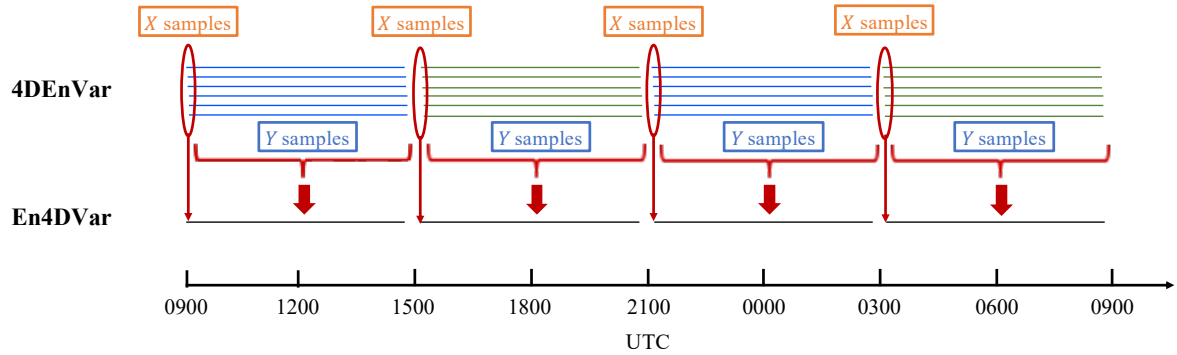
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(a)



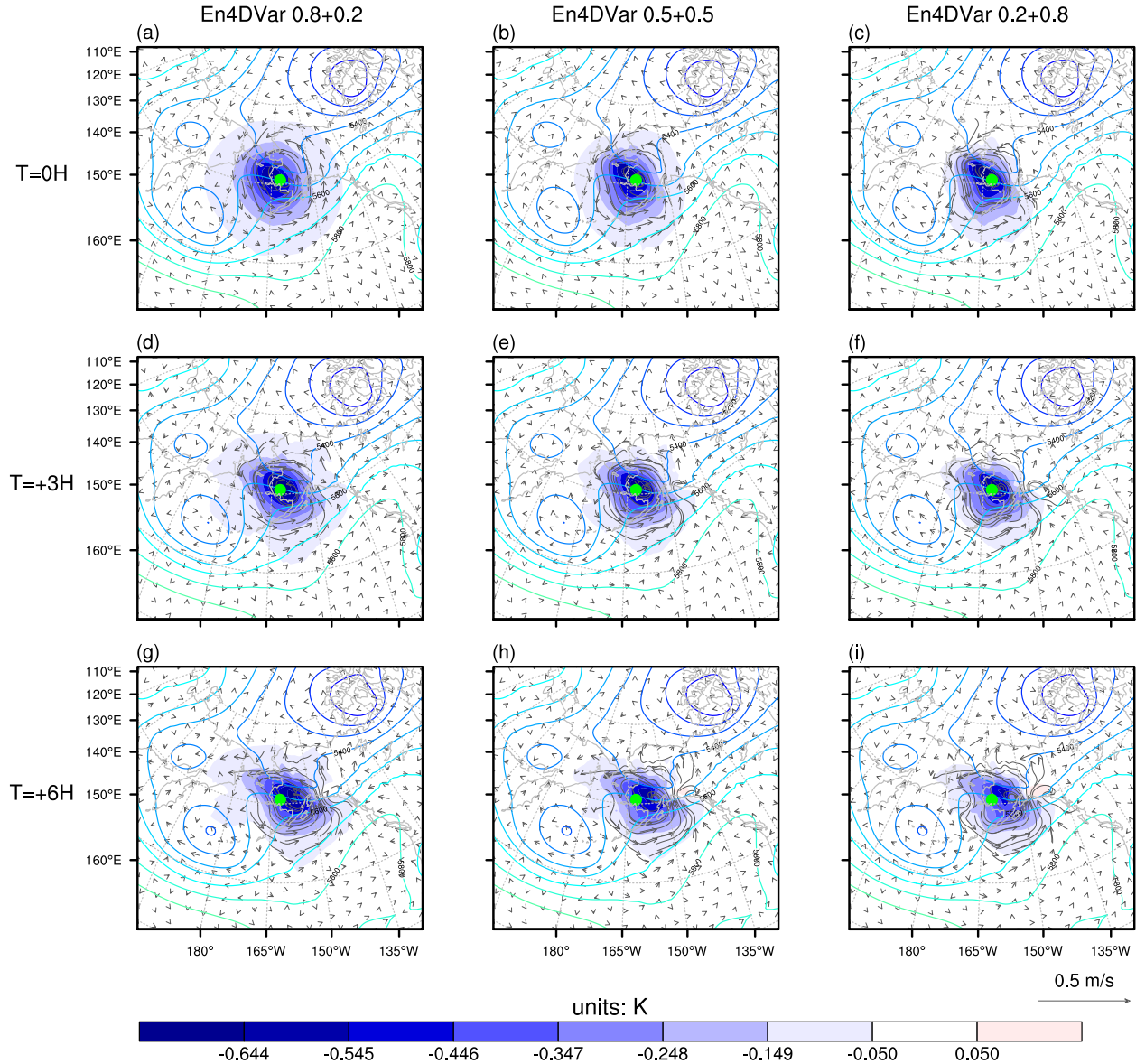
(b)



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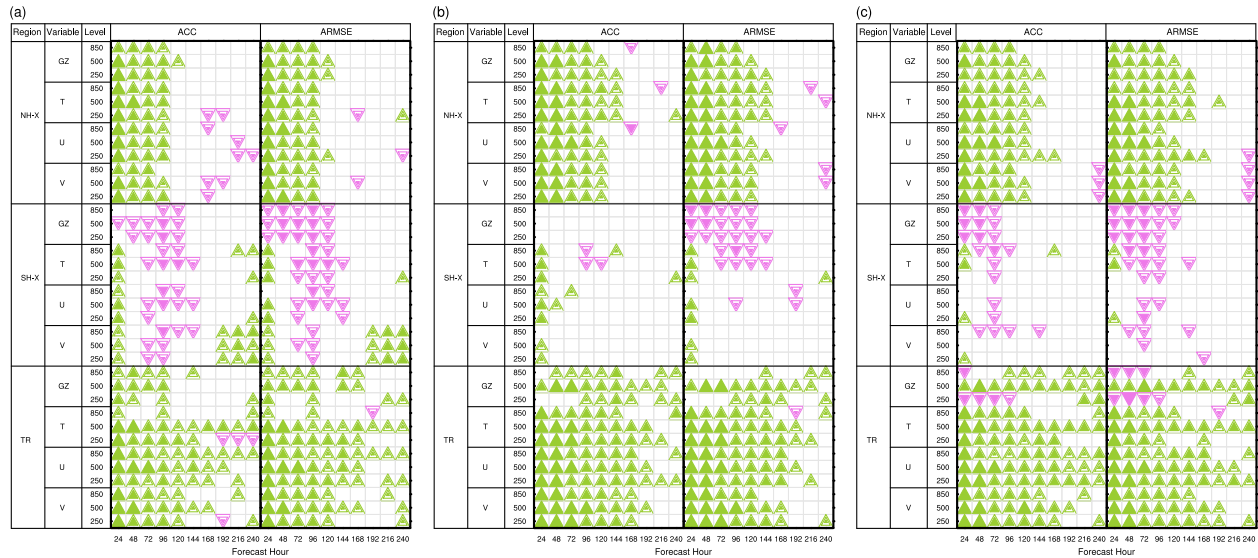
791 **Figure 1.** Schematic of the En4DVar system developed in this study. The key components and  
 792 techniques of the En4DVar system are shown in (a), and the exchange of information between the  
 793 4DEnVar system and the En4DVar system on the timeline during the assimilation cycle is shown  
 794 in (b).





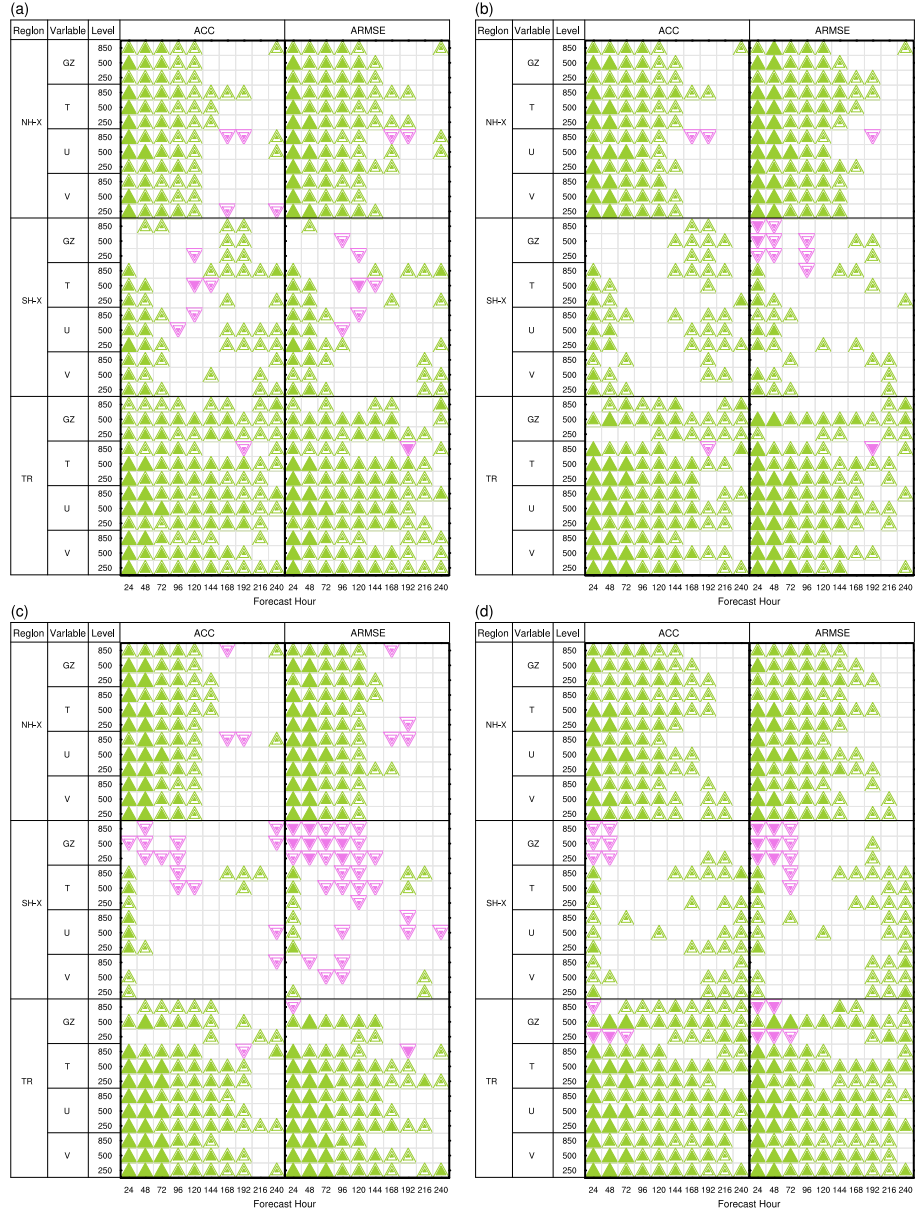
**Figure 2.** The temperature (shading; units: K) and vector wind (vector; units: m/s) analysis increments valid at the (top) beginning, (middle row) middle, and (bottom) end of the assimilation window resulting from assimilating the single-point temperature observation valid at the middle of the assimilation window for the En4DVar system adopting the linear combination coefficients of (left) ( $\gamma_c = 0.8, \gamma_e = 0.2$ ), (middle column) ( $\gamma_c = 0.5, \gamma_e = 0.5$ ) and (right) ( $\gamma_c = 0.2, \gamma_e = 0.8$ ) on the model level closest to the assimilated observation (marked with a green dot). The solid contour is the 500hPa background field geopotential height (units: gpm) valid at the (top) beginning, (middle row) middle, and (bottom) end of the assimilation window.





**Figure 3** The scorecard of the ACC and ARMSE calculated for the forecasts initialized by the En4DVar system adopting the linear combination coefficients of (a)  $(\gamma_c = 0.8, \gamma_e = 0.2)$ , (b)  $(\gamma_c = 0.5, \gamma_e = 0.5)$  and (c)  $(\gamma_c = 0.2, \gamma_e = 0.8)$  against those initialized by the 4DVar system with identical settings, respectively. If the former forecast has a significantly higher / smaller (lower / larger) ACC / ARMSE than the latter, a green upward-pointing (red downward-pointing) triangle is marked. The large, medium and small filled triangles respectively indicate that the differences of ACC or ARMSE are greater than 3 times, between 1 times and 3 times, and between 0.5 times and 1 times the t value of the 95% confidence level, i.e., fairly significant, significant, and insignificant. No triangles are shown when the differences are less than 0.5 times the t value of the 95% confidence level, indicating equivalent.

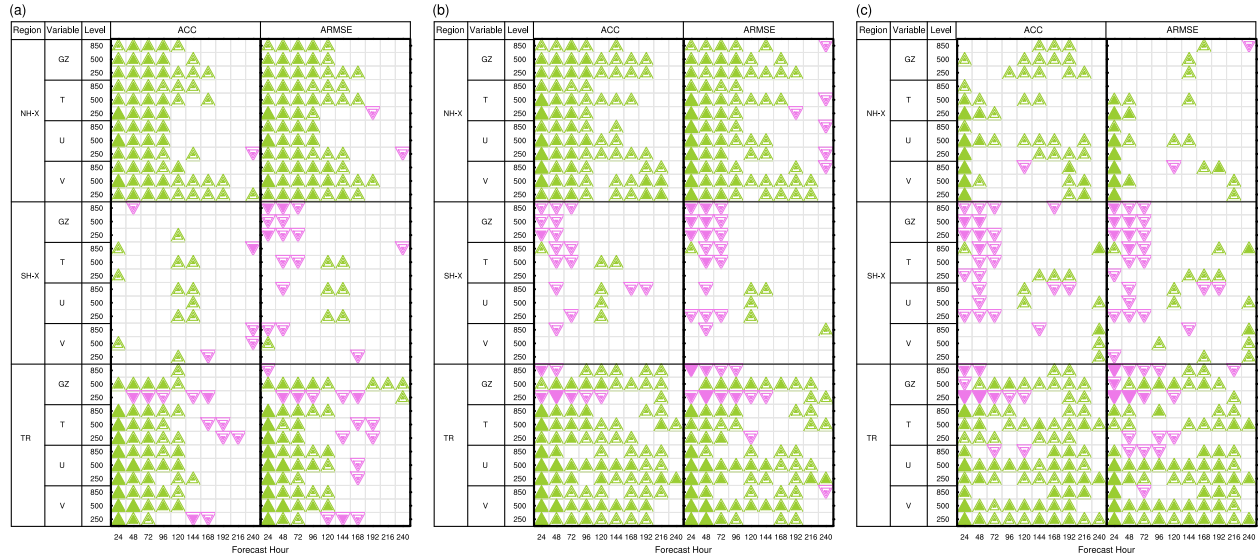




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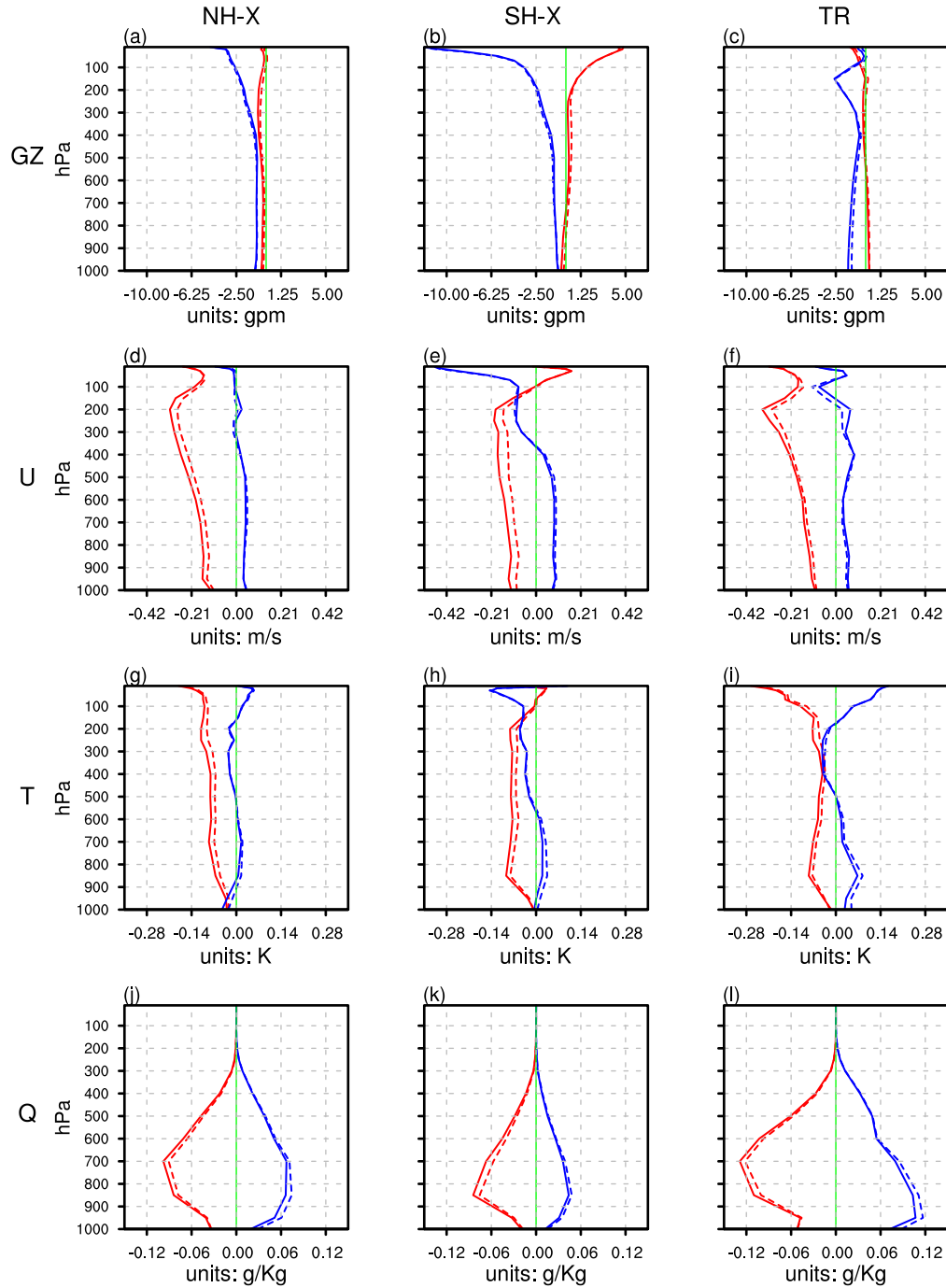
816 **Figure 4.** Same as Figure 3, except for the linear combinations of (a) ( $\gamma_c = 0.8, \gamma_e = 0.25$ ), (b)  
 817 ( $\gamma_c = 0.6, \gamma_e = 0.5$ ), (c) ( $\gamma_c = 0.5, \gamma_e = 0.6$ ) and (d) ( $\gamma_c = 0.25, \gamma_e = 0.8$ ).





**Figure 5.** Same as Figure 3, except for the forecasts initialized by the En4DVar system adopting the linear combinations of (a) ( $\gamma_c = 0.6, \gamma_e = 0.5$ ) and (b) ( $\gamma_c = 0.25, \gamma_e = 0.8$ ) against those using the linear combination of ( $\gamma_c = 0.8, \gamma_e = 0.25$ ), and (c) ( $\gamma_c = 0.25, \gamma_e = 0.8$ ) against those using the linear combination of ( $\gamma_c = 0.6, \gamma_e = 0.5$ ).

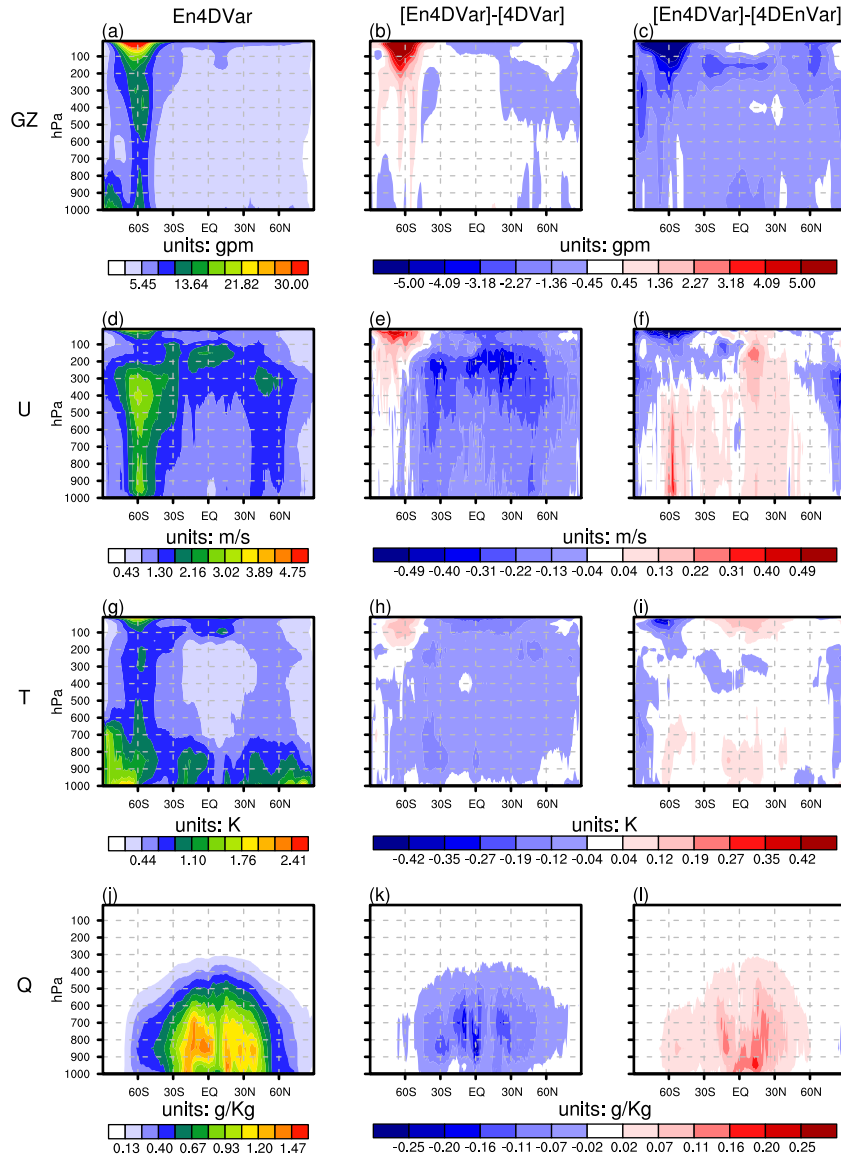




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824 **Figure 6.** Vertical profiles of the ARMSE (verified against the “truth” state) differences of the  
 825 background (dashed line) and analysis (solid line) fields of the geopotential height (row 1; units:  
 826 gpm), zonal wind (row 2; units: m/s), temperature (row 3; units: K) and specific humidity (row 4;  
 827 units: g/Kg) in the Northern Extratropics (20°N~90°N, 180°W~180°E; left), Southern Extratropics  
 828 (20°S~90°S, 180°W~180°E; middle column) and Tropics (20°S~20°N, 180°W~180°E; right). The  
 829 red (blue) lines show the ARMSE differences between the En4DVar and 4DVar (4DVar  
 830 ensemble mean) background and analyses.

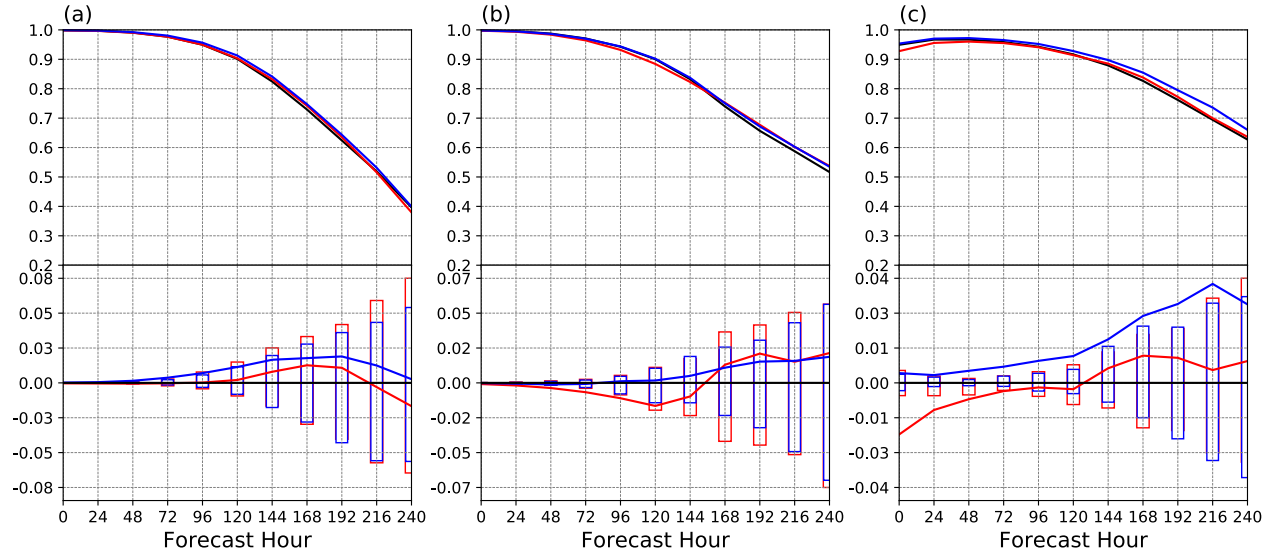




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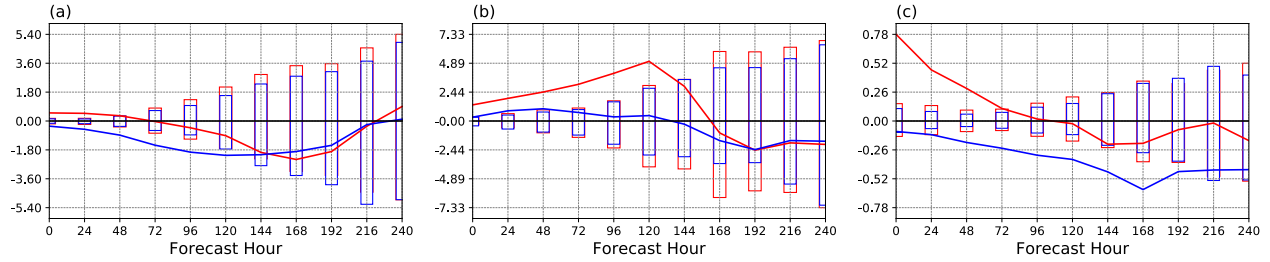
832 **Figure 7.** The pressure versus latitude plots of the ARMSEs (verified relative to the “truth” state)  
 833 of the geopotential height (row 1; units: gpm), zonal wind (row 2; units: m/s), temperature (row 3;  
 834 units: K) and specific humidity (row 4; units: g/Kg) analyses from the En4DVar (left), and the  
 835 ARMSE differences between En4DVar and 4DVar (middle column) and between En4DVar and  
 836 4DVar (left), respectively.





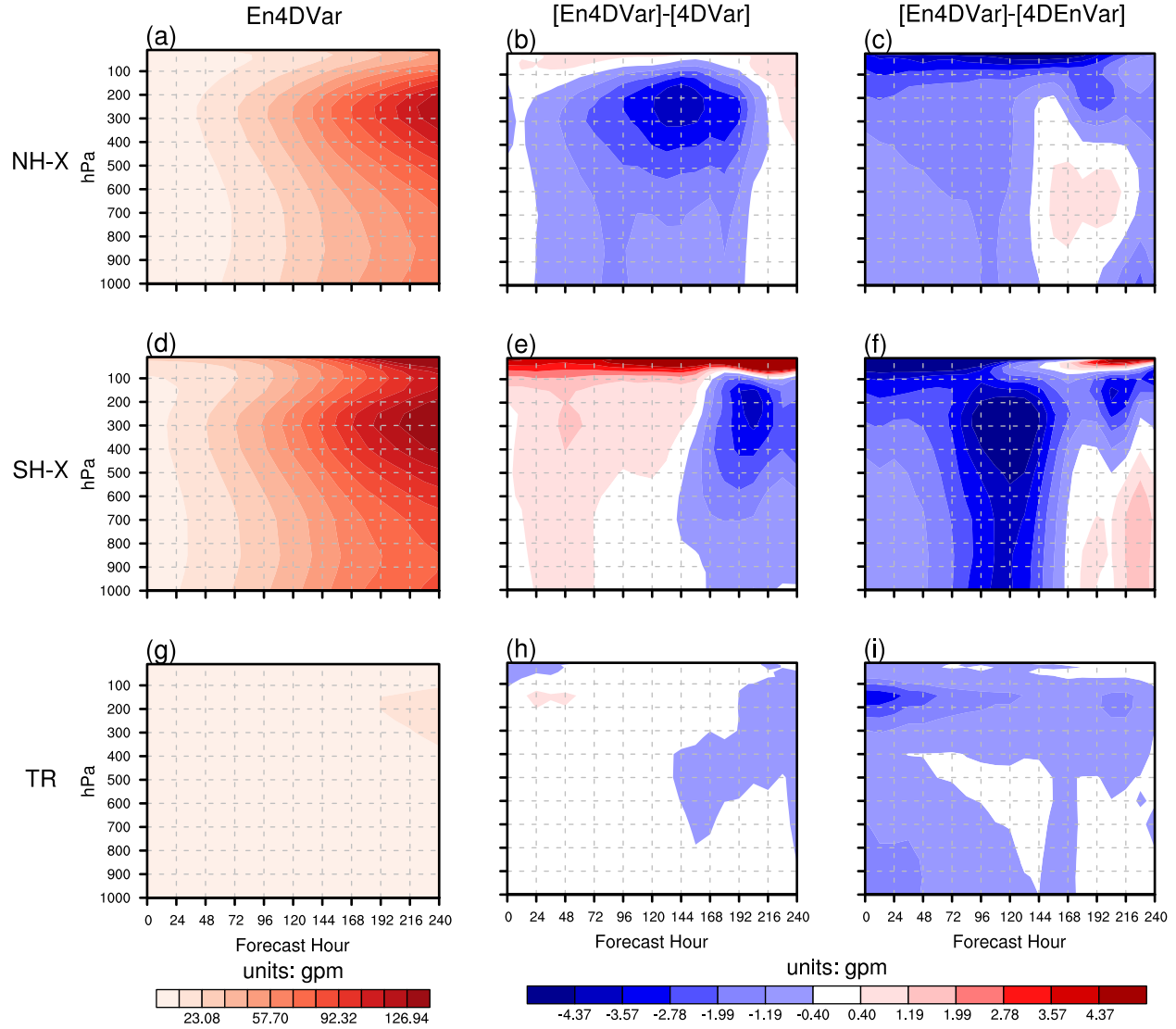
**Figure 8.** The anomaly correlation coefficients (ACCs) of the forecasts of the 500hPa geopotential height respectively initialized from the 4DVar (black line), 4DVar ensemble mean (red line) and En4DVar analyses (blue line) against the “truth” state in the (a) Northern Extratropics (20°N~90°N; 180°W~180°E), (b) Southern Extratropics (20°S~90°S; 180°W~180°E) and (c) Tropics (20°S~20°N, 180°W~180°E). The corresponding ACC differences between the forecasts initialized from the 4DVar ensemble mean and 4DVar analyses (red line) and between those initialized from the En4DVar and 4DVar analyses (blue line), with the 95% confidence threshold, are also plotted in the bottom.





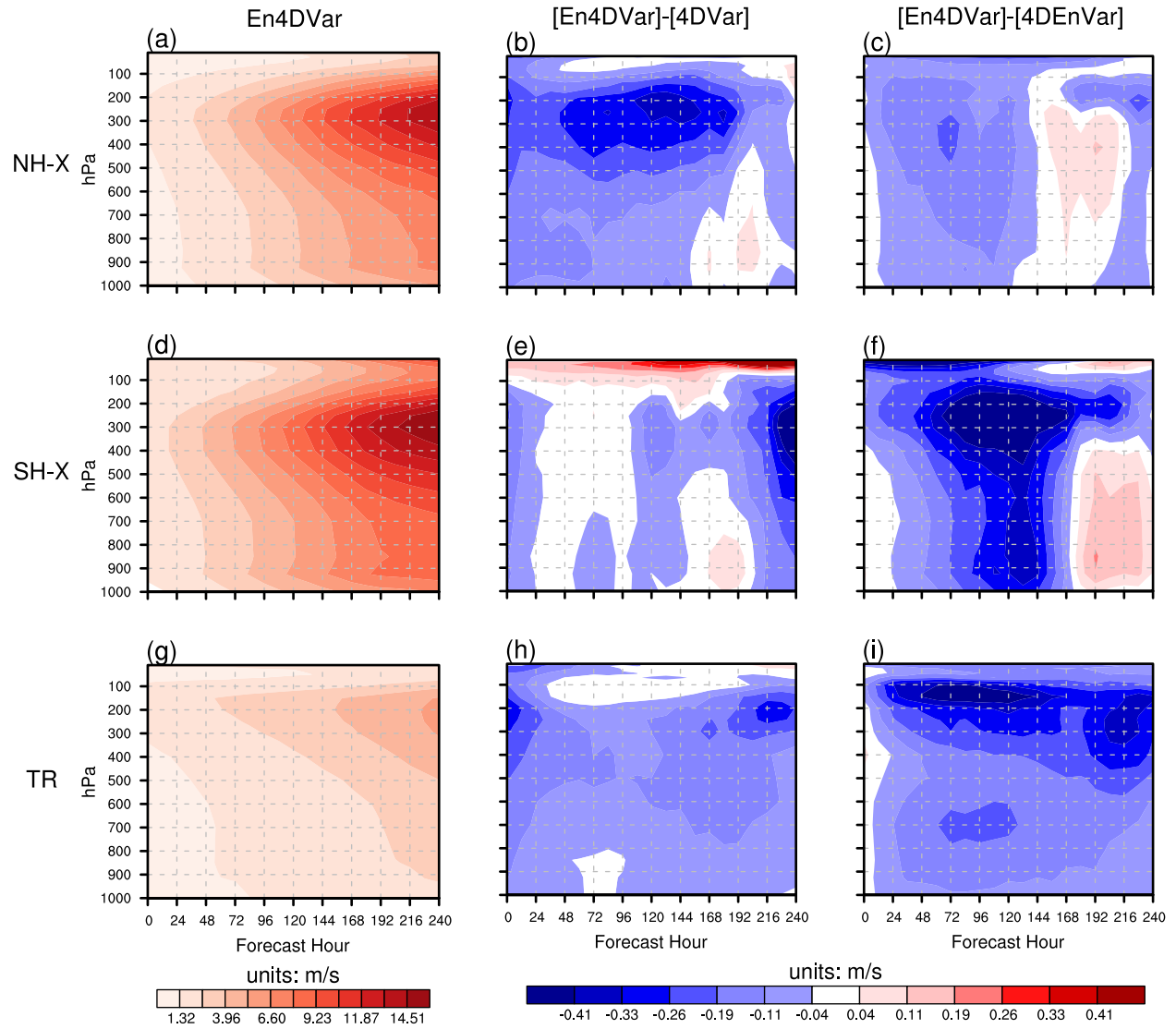
**Figure 9.** The ARMSE differences between the forecasts of the 500hPa geopotential height initialized from the 4DVar ensemble mean and 4DVar analyses (red line) and between those initialized from the En4DVar and 4DVar analyses (blue line) against the “truth” state in the (a) Northern Extratropics ( $20^{\circ}\text{N}\sim 90^{\circ}\text{N}$ ;  $180^{\circ}\text{W}\sim 180^{\circ}\text{E}$ ), (b) Southern Extratropics ( $20^{\circ}\text{S}\sim 90^{\circ}\text{S}$ ;  $180^{\circ}\text{W}\sim 180^{\circ}\text{E}$ ) and (c) Tropics ( $20^{\circ}\text{S}\sim 20^{\circ}\text{N}$ ,  $180^{\circ}\text{W}\sim 180^{\circ}\text{E}$ ). The bar charts show the 95% confidence threshold.





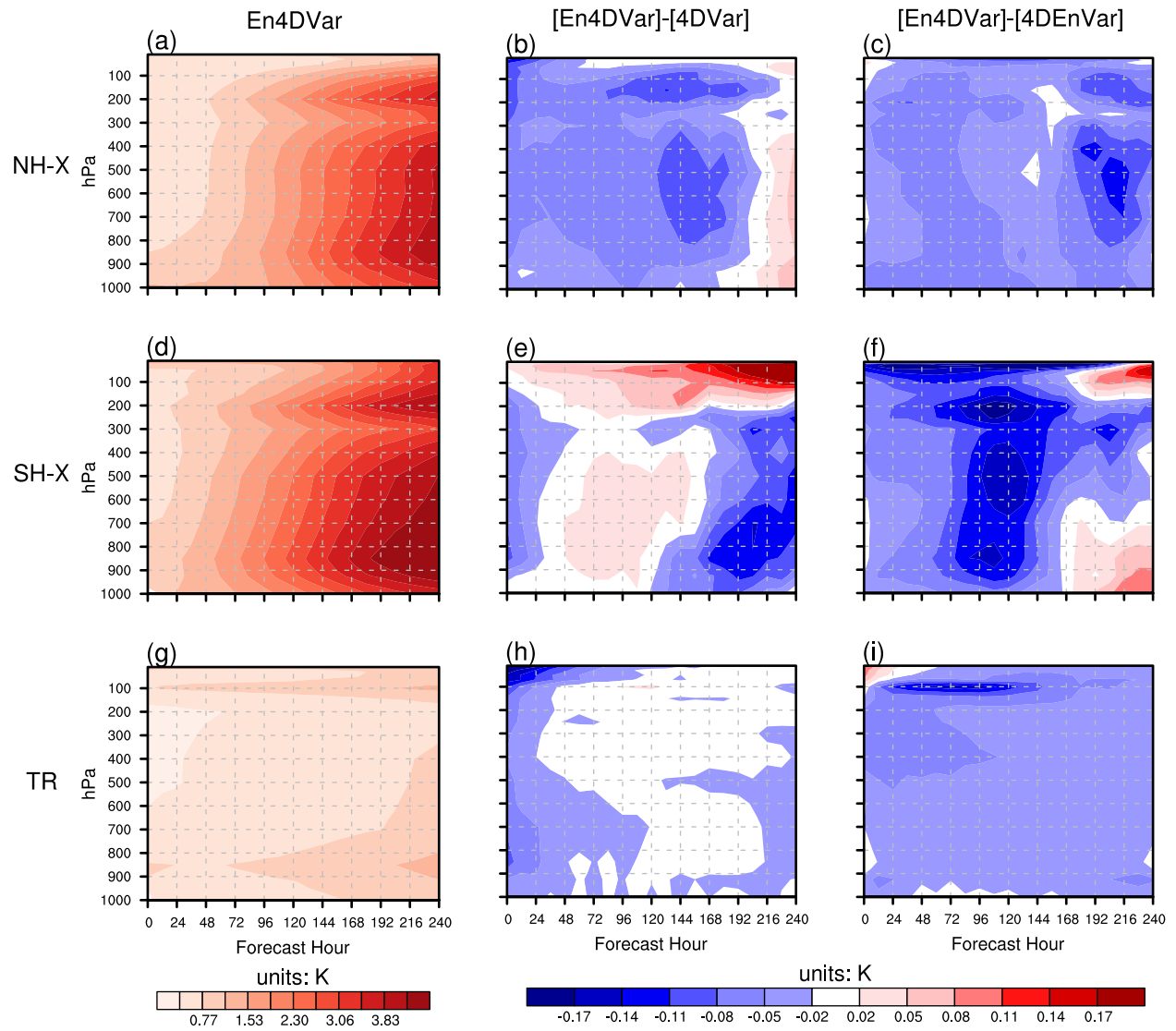
**Figure 10.** The ARMSEs of the geopotential height forecasts (units: gpm) initiated from the 1200 UTC analyses of the En4DVar experiment as a function of lead time (left column) in the (a) Northern Extratropics (20°N~90°N; 180°W~180°E), (d) Southern Extratropics (20°S~90°S; 180°W~180°E) and (g) Tropics (20°S~20°N, 180°W~180°E). The differences of ARMSE between the En4DVar- and 4DVar-(4DEnVar-)initialized (deterministic) forecasts are plotted in the middle (right) column.





**Figure 11.** Sam as Figure 10, except for the zonal wind forecasts (units: m/s).

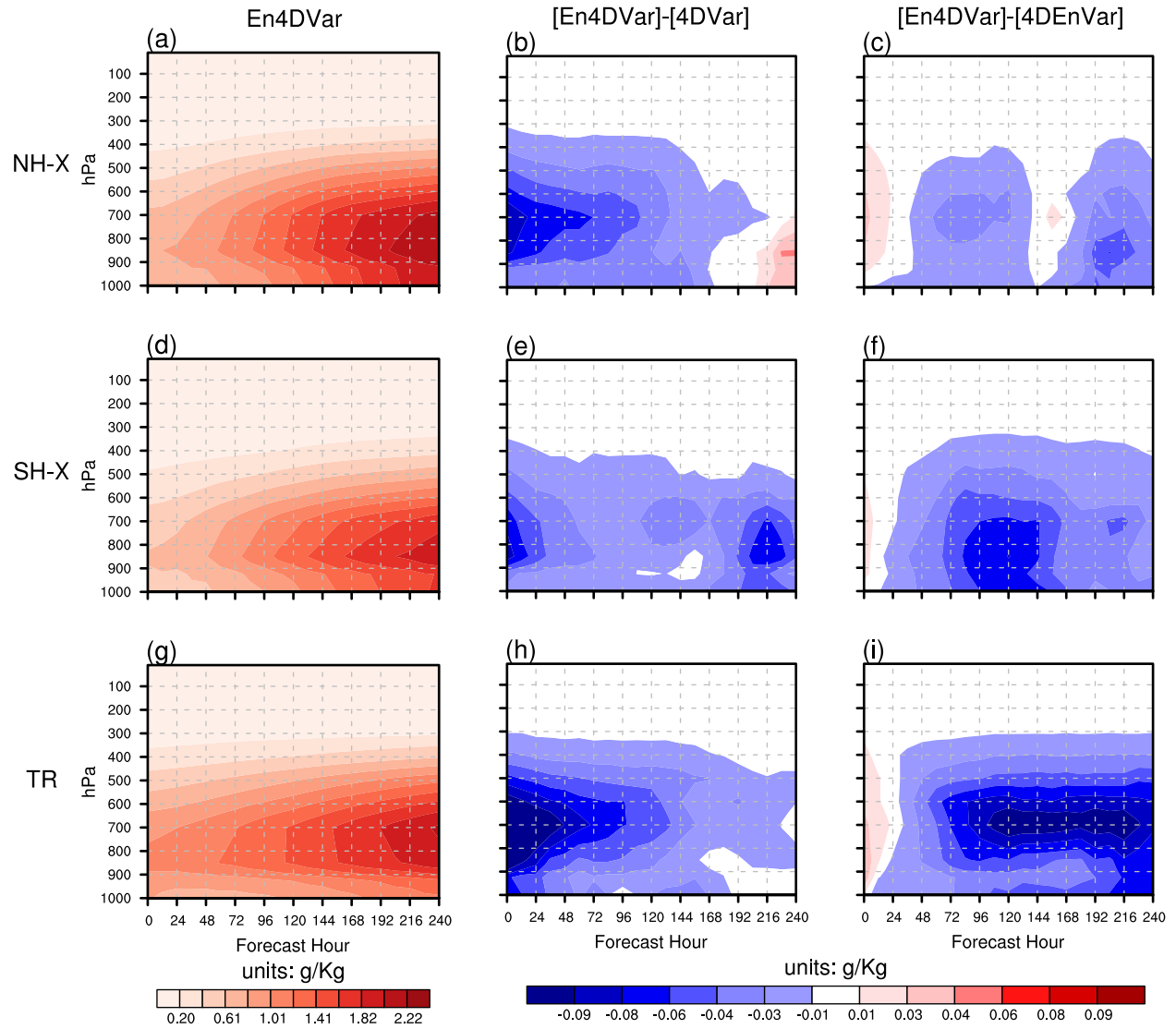




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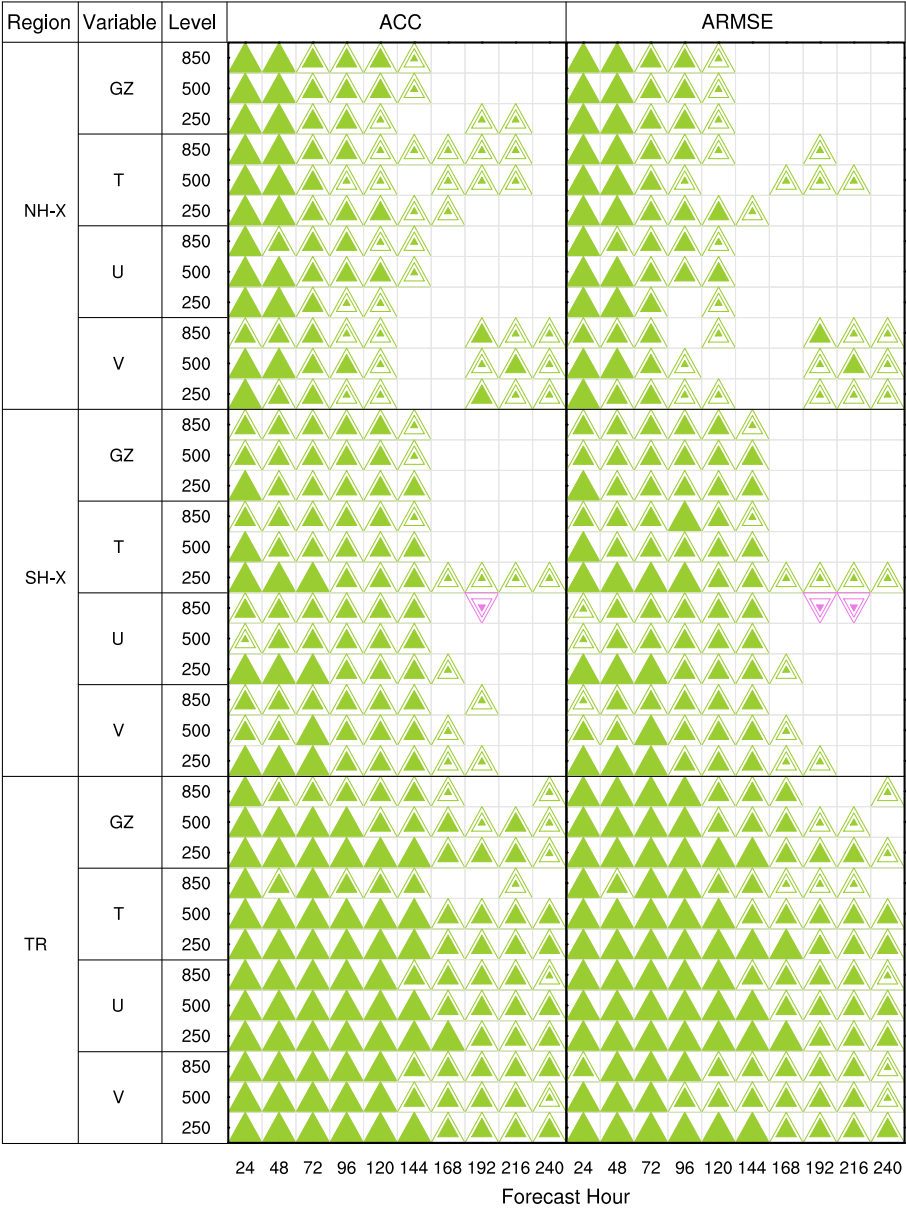
863 **Figure 12.** Sam as Figure 10, except for the temperature forecasts (units: K).





**Figure 13.** Sam as Figure 10, except for the specific humidity forecasts (units: g/kg).





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867 **Figure 14.** Same as Figure 3, except for the forecasts initialized by the En4DVar system adopting  
868 the linear combination coefficients of ( $\gamma_c = 0.25, \gamma_e = 0.8$ ) against the 4DEnVar-initialized  
869 deterministic forecasts.