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# Accounting for model error from unresolved scales in ensemble Kalman filters by stochastic parametrization

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#### ABSTRACT

We investigate by numerical experiment the use of discrete-time stochastic parametrization to account for model error due to unresolved scales in ensemble Kalman filters. The parametrization quantifies the model error and produces an improved non-Markovian forecast model, which generates high-quality forecast ensembles and improves filter performance. We compare this with the methods of dealing with model error through covariance inflation and localization (IL), using as example the two-layer Lorenz 96 system. The numerical results show that when the ensemble size is sufficiently large, the parametrization is more effective in accounting for the model error than IL; if the ensemble size is small, IL are needed to reduce sampling error, but the parametrization further improves the performance of the filter. This suggests that in real applications where the ensemble size is relatively small, the filter can achieve better performance than pure IL if stochastic parametrization methods are combined with IL.

#### 1. Introduction

Model error due to unresolved scales can degrade the performance of data assimilation schemes. Such model error can arise from failure to represent sub-grid processes correctly, from computational resources too limited to resolve all scales, and from discretization and truncation errors.

Various methods have been proposed for taking model error into account. One can roughly divide them into direct and indirect approaches. In an indirect approach, one accounts for model error in ensemble data assimilation by correcting the ensemble in the assimilation step. The most widely used indirect methods are covariance inflation and localization (IL) algorithms, which correct the sample covariance (Houtekamer and Mitchell 1998; Anderson and Anderson 1999; Mitchell and Houtekamer 2000; Hamill et al. 2001). These algorithms were originally introduced to reduce sampling errors in the sample covariance due to insufficient ensemble size. Nevertheless, they have been found to compensate effectively for model errors and have been widely used for that purpose (see e.g. Mitchell and Houtekamer (2000); Hamill and Whitaker (2005); Anderson (2007a, 2009)). Other examples of indirect methods include covariance relaxation (Zhang et al. 2004) and bias correction methods that use innovation from data to remove bias in the forecast ensemble (Dee and Da Silva 1998). The drawbacks of these indirect methods are that they need empirical tuning, and more important, that the deficiency of the forecast model remains.

In a direct approach, one seeks a representation of the model error to augment and improve the forecast model, so that the forecast ensemble has correct statistics and dynamics. Examples include deterministic and stochastic parametrization methods (Palmer 2001; Meng and Zhang 2007; Berry and Harlim 2014; Mitchell and Carrassi 2015), additive random perturbations (Hamill and Whitaker 2005; Houtekamer et al. 2009), low dimensional method (Li et al. 2009), and averaging and homogenization methods (Pavliotis and Stuart 2008; Mitchell and Gottwald 2012; Gottwald and Harlim 2013). Representations of the model error can be derived either within data assimilation using the noisy observations, or before data assimilation using noiseless training data. In the latter case, numerous results demonstrate that stochastic

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parametrization is preferable to deterministic parametrization (Buizza et al. 1999; Palmer 2001; Pavliotis and Stuart 2008), and that a non-Markovian model is preferable to a Markovian model in the absence of scale separation, see e.g. (Wilks 2005; Crommelin and Vanden-Eijnden 2008; Danforth and Kalnay 2008; Chekroun et al. 2011; Majda and Harlim 2013; Kondrashov et al. 2015). These findings are consistent with the Mori-Zwanzig analysis (Zwanzig 1973, 2001; Chorin and Hald 2013; Chorin et al. 2000, 2002; Gottwald et al. 2015) in statistical physics, which shows that a closed system of equations for a subset of variables in a given problem consists of a Markovian term, a non-Markovian memory term, and a stochastic noise term. The above-mentioned methods face challenges in deriving an effective non-Markovian model, due to difficulties in inferring a continuous-time model from partial discrete data and then deriving an accurate discretization for it. A novel, efficient, discrete-time non-Markovian stochastic parametrization scheme for quantifying model error was introduced in (Chorin and Lu 2015). This method is fully discrete, readily takes memory effects into account, simplifies the inference from discrete data, and requires no discretization. It leads to an improved non-Markovian forecast model that can capture key statistical and dynamical features of the resolved scales.

It is natural to ask whether the direct approach can be as good or better than the methods of IL in accounting for model error in ensemble Kalman filters (EnKF). Several direct methods have been studied for this purpose. Additive error representations were shown to improve the performance of the ensemble square root Kalman filter in (Hamill and Whitaker 2005); bias removal methods augmented by additive noise were shown to outperform pure inflation schemes in the local ensemble transform Kalman filter in (Li et al. 2009); time-varying and timeconstant model error representations were shown to reduce the tuning of IL in the ensemble transform Kalman filter in (Mitchell and Carrassi 2015).

In the present study we examine the discrete-time parametrization and compare it with covariance inflation and localization in accounting for model error in the EnKF. We assume that offline noiseless training data of the resolved scales can be generated, and used either to tune inflation and localization or to infer parameters in the parametrization. We examine both cases where the ensemble is large enough so that sampling error is negligible, and where the sample is small and sampling error needs to be reduced by IL. We carry out numerical tests on the two-layer Lorenz 96 system (Lorenz 1996), a simplified nonlinear model of atmospheric dynamics involving interacting resolved and unresolved scales of motion. A forecast model in the EnKF is a truncated model of the large scales alone, and its model error comes from the unresolved small scales. The parametrization directly accounts for the model error by constructing an improved forecast model for the filter, and is compared with the IL approach.

The numerical results show that when the ensemble size is large, the parametrization outperforms IL in accounting for model error. To the best of our knowledge, this is the first comparison made in a case where the ensemble size is large enough for sampling error to be negligible, so that both methods account exclusively for model error and their performance can be compared clearly. The numerical results also show that when the ensemble size is small, IL are needed to reduce sampling error, but the parametrization further improves filter performance. This result is in line with the previous findings in (Hamill and Whitaker 2005; Li et al. 2009; Mitchell and Carrassi 2015) that with the combination of stochastic methods and IL, the filter can achieve better performance than pure IL in practical small ensemble size.

The paper is organized as follows. In section 2 we provide a quick review of the EnKF. In section 3 we review covariance inflation and localization algorithms and discrete-time non-Markovian stochastic parametrization. We devote section 4 to a numerical study using the two-layer Lorenz 96 system, and conclude with a discussion of the results in section 5.

#### 2. The ensemble Kalman filter

The Ensemble Kalman Filter (EnKF) is a Monte-Carlo implementation of Bayesian filtering with the Kalman filter update (Evensen 1994; Evensen and Van Leeuwen 1996; Houtekamer and Mitchell 1998; Burgers et al. 1998). It uses an ensemble of random samples, also called particles, to approximate the forecast and analysis distributions by Gaussian distributions whose means and covariances are given by ensemble means and covariances. Among various EnKF algorithms, we choose to consider only the version with perturbed observations, introduced in (Burgers et al. 1998; Houtekamer and Mitchell 1998), and we refer to (Lei et al. 2010) for a comparison of different versions of EnKF algorithms.

Suppose the filter uses a forecast model

$$\mathbf{x}_n = \mathbf{F}_n(\mathbf{x}_{n-l:n-1}),\tag{1}$$

where  $\mathbf{x}_n \in \mathbb{R}^{d_x}$  is the state variable,  $\mathbf{x}_{n-l:n-1} = (\mathbf{x}_{n-l}, \dots, \mathbf{x}_{n-1})$ , and  $\mathbf{F}_n$  is a forecast operator at time *n* which maps  $\mathbb{R}^{l \times d_x}$  to  $\mathbb{R}^{d_x}$  with  $1 \le l \le n-1$ . The forecast model can be either stochastic or deterministic, and either Markovian (e.g. l = 1) or non-Markovian (e.g. l > 1). The state variable is observed through a linear observation operator with Gaussian noise:

$$\mathbf{z}_n = H\mathbf{x}_n + \varepsilon_n$$

where  $H \in \mathbb{R}^{d_z \times d_x}$  is the observation matrix, and the  $\varepsilon_n \sim N(0, R)$  are independent Gaussian noises. In this study, we assume that the observation matrix R is known.

#### a. The standard EnKF

The EnKF iterates the following two steps, with an initial ensemble of particles  $\{\mathbf{x}_0^{a,(i)}, i = 1,...,M\}$  sampled from the forecast distribution of the state variable **x** (e.g. the stationary distribution of the forecast model).

- 1. Forecast step: from the ensemble  $\{\mathbf{x}_{1:n-1}^{a,(i)}\}$  at time n-1, generate a forecast ensemble  $\{\mathbf{x}_{n}^{f,(i)}\}$  using the forecast model in (1), i.e.  $\mathbf{x}_{n}^{f,(i)} = F_{n}(\mathbf{x}_{n-l:n-1}^{a,(i)})$ . Here the superscript in  $\mathbf{x}_{n}^{f}$  denotes the ensemble from the forecast model, and the superscript in  $\mathbf{x}_{n}^{a}$  denotes the ensemble of the posterior distribution after assimilating data in the following analysis step. If the forecast model is stochastic, independent realizations should be used at different times.
- 2. Analysis step. Given new observation  $\mathbf{z}_n$ , update the forecast ensemble to get a posterior ensemble of  $\mathbf{x}_n$ ,

$$\mathbf{x}_{n}^{a,(i)} = \mathbf{x}_{n}^{f,(i)} + K_{n}(\mathbf{z}_{n}^{(i)} - H\mathbf{x}_{n}^{f,(i)}), \qquad (2)$$

for i = 1, ..., M, where the Kalman gain matrix is

$$K_n = C_n^f H^T (H C_n^f H^T + R)^{-1}, \qquad (3)$$

where the matrix  $C_n^f$  is the sample covariance of the forecast ensemble:

$$C_n^f = \frac{1}{M-1} \sum_{i=1}^M \left( \mathbf{x}_n^{f,(i)} - \overline{\mathbf{x}_n^f} \right) \left( \mathbf{x}_n^{f,(i)} - \overline{\mathbf{x}_n^f} \right)^T,$$

where  $\overline{\mathbf{x}_n^f} = \frac{1}{M} \sum_{i=1}^M \mathbf{x}_n^{f,(i)}$  and the  $\mathbf{z}_n^{(i)}$  are obtained by adding random perturbations  $\varepsilon_n^{(i)} \sim N(0,R)$  to  $\mathbf{z}_n$ :

$$\mathbf{z}_n^{(i)} = \mathbf{z}_n + \boldsymbol{\varepsilon}_n^{(i)}.$$

#### b. A block update algorithm

At each time *n*, only the current state  $\mathbf{x}_n^{(i)}$  of the *i*-th particle is updated in the analysis step in the above standard EnKF, and the past trajectory  $\mathbf{x}_{1:n-1}^{(i)}$  of the particle remains unchanged. Therefore, the time correlation between  $\mathbf{x}_n$  and  $\mathbf{x}_{1:n-1}$  is not properly represented by the ensemble. For a Markovian forecast model, this works fine, because the next state  $\mathbf{x}_{n+1}$  depends only on the current state  $\mathbf{x}_n$ . For a non-Markovian model with lag *l*, however, the next state  $\mathbf{x}_{n+1}$  depends directly on a block of past trajectory  $\mathbf{x}_{n-l+1:n}$ . This requires the ensemble to properly represent the space-time correlation of  $\mathbf{x}_{n-l+1:n}$ , and therefore the states  $\mathbf{x}_{n-l+1:n}$  should be updated as a whole at time *n*. Inspired by the block sampling algorithm of Doucet et al. (2006), we introduce the following block update algorithm that updates a block  $\mathbf{x}_{n-L+1:n}$  with  $L \ge l$ 

in the analysis step of the EnKF. This block update algorithm is akin to the fixed-lag smoother using EnKF (Khare et al. 2008), which is an implementation of the ensemble Kalman smoother (EnKS) discussed in Evensen and Van Leeuwen (2000) and Whitaker and Compo (2002).

Choose a block length  $L \ge 1$ , and define the augmented observation matrix  $\widetilde{H} \in \mathbb{R}^{Ld_z \times Ld_x}$  and the augmented noise covariance  $\widetilde{R} \in \mathbb{R}^{Ld_z \times Ld_z}$  as

$$\widetilde{H} = \operatorname{diag}(0, \dots, 0, H), \quad \widetilde{R} = \operatorname{diag}(0, \dots, 0, R).$$
 (4)

For n < L, use the above EnKF method. At time  $n \ge L$ , after obtaining the forecast ensemble  $\{\mathbf{x}_n^{f,(i)}\}$ , update the ensemble of the block path  $\mathbf{X}_n^{f,(i)} = (\mathbf{x}_{n-L+1:n-1}^{a,(i)}, \mathbf{x}_n^{f,(i)})$ :

$$\mathbf{X}_{n}^{a,(i)} = \mathbf{X}_{n}^{f,(i)} + \widetilde{K}_{n}((\mathbf{z}_{n}^{(i)} - \widetilde{H}\mathbf{X}_{n}^{f,(i)}),$$

for i = 1, ..., M, where the Kalman gain matrix is computed as

$$\widetilde{K}_n = \widetilde{C}_n^f \widetilde{H}^T (\widetilde{H} \widetilde{C}_n^f \widetilde{H}^T + \widetilde{R})^{-1}.$$

Here the matrix  $\widetilde{C}_n^f$  is the sample covariance of the forecast ensemble:

$$\widetilde{C}_{n}^{f} = \frac{1}{M-1} \sum_{i=1}^{M} \left( \mathbf{X}_{n}^{f,(i)} - \overline{\mathbf{X}_{n}^{f}} \right) \left( \mathbf{X}_{n}^{f,(i)} - \overline{\mathbf{X}_{n}^{f}} \right)^{T},$$

where  $\overline{\mathbf{X}_{n}^{f}} = \frac{1}{M} \sum_{i=1}^{M} \mathbf{X}_{n}^{f,(i)}$ . Then update the current *L*-step block by setting  $\mathbf{x}_{n-L+1:n}^{a,(i)} = \mathbf{X}_{n}^{a,(i)}$ .

When L = 1, the above algorithm is the same as the standard EnKF. When L > 1, it updates a block of the trajectory using the new observation. A natural choice of block length L is the length l of the memory in the forecast operator  $f_n(\mathbf{x}_{n-l:n-1})$ . This is the choice we make in this paper, and we leave it as future work to discuss of the optimal choice of L as well as of other issues such as covariance inflation and localization for this block update algorithm and its variants in applications to non-Markovian models.

#### 3. Methods to account for model error

Let a forecast model at our disposal be represented as

$$\mathbf{x}_n = \mathbf{f}_0(\mathbf{x}_{n-1}),\tag{5}$$

where  $\mathbf{x_n}$  is a vector in  $\mathbb{R}^{d_x}$  representing the resolved scales at time  $t_n$ , and  $\mathbf{f}_0$  is a forecast operator independent of time. This is a reduced model of a more complicated full model of the form:

$$\begin{cases} \widehat{\mathbf{x}}_n = \widehat{\mathbf{F}}(\widehat{\mathbf{x}}_{n-1}, \widehat{\mathbf{y}}_{n-1}), \\ \widehat{\mathbf{y}}_n = \widehat{\mathbf{G}}(\widehat{\mathbf{x}}_{n-1}, \widehat{\mathbf{y}}_{n-1}), \end{cases}$$
(6)

where  $\widehat{\mathbf{x}}_n \in \mathbb{R}^{d_x}$  and  $\widehat{\mathbf{y}}_n \in \mathbb{R}^{d_y}$  are the resolved and unresolved scales at time  $t_n$  respectively, with  $d_x << d_y \le \infty$ ,

and where the functions  $\widehat{\mathbf{F}}$  and  $\widehat{\mathbf{G}}$  map the states from time  $t_{n-1}$  to  $t_n$ . In general, this full model is a discrete representation of a system of differential equations. The reduced model is used when the full system is too difficult to solve or possible not fully understood, and it is often obtained by truncating the full system. The difference between the solutions of the reduced model (5) and the full model (6) is the model error due to unresolved scales.

#### a. Covariance inflation and localization

**Covariance localization.** Covariance localization was originally designed to remove poorly estimated longrange spatial correlations due to insufficient ensemble size (Houtekamer and Mitchell 1998; Gaspari and Cohn 1999; Furrer and Bengtsson 2007; Anderson 2007b). The standard implementation of localization is through the Schur product (entry-wise product, also known as Hadamard product) of the forecast covariance  $C_n^f$  by a localization matrix  $C_{loc}$ , which is a symmetric positive definite matrix with entries obtained from a predefined correlationlength function, known as taper function. In this study, we use the widely used Gaspari-Cohn taper function (Gaspari and Cohn 1999), which is a function with compact support given by

$$g(s) = \begin{cases} 1 - \frac{5}{3}s^2 + \frac{5}{8}s^3 + \frac{1}{2}s^4 - \frac{1}{4}s^5, & \text{if } 0 \le s \le 1; \\ -\frac{2}{3s} + 4 - 5s + \frac{5}{3}s^2 + \frac{5}{8}s^3 - \frac{1}{2}s^4 + \frac{1}{12}s^5, & \text{if } 1 \le s \le 2; \\ 0, & \text{if } s \ge 2. \end{cases}$$
(7)

The corresponding localization matrix is

$$C_{r_{loc}}(i,j) = g(|i-j|/r_{loc}),$$
 (8)

where  $r_{loc}$  is the localization radius. We refer to (Furrer and Bengtsson 2007; Anderson 2007b; Sakov and Bertino 2011) for analysis and comparisons between different localization methods, and refer to (Bishop and Hodyss 2007; Anderson 2012) and the references therein for recent developments in adaptive localization methods.

**Covariance inflation.** Covariance inflation algorithms account for the underestimation in the covariance of the forecast ensemble. There are two main types of covariance inflation, additive and multiplicative inflation. In additive inflation algorithms (Hamill and Whitaker 2005; Tong et al. 2016), the forecast covariance  $C_n^f$  in the EnKF is replaced by

$$\widehat{C}_n^f = C_n^f + \lambda I,$$

for some  $\lambda > 0$ . In multiplicative inflation algorithms (Anderson and Anderson 1999; Hamill et al. 2001), the spread of the forecast ensemble is inflated by replacing  $\mathbf{x}_n^{f,(i)}$  with  $\mathbf{x}_n^{f,(i)} + \sqrt{1+\lambda} \left( \mathbf{x}_n^{f,(i)} - \overline{\mathbf{x}_n^{f,(i)}} \right)$  for some  $\lambda > 0$ 

in the analysis step, which is equivalent to replacing the covariance  $C_n^f$  by

$$\widehat{C}_n^f = (1+\lambda)C_n^f.$$

This increases the covariance of the forecast ensemble, so as to account for the underestimation of covariance. Inflation has the effect of weighting the observations more than the deficient forecast model, and pulling the filter back towards the observations so as to avoid filter divergence. Optimization of the inflation parameter  $\lambda$  is usually done by numerical tuning. To avoid ad-hoc tuning and to account for the dynamical changes in the model error, adaptive inflation algorithms have been recently developed in (Anderson 2007a, 2009) for multiplicative inflation, and in (Kelly et al. 2014; Tong et al. 2015, 2016) for additive inflation.

In the numerical experiments that follow, we use inflation and localization simultaneously, test both additive and multiplicative inflation, and select the best combinations. The main cost is the generation of training data to tune the inflation parameter and the localization radius.

#### b. Discrete-time stochastic parametrization

The model error in the forecast model (5) is  $\widehat{\mathbf{F}}(\widehat{\mathbf{x}}_{n-1}, \widehat{\mathbf{y}}_{n-1}) - \mathbf{f}_0(\widehat{\mathbf{x}}_{n-1})$ , which can be seen by rewriting the first equation in the full system (6)

$$\widehat{\mathbf{x}}_n = \mathbf{f}_0(\widehat{\mathbf{x}}_{n-1}) + [\widehat{\mathbf{F}}(\widehat{\mathbf{x}}_{n-1}, \widehat{\mathbf{y}}_{n-1}) - \mathbf{f}_0(\widehat{\mathbf{x}}_{n-1})].$$

The discrete-time stochastic parametrization method quantifies the model error and produces an improved forecast model. It constructs a non-Markovian NARMA (nonlinear autoregression moving average) forecast model of the form

$$\mathbf{x}_n = \mathbf{f}_0(\mathbf{x}_{n-1}) + \Phi(\mathbf{x}_{n-p:n-1}, \xi_{n-q:n-1}) + \xi_n, \quad (9)$$

where the  $\{\xi_n\}$  are independent Gaussian random variables with mean zero and covariance diag $(\sigma_{\xi}^2)$ . The function  $\mathbf{f}_0$  comes from the original forecast model (5), and  $\Phi(\mathbf{x}_{n-p:n-1}, \xi_{n-q:n-1})$  is a parametric function of the form

$$\Phi_{n}: = \Phi(\mathbf{x}_{n-p:n-1}, \xi_{n-q:n-1})$$
(10)  
$$= \sum_{j=1}^{p} a_{j} \mathbf{x}_{n-j} + \sum_{i=0}^{r} \sum_{j=1}^{p} b_{i,j} \mathbf{f}_{i}(\mathbf{x}_{n-j}) + \sum_{j=1}^{q} c_{j} \xi_{n-j},$$

where  $\{a_j, b_{i,j}, c_j, \sigma_{\xi}^2\}$  are parameters to be estimated, and  $\{\mathbf{f}_i, i = 1, ..., r\}$  are functions to be provided by modelers. The appearance of  $\mathbf{f}_0$  in  $\Phi$  has the effect of modifying the coefficient of  $\mathbf{f}_0(\mathbf{x}_{n-1})$  from what it was the original forecast model.

The NARMA model can capture key statistical and dynamical features of the resolved scales, and generate high quality forecast ensembles which have correct mean and covariance if the ensemble size is sufficient. We emphasize that this is different from just correcting the ensemble, because the forecast model is improved, and this treats the root of the model error problem.

The main difficulty in this construction is deriving and selecting the ansatz (i.e. the functions  $\{\mathbf{f}_i\}$  and the orders  $\{p, r, q\}$ ) of the NARMA model. The ansatz may be derived from the physical properties of the full system, and it may depend on the numerical scheme used in the original reduced model. We refer to (Crommelin and Vanden-Eijnden 2008; Majda and Harlim 2013; Kondrashov et al. 2015; Harlim 2016; Lu et al. 2017, 2016) for further discussion.

Once {**f**<sub>*i*</sub>} and the orders {*p*,*r*,*q*} are fixed, the parameters  $\theta = \{a_j, b_{i,j}, c_j, \sigma_{\xi}^2\}$  are estimated by conditional likelihood methods. We first solve the full system (6) offline to generate a time series { $\hat{\mathbf{x}}_n$ }<sup>*N*</sup><sub>*n*=1</sub> for a large *N*. Then the parameters are estimated as follows. Conditional on  $\xi_1, \ldots, \xi_m$ , the negative log-likelihood of { $\mathbf{x}_n = \hat{\mathbf{x}}_n$ }<sup>*N*</sup><sub>*n*=*m*+1</sub> is

$$L(\theta|\xi_{1},...,\xi_{m}) = \sum_{k=1}^{d_{x}} \sum_{n=m+1}^{N} \frac{\left(\mathbf{x}_{n,k} - \Phi_{n,k}\right)^{2}}{2\sigma_{\xi,k}^{2}} + \frac{N-q}{2}\log\sigma_{\xi,k}^{2}$$
(11)

where  $m = \max\{p, q\}$ ,  $\theta = (a_j^k, b_{i,j}^k, c_j^k, \sigma_{\xi,k}^2)$ . For a given value of  $\theta$ , if q = 0, the values of  $\{\Phi_n\}_{n=m+1}^N$  can be computed directly from data  $\{\mathbf{x}_n\}_{n=1}^N$ . If q > 0, the values of  $\{\Phi_n\}_{n=m+1}^N$  and  $\{\xi_n\}_{n=m+1}^N$  can be computed recursively, conditional on  $\xi_1 = \cdots = \xi_m = 0$ . That is, one computes  $\Phi_{m+1}$  from  $\xi_{m-q+1:m}$  using equation (10), and computes  $\xi_{m+1}$  from  $\Phi_{m+1}$  using equation (9); and repeats this process for the rest times  $n \ge m+1$ . The maximum likelihood estimator (MLE) of the parameter is the minimizer of the negative log-likelihood

$$\widehat{\theta}_N = \arg\min_{\boldsymbol{\theta}} L_N(\boldsymbol{\theta}|\boldsymbol{\xi}_1,\ldots,\boldsymbol{\xi}_m).$$

If q = 0, the minimization reduces to least squares regression. If q > 0, the minimization can be done by iterative least squares (Ding and Chen 2005) or other optimization methods.

As in covariance inflation and localization algorithms, the main cost of the discrete-time stochastic parametrization method is the generation of training data. This requires solving the full system offline for a time interval long enough so that the maximum likelihood estimator, which converges at the rate  $1/\sqrt{N}$ , is close to its limit. The cost of parameter estimation depends on the NARMA model. It is negligible if the model does not have a moving average term, i.e. if q = 0. In this case the maximum likelihood estimator is equivalent to the least squares estimator. The cost varies when  $q \neq 0$  since the minimization may need many iterations.

#### 4. Numerical experiments on the Lorenz 96 system

In this section we carry out numerical experiments on the two-layer Lorenz 96 system (Lorenz 1996), which consists of K resolved variables  $x_k$  coupled to  $J \times K$  unresolved variables  $y_{j,k}$ 

$$\frac{d}{dt}x_k = x_{k-1}(x_{k+1} - x_{k-2}) - x_k + F + z_k,$$
  
$$\frac{d}{dt}y_{j,k} = \frac{1}{\varepsilon}[y_{j+1,k}(y_{j-1,k} - y_{j+2,k}) - y_{j,k} + h_y x_k].$$

where  $z_k = \frac{h_x}{J} \sum_j y_{j,k}$ , and  $k = 1, \dots, K$ ,  $j = 1, \dots, J$ . The indices are cyclic,  $x_k = x_{k+K}$ ,  $y_{j,k} = y_{j,k+K}$  and  $y_{j+J,k} =$  $y_{i,k+1}$ . The system is invariant under spatial translations, and the statistical properties are identical for all  $x_k$ . The formulation here is equivalent to the original formulation by Lorenz (see e.g. Fatkulin and Vanden-Eijnden (2004); Crommelin and Vanden-Eijnden (2008); Kwasniok (2012)). The parameter  $\varepsilon$  measures the scale separation between the resolved variables  $x_k$  and the unresolved variables  $y_{i,k}$ . We set  $\varepsilon = 0.5$ , so that there is no significant scale separation between resolved and unresolved processes, as is both more realistic and more difficult to handle for parameterizations (see (Fatkulin and Vanden-Eijnden 2004) and references therein). We take  $K = 18, J = 20, F = 10, h_x = -1$  and  $h_y = 1$ . Here one model time unit is approximately equal to five atmospheric days, deduced by comparing the error doubling time of the model to that observed in the atmosphere (Lorenz 1996; Arnold et al. 2013; Mitchell and Carrassi 2015).

In the experiments, we take a trajectory of the resolved variables *x* in the full system to be the truth. We solve the full system by a fourth-order Runge-Kutta method with a time-step dt = 0.001, and make recordings every 50 steps, i.e. with observation spacing h = 0.05, approximately six atmospheric hours. To eliminate transients, we begin to make observations after running the full model for 100 time units. To create noisy observations we add to the recorded trajectory independent Gaussian random vectors with mean zero and covariance  $R = \sigma_{F}^{2}I$ .

In the data assimilation, we assume that we cannot afford to solve the full Lorenz 96 system for ensemble forecasts, and use a reduced system obtained by discarding the y variables:

$$\frac{d}{dt}x_k = x_{k-1}(x_{k+1} - x_{k-2}) - x_k + F,$$

for k = 1, ..., K. After discretization by a fourth-order Runge-Kutta method with time-step *h* (i.e. the observation spacing), one obtains a system of difference equations:

$$x_{k,n} = x_{k,n-1} + f_k^h(x_{\cdot,n-1}), \tag{12}$$

for k = 1, ..., K, where  $x_{k,n}$  is the value of the component  $x_k$  at time *n*. Hereafter we refer to this reduced discretized

model as *the L96x model*, and we refer to the discrete representation of the full L96 system as *the full model*.

**This paragraph will be deleted.** The model error in the L96x model comes from the unresolved *y* variables. It has been shown to have a mean close to zero (see e.g. (Arnold et al. 2013; Chorin and Lu 2015; Mitchell and Carrassi 2015)), hence the biases in the means of forecast ensembles are negligible. This removes a concern about ensemble bias in the use of covariance inflation and localization to account for such model error (Dee and Da Silva 1998; Li et al. 2009).

In the following, we first implement the two methods reviewed in Section 3 to account for such model error in Sections a-b, and then compare their filtering and forecasting performance in Sections c-d.

#### a. Accounting for model error by discrete-time stochastic parametrization

Discrete-time stochastic parametrization quantifies the model error of the L96x model and produces an improved forecast model, which we call the NARMA model, as introduced in section b. Specifically, this is done by using the conditional likelihood method to fit a NARMA model to a set of training data, which is generated by solving the full model for a long time. The initial conditions in the simulation that generates training data can be arbitrary, because the estimated parameters of the NARMA model will converge as the length of the training data increases, due to ergodicity of the full system (Chorin and Lu 2015). According to the results in (Chorin and Lu 2015), we use a NARMA(2,0) model

$$x_{k,n} = \sum_{j=1}^{2} (a_j x_{k,n-j} + b_j f_k^h(x_{\cdot,n-j})) + c_0 + c_1 x_{k,n-1}^2 + c_2 x_{k,n-j}^2$$

where  $f_k^h(x)$  comes from the right hand side of (12), and  $\{\xi_{\cdot,n}\}$  is a sequence of independent Gaussian random vectors with mean zero and covariance  $\sigma_{\xi}^2 I$ . The parameters in the different components are the same due to the symmetry in the equations.

The main cost in deriving the NARMA representation is the generation of training data. The cost of the NARMA parameter estimation is negligible compared with cost of generating training data, because the model does not have moving average terms and the optimization reduces to linear least squares. In our tests, the training data were generated by solving the full system with step size dt = 0.001and recording data every 50 steps, i.e. with observation spacing h = 0.05. Table 1 shows the values of the parameters  $(a_j, b_j, c_j, \sigma_{\xi})$  estimated from a training dataset of length  $N = 10^5$ , i.e. 5000 time units, approximately equal to 69 atmospheric years. Further tests showed that a datalength of  $N = 10^4$  could also lead to models with good statistical properties. The minimum data-length necessary to identify a NARMA model is problem dependent, and a general criterion is beyond the scope of the current study.

TABLE 1. Values of the parameters in the NARMA model.

$a_1$	$a_2$	$b_1$	$b_2$
1.8992	-0.9022	0.9946	-0.9058
$c_0$	$c_1 \; (\times 10^{-5})$	$c_2 \; (\times 10^{-5})$	$\sigma_{\xi}$
0.0024	-0.3903	0.9396	0.0084

NARMA as an improved forecast model for the L96x model. Figure 1 shows the empirical probability density function (PDF) and the autocorrelation function (ACF) of the full model, the L96x model and the NARMA model, computed from time averaging of a long trajectory of each model. The NARMA model reproduces the PDF and the ACF faithfully, while the L96x model misses the shape of the PDF and the oscillation of the ACF. The PDF approximates the invariant measure of the large-scale variables, and the ACF approximates the dynamical transition. Hence, the NARMA model captures the statistical and dynamical features of the large-scale variables much better than the L96x model.

By accounting for the model error, the NARMA model significantly improves state estimation of the filters over the L96x model. Table 2 shows the mean and standard deviation of the relative errors of state estimation on 100 simulations, in which the variance of observation noise is  $\sigma_{\varepsilon} = 0.2$  and the ensemble size is M = 1000. Here we judge the quality of the state estimates by the relative error in the ensemble means, that is, the relative difference between the ensemble means and the truth,

$$e_{rel} = \left(\sum_{\substack{n=N_0+1\\k,n-1}}^{N} \sum_{k=1}^{K} |\overline{x_{k,n}} - x_{k,n}|^2 / \sum_{\substack{n=N_0+1\\k=1}}^{N} \sum_{k=1}^{K} |x_{k,n}|^2 \right)^{1/2},$$
(14)

where  $(\overline{x_{k,n}}, n = N_0 + 1, ..., N)$  are the ensemble means, and  $(x_{k,n}, n = N_0 + 1, ..., N)$  are the true state values. We skipped the first  $N_0$  steps so as to eliminate the transients in assimilation. In the tests, it took only a few steps for the filters to reach a stationary state, so we took N = 400and  $N_0 = 200$ . We implemented both the standard EnKF and the EnKF with block update using block length L = 2. In both cases, the NARMA model successfully reduced the relative error in the state estimation to below 2.10%, which is the relative uncertainty induced by the observation noise; the filter with L96x model performs very poorly, due to the model error.

We also tested a parametrization using a Markovian model in the form of NARMA (1,0) similar to equation (13). The Markovian model reproduced the empirical PDF and ACF well, but is slightly inferior to the NARMA model (data not shown here). The Markovian model successfully reduced the relative error to  $0.0210\pm 0.0022$  in the above 100 simulations, which is slightly larger than those of the NARMA model ( $0.0156\pm 0.0019$ ). Also, the NARMA model yielded better forecast performance than the Markovian model. Therefore it is important to choose

TABLE 2. The mean and standard deviation of the relative errors of state estimation on 100 simulations, in which the ensemble size is M = 1000 and the variance of the observation noise is  $\sigma_{\varepsilon} = 0.2$ . Both the standard EnKF and the EnKF with the block update algorithm are implemented, with the L96x model and the NARMA model as forecast model.

	Standard EnKF	EnKF with Block Update
L96x	$0.7884 \pm 0.0774$	$0.8022 \pm 0.0818$
NARMA	$0.0182 \pm 0.0016$	$0.0156 \pm 0.0011$

a good model for the model error, and we consider only the NARMA model in this study.

These results show that discrete-time stochastic parametrization can effectively account for model error, and therefore improve the performance of ensemble filter.

Note also that the block update algorithm reduces the error of state estimation for the NARMA model, but it does not improve the performance of the filter with the L96x model. Hence, in the following tests, we use the block update algorithm for the NARMA model and the standard EnKF for the L96x model.

#### b. Accounting for model error by tuning inflation and localization

Covariance inflation and localization (denoted by IL hereafter) can account for both model error and sampling error, but the parametrization can only reduce model error. To compare their effectiveness in accounting for model error, we consider two situations, one with an ensemble sufficiently large for sampling error to be negligible, and one with a practical small ensemble. In the first situation, we compare filter performance of the NARMA model using no IL, with the performance of the L96x model using best tuned IL. This highlights the impact of the two methods on accounting for model error. In the second situation, we apply IL to both the L96x and the NARMA models; in the L96x model, IL accounts for both sampling error and model error; in the NARMA model, IL accounts mainly for sampling error.

We also test the standard EnKF using the full model, which has no model error, as forecast model, so as to provide a useful yardstick for assessing the results.

We carry out the covariance localization with the localization matrix  $C_{r_{loc}}$  defined in (8), using the Gaspari–Cohn taper function (7), where  $r_{loc}$  is the localization radius. We also tested a Toeplitz circulant matrix with exponential spectrum decay, but there is no clear improvement in filter performance over the Gaspari–Cohn matrix (data not shown here). In the EnKF with block update, the localization matrix is an array containing *L* copies of  $C_{r_{loc}}$  in the row and column dimensions.

We tune the localization and inflation by trying different values of  $r_{loc}$  and  $\lambda$  for filtering a single set of observations with noise variance  $\sigma_{\varepsilon} = 0.2$ . Both additive and

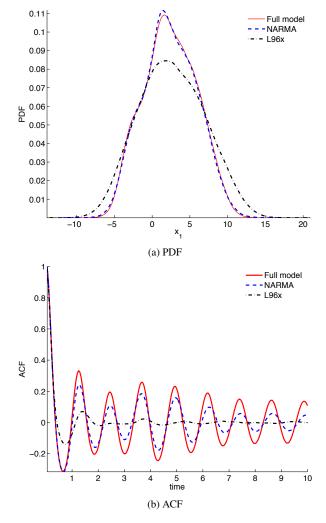


FIG. 1. Empirical probability density function (PDF) and autocorrelation function (ACF) of the full model, the L96x model and the NARMA model.

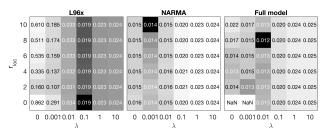


FIG. 2. Relative error of the ensemble fitter for different covariance localizations and additive inflations, with ensemble size M = 10 for the full model, and M = 1000 for the reduced models. The letters NaN indicates that the filter diverged. Here a localization radius  $r_{loc} = 0$  means no localization. An additive inflation  $\lambda = 0$  means no inflation.

multiplicative inflation were tested, and additive inflation led to slightly better filter performance for both the full and the L96x models (data are not shown here). Hence in the following we only consider additive inflation.

TABLE 3. The best tuned values of localization radius  $r_{loc}$  and additive inflation parameter  $\lambda$  for the three models using ensemble size M = 10.

	L96x	NARMA	Full model
Localization radius rloc	2	2	2
Additive inflation $\lambda$	0.1	0.01	0.01

**Tuning in the case of sufficient ensemble size.** We first discuss tuning in the case where the sample size is sufficiently large for sampling error to be negligible. Here, a large ensemble with M = 1000 members is found to be sufficient. For the computational cost to be similar to that of the L96x and NARMA models, the full model uses an ensemble of size M = 10, with IL to account for the sampling error due to insufficient size. Tests showed that IL were able to effectively account for the sampling error, yielding state estimations almost as accurate as the full model with an ensemble size M = 1000.

Figure 2 shows the relative errors in scaled colors (the darker the color, the smaller the relative error in state estimation) for different  $r_{loc}$  and additive inflation  $\lambda$ . Here a localization radius  $r_{loc} = 0$  means no localization, and an additive inflation value  $\lambda = 0$  means no inflation. To demonstrate the need of tuning for different models, common values of  $r_{loc}$  and  $\lambda$  are plotted. The best tuned values shown here may not be optimal, but they are close to the optimal values in finer tuning.

The left plot shows the relative errors of the L96x model with IL. Because of model error, the L96x model performs poorly without IL ( $r_{loc} = 0, \lambda = 0$ ). As the additive inflation parameter  $\lambda$  increases, the relative error in state estimation first sharply decreases and then slightly increases; a similar pattern can be observed as the localization radius  $r_{loc}$  increases. To select the best values for  $r_{loc}$  and  $\lambda$ , we do not choose the pair  $(r_{loc}, \lambda)$  which produces the smallest relative error in the array, but rather the pair at the intersection of the column and the row which have the smallest sum of relative errors among the columns and rows respectively. This is because tests show that the pair that yields the smallest error is sensitive to various factors, such as the number of observations and the initial conditions used to generate the training data, while the pairs at the intersection are much more robust to these factors. For the L96x model, this strategy yields  $(r_{loc}, \lambda) = (2, 0.1)$ .

In the middle plot we show the parameter values for tuning IL for the NARMA model. IL bring negligible improvements for the NARMA model: the relative error decreases only from 0.016 to 0.014 in this simulation (results are similar for other simulations). This suggests that the NARMA model has accounted for the model error so well that IL cannot help much.

The right plot shows the relative errors in filtering with the full model. Due to sampling error caused by the small ensemble size, the EnKF with the full model diverges if no localization or inflation is used. IL accounts for the sampling error, stabilizes the filter and leads to accurate state estimation with relative error 0.013, while the relative error of the full model with M = 1000 is 0.011. The best values for the IL parameters in this setup are  $r_{loc} = 2$  and  $\lambda = 0.01$ .

In summary, when comparing filter performance in the case of large ensemble size in section c, we use  $r_{loc} = 2$  and  $\lambda = 0.1$  for the L96x model, and  $r_{loc} = 2$  and  $\lambda = 0.01$  for the full model. For the NARMA model, we use a block updating algorithm without any localization or inflation. We found that even with tuned IL, the filter with the full model may diverge (with a frequency of about 2 out of 100 simulations). Since the full model only serves as a reference, we drop the simulation when the filter diverges.

Tuning in the case of small ensemble size. We use the same tuning strategy as above for different small ensemble sizes, ranging from 10 to 100. Table 3 shows the best pair of the localization radius  $r_{loc}$  and the additive inflation parameter  $\lambda$  in the case of ensemble size M = 10. The best pair  $(r_{loc}, \lambda)$  for the L96x model did not change much when ensemble size changed. The best pairs of  $(r_{loc}, \lambda)$  for the NARMA model and the full model were sensitive to changes in ensemble size, with  $\lambda$  varying between 0.001 and 0.01 and  $r_{loc}$  varying between 2 to 10. But the relative errors corresponding to these pairs in the array were very close to each other (data not shown here, but this can be readily seen from the middle and right plots in Figure 2). Therefore, we accept these suboptimal pairs and use them in the table for other ensemble sizes when comparing filter performance in section d.

# c. Filter performance comparison: the case of sufficient ensemble size

We consider first the case of a large ensemble size M = 1000. This setup aims to answer the main question of this paper: whether the parametrization can be as effective as IL in accounting for the model error due to unresolved scales. With this M, the sampling error in the ensemble covariance is negligible compared to the model error, therefore the filter performance depends on how well the two methods can account for the model error.

Their performance is measured by the resulting state estimates and ensemble forecasts. We first compare them in a single simulation, and then consider the statistics of the errors over 100 simulations. Results from the full model, with ensemble size M = 10 and IL with  $(r_{loc}, \lambda) = (2, 0.01)$  are included to provide a sense of the best possible results at a comparable computational cost.

**State Estimation.** The trajectories in a short single simulation with observation noise  $\sigma_{\varepsilon} = 0.2$  are shown in Figure 3. The filtered trajectories (the magenta lines) are in the time interval [0,6]. The ensemble and its mean (the black dash dot lines) follow the true trajectory (the blue

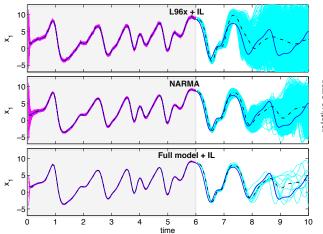


FIG. 3. Ensembles of trajectories in filtering and forecasting. Each plot contains a true trajectory (blue line), an ensemble of filtering trajectories (magenta lines) in the time interval [0, 6] (in gray shade) and forecasting trajectories (cyan lines) in the time interval (6, 10], and the ensemble mean (black dash-dot line). Covariance inflation and localization (IL) accounts for the model error of the L96x model in the filter, and the parametrization reduces the model error through the NARMA model, in the case of a large ensemble size M = 1000. The full model provides a yardstick for performance at a comparable cost by using tuned IL with ensemble size M = 10.

line) relatively well for all the three forecast models. The relative errors of state estimation are 1.91%, 1.59% and 1.31% for the L96x, NARMA and full model, respectively.

The difference in state estimation is clear in the statistics of the relative error in 100 simulations, as shown in Figure 4. To test the robustness of the filter, we consider different variances of observation noise, with  $\sigma_{\varepsilon}$  taking the values  $\{0.1, 0.2, 0.4, 0.8\}$ , for which the relative error of the observation noise ranges from 1.05% to 8.40%. The NARMA model, using no covariance localization or inflation, has smaller errors than the L96x model using tuned IL. For example, in the case  $\sigma_{\varepsilon} = 0.2$ , the average relative errors are 1.73%, 1.33% and 1.11% for the L96x, NARMA and full model, respectively. The relative error of the L96 model is about 1.3 times the relative error of the NARMA model. This shows that the stochastic parametrization is more effective than IL in dealing with model error. On the other hand, with the help of IL, the full model with a small ensemble size has slightly smaller errors than the NARMA model. This indicates that (i) tuned covariance IL are effective in dealing with sampling error, (ii) there is still model error in the NARMA model.

**Forecasting.** The goal of state estimation is to provide initial conditions for the forecast model to use in forecasting the future evolution of the resolved scales. After assimilating the last observation, the filtering ensemble provides the desired initial conditions, and by running the forecast model, we obtain a forecasting ensemble.

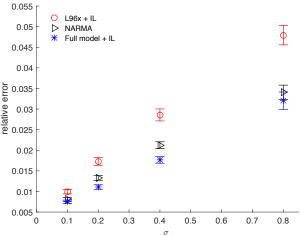


FIG. 4. Mean and standard deviation of the relative error of state estimation calculated with 100 simulations for different variances of observation noise. The ensemble size is 1000 for the L96x and NARMA model, and 10 for the full model. The L96x model and the full model use tuned inflation and localization (IL), and the NARMA uses neither.

The difference in the ensemble forecasts of these models is clear in the single simulation shown in Figure 3. The forecasting trajectories (the cyan lines) are in the time interval (6,10]. It is desirable that the ensemble of forecasting trajectories follow the true trajectory as long as possible before spreading out. The ensemble of the full model follows the true trajectory for about 2.5 time units (from t = 6 to t = 8.5), and the L96x and NARMA models for about 1 and 1.8 time units respectively. The ensemble means keep following the true trajectory slightly longer. This shows that the NARMA model has better prediction skills than the L96x model in this simulation.

The improved forecast of NARMA model over the L96x + IL combination can be attributed to two factors: a better forecast model and more accurate two-step initial distributions. To dis-entangle these two factors, we tested a Markovian model in the form of NARMA(1,0) simultaneously with the above non-Markovian NARMA and L96x model. Results showed that the Markovian NARMA(1,0) model made forecast slightly inferior to the NARMA model but much better than L96x + IL, while it has relative errors in state estimation similar to L96x+IL. This suggests that the improvement of the forecast of the NARMA model over L96x + IL comes mainly from the better forecast model.

We further compare the forecast performance on 100 simulations, by studying the root mean square error (RMSE) and the anomaly correlation (ANCR) between the mean trajectories of the forecast ensembles and the true trajectories. The RMSE measures the average difference between trajectories whereas the ANCR measures the average correlation between them (Crommelin and Vanden-Eijnden 2008). Figure 5 shows the RMSE and

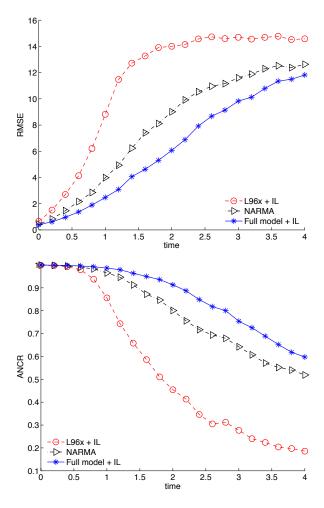


FIG. 5. RMSE and ANCR of ensemble forecasting on 100 simulations, with  $\sigma_{\varepsilon} = 0.2$ . The ensemble size is 1000 for the L96x model and the NARMA model, and the ensemble size is 10 for the full model. The L96x model and the full model use tuned inflation and localization (IL), and the NARMA uses neither.

the ANCR of the forecast ensemble in the 100 simulations, when  $\sigma_{\varepsilon} = 0.2$ . A small and slowly increasing RMSE, combined with a large and slowly decreasing ANCR, indicate a good forecast performance. The NARMA model shows a significant improvement over the L96x model, and is close to the full model, which has the smallest RMSE and the largest ANCR. With the threshold of RMSE less than 9 and the ANCR larger than 0.8, the forecast time of the NARMA model is about two time units (approximately 10 atmospheric days), which is double of the L96x model's one time unit (approximately five atmospheric days), and is slightly less than the full model's 2.5 time units (approximately 13 atmospheric days). We also computed the rank histogram (Crommelin and Vanden-Eijnden 2008) at lead time 1.6, see Figure 6. The rank histogram of the full model is almost flat as desired, NARMA has a rank histogram close to flat, but L96x

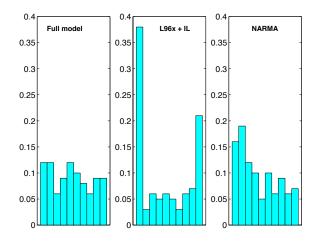


FIG. 6. Rank histograms of the 100 simulations at lead time  $\tau = 1.6$ . An ideal rank histogram should be flat. The full model has the flattest rank histogram, NARMA's rank histogram is close to flat, but L96x + IL has a U-shaped rank histogram.

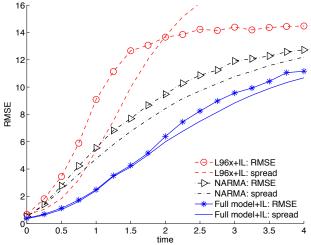


FIG. 7. Comparison of RMSE with ensemble spread (i.e. the trace of the ensemble covariance). The ensemble spread of the full model matches the RMSE well, and the ensemble spread of NARMA is close to the RMSE, but there is a big mismatch between the ensemble spread and the RMSE for L96x+IL.

+ IL has a U-shaped rank histogram. We also compared the RMSE with ensemble spread (i.e. the trace of the ensemble covariance) in Figure 7. The ensemble spread of the full model matches the RMSE well, and the ensemble spread of NARMA is close to the RMSE, but there is a big mismatch between the ensemble spread and the RMSE for L96x + IL. The results for the other values of  $\sigma_{\varepsilon}$  are similar (data not shown here).

In short, the NARMA model has significantly better state estimation and prediction performance than the L96x

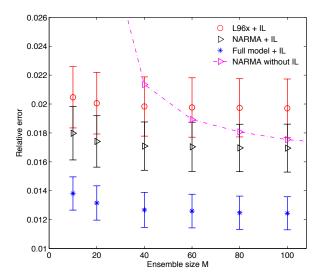


FIG. 8. Mean and standard deviation of the relative error of state estimation in the EnKF with different ensemble sizes on 100 simulations. All the three models use inflation and localization (IL). The mean of the NARMA model without IL is also plotted to indicate that sampling error decreases as ensemble size increases.

model, and its performance is close to that of the full model. Recall that the NARMA accounts for the model error by discrete-time stochastic parametrization of the unresolved scales, while the L96x model accounts for the model error by covariance inflation and localization. This suggests that the discrete-time stochastic parametrization is more effective in dealing with model error than covariance inflation and localization.

### d. Filter performance comparison: the case of small ensemble size

Due to limited computational resources, in many applications one can afford only a small ensemble, and significant sampling error may be present. In this case, localization and/or inflation are needed to account for the sampling error.

In this subsection, we compare the filter performance for several small ensemble sizes, ranging from M = 10 to M = 100, with all the models using tuned IL with parameters given in Table 3. In all of them, the variance of the observation noise is  $\sigma_{\varepsilon} = 0.2$ .

**State estimation.** Figure 8 shows the means and standard deviations of the relative errors in state estimation on 100 simulations, with several small ensemble sizes. With tuned IL, the NARMA model (black triangle) has smaller errors than the L96x model (red circle) for all sizes. Recall that IL account for both sampling error and model error for the L96x model, while in the filter with the NARMA model, they mainly account for the sampling error while the stochastic parametrization accounts for model error.

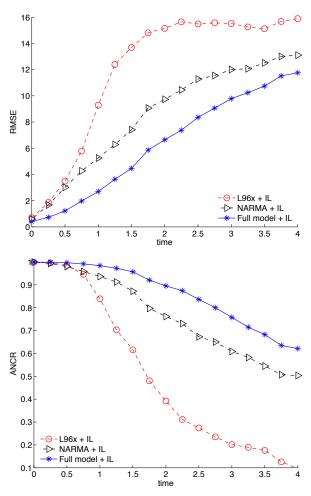


FIG. 9. RMSE and ANCR of ensemble forecasting on 100 simulations, with  $\sigma_{\varepsilon} = 0.2$ . All the models use ensemble size M = 10 and tuned inflation and localization.

This shows that the parametrization treats the model error more effectively than IL and improves the filter performance.

We also tested the NARMA model without using inflation or localization (cyan triangle with dash-dot line). Its error decreases much faster than those using inflation and localization as ensemble size increases. In particular, it has smaller errors than L96x with tuned IL when the ensemble size is larger than 60. Also, its performance becomes close to the NARMA with IL when the ensemble size is 100. This indicates that (i) the NARMA model has effectively reduced the model error of the L96x model; (ii) the sampling error becomes small when ensemble size reaches M = 100 (It also verifies that the size M = 1000 used in section c is sufficiently large to make the sampling error negligible). **Forecasting.** Figure 9 shows the RMSE and the ANCR of the forecast ensemble in 100 simulations, with all models using ensemble size M = 10 and tuned IL. The NARMA model is a clear improvement over the L96x model in forecasting: its RMSE increases much slower, and its ANCR decreases much slower. But the gap between the NARMA model and the full model is slightly larger than the gap in Figure 5, where a large ensemble size was used. Here the forecast time of the NARMA model is about 1.5 time units (approximately eight atmospheric days), which is 50% more than the L96x model's one time unit (approximately five atmospheric days), and it is less than the full model's 2.5 time units (approximately 13 atmospheric days).

In short, in case of insufficient ensemble size, the NARMA model has better state estimation and prediction properties than the L96x model, when both use tuned IL. Covariance inflation and localization account for both sampling error and model error for the L96x model; they mainly account for sampling error for the NARMA model, which has quantified the model error by parametrization. Hence, the discrete-time stochastic parametrization can be combined with covariance inflation and localization to improve filter performance.

#### 5. Summary and discussion

We have examined discrete-time stochastic parametrization as a way to account for model error due to unresolved scales in the version of EnKF with perturbed observations and compared it with covariance inflation and localization algorithms.

We carried out numerical experiments on the two-layer Lorenz 96 system, with the goal of predicting the future evolution of the observed variables on the basis of noisy observations of these variables. We assumed that a forecast model in the filter was a truncated system in which the unobserved variables were unresolved. The model error comes from this underresolution. We analyzed how the two methods accounted for this error. The stochastic parametrization method directly quantified the model error and led to an improved forecast model, while covariance inflation and localization corrected the ensemble covariance in the analysis step in the filter. When the ensemble size was sufficiently large for the sampling error to be negligible, the improved forecast model, without any inflation or localization, achieved significantly better performance in state estimation and prediction than the unmodified truncated forecast model with tuned inflation and localization. When the ensemble size was small, covariance inflation and localization were needed to account for the sampling error, but the improved forecast model provided further improvement in filter performance. These results

show that the discrete-time stochastic parametrization approach was more effective than the inflation and localization approach in dealing with model error from unresolved scales.

As a consequence of this study, we advocate the direct approach, which works on the root of the problem: the deficiency of the model. The direct approach improves the forecast model, and therefore improves the overall quality of the forecast ensemble as well as filtering and prediction performance (Harlim 2016; Chorin et al. 2016). This is fundamentally different from the covariance inflation and localization approach, which corrects the sample covariance to improve ensemble quality, but the model deficiency remains. However, the parametrization can only account for model error, but covariance inflation and localization can account for both sampling and model error. When there are both model error and sampling error because of small ensemble size, these two methods can work together to achieve better performance than inflation/localization used alone.

This study has been carried out in a setting where the full model can be solved offline, and its solution used to tune inflation and localization or to infer parameters in stochastic parametrization. A more challenging and realistic setting would be one where the full model is unknown, and one has to use noisy observations to infer a parametrization (Li et al. 2009; Berry and Harlim 2014; Harlim 2016). This is the challenging topic of parameter estimation for hidden Markov and non-Markov models (Kantas et al. 2009). We leave it to future work.

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