1	Impact of perturbation schemes on the ensemble prediction
2	in a coupled Lorenz model
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#### ABSTRACT

22 Based on a simple coupled Lorenz model, we investigate how to consider a 23 suitable initial perturbation scheme for ensemble forecasting in a multiscale system 24 involving slow dynamics and fast dynamics. Four initial perturbation approaches are 25 used in the ensemble forecasting experiments: random perturbation (RP), the bred 26 vector (BV), the ensemble transform Kalman filter (ETKF) and the nonlinear local 27 Lyapunov vector (NLLV) methods. Results show that, regardless of the method used, the ensemble averages behave indistinguishably from the control forecasts during the 28 first few time steps. Due to different error growth in different time-scale systems, the 29 30 ensemble averages perform better than the control forecast after a very short period of 31 lead time in a fast subsystem, but after a relatively long period of time in a slow subsystem. As a result of coupled dynamic processes, whether adding perturbations to 32 33 fast variables or to slow variables can contribute to an improvement in the forecasting 34 skill for fast variables and slow variables. When it comes to the initial perturbation approaches, the NLLVs show higher forecasting skill than BVs or RPs overall. 35 NLLVs and ETKFs had nearly equivalent prediction skill, and NLLVs won by a 36 narrow margin. In particular, when adding perturbations to slow variables, 37 independent perturbations (NLLVs and ETKFs) perform much better in the ensemble 38 39 prediction. These results are simply implied in a real coupled air-sea model. For the 40 prediction of oceanic variables, independent perturbations (NLLVs) and adding

41	perturbations to oceanic variables will be expected to perform better in the ensemble
42	prediction.
43	Key words: Ensemble prediction; The nonlinear local Lyapunov vector (NLLV); The
44	ensemble transform Kalman filter (ETKF); Coupled air-sea models
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46	Article Highlights:
47	• This study explores ensemble prediction in a multiscale system which involve
48	slow dynamics and fast dynamics by multiple initial perturbation schemes;
49	• The advantages of an ensemble forecast become apparent after a very short
50	period of time in a fast subsystem, but after a relatively long period of time in a
51	slow subsystem.
52	• When adding perturbations to slow variables in a multiscale system, independent
53	perturbations (NLLVs and ETKFs) perform much better in the ensemble
54	prediction.
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#### 67 1. Introduction

68	In recent years, air-sea coupled models which describe the interactions between
69	the atmosphere and the ocean have been more extensively applied to simulate weather
70	and climate phenomena (Bender et al. 2007; Larson and Kirtman 2017; Mogensen et
71	al. 2017; Zou et al. 2016). Air-sea coupling plays an important role in the simulation
72	of weather and climate (Dong et al. 2017; Thompson et al. 2018). In the air-sea
73	interface, it involves material and energy exchange, with a lot of complex physical
74	processes (Soloviev et al. 2014). The coupled models can describe these coupled
75	feedback processes better than atmosphere-only models (Perlin et al. 2020). Hence,
76	the simulation of the weather and climate phenomena can be improved by using a
77	coupled air-sea model (Dong et al. 2017; Fu and Wang 2004; Ratnam et al. 2008;
78	Wang et al. 2005).

79 However, the simulation of weather and climate phenomena using coupled airsea models involves many uncertainties, including initial condition uncertainty 80 (Lorenz 1969, 1982) and model uncertainty (Leutbecher and Palmer 2008). The 81 Ensemble prediction technology has been developed to deal with these uncertainties 82 83 (Demeritt et al. 2007; Ehrendorfer 1997; Leith 1974). It generates ensemble members 84 by adding perturbations to the analysis state (Magnusson et al. 2008). The ensemble 85 mean of ensemble members can reduce the errors compared to a single forecast, and 86 we can quantitatively estimate the probability density of a forecast state with a finite 87 number of ensemble members (Feng et al. 2014; Froude et al. 2007; Leutbecher and 88 Palmer 2008).

89 Here, we mainly focus on the ensemble prediction in relation to initial condition 90 uncertainty. The key to constructing initial perturbations is to generate several initial 91 states which can represent real initial uncertainty (Zhang and Krishnamurti 1999). 92 Many ensemble initial perturbation methods have been developed in succession, such 93 as the Monte Carlo method (also called the random perturbation (RP) method (Leith 94 1974)), the bred vector (BV) method (Toth and Kalnay 1993, 1997), the singular 95 vector (SV) method (Palmer 1992), the ensemble transform Kalman filter (ETKF) 96 method (Wang and Bishop 2003), the ensemble transform with rescaling (ETR) method (Wei et al. 2008; Wei et al. 2006), the conditional nonlinear optimal 97 perturbations (CNOPs) method (Mu and Jiang 2008) and the nonlinear local 98 Lyapunov vector (NLLV) method (Ding et al. 2017; Feng et al. 2014; Feng et al. 99 2016; Feng et al. 2018). 100

A surge of studies have focused on ensemble prediction in atmosphere-only or 101 102 ocean-only models, but it has not been explored extensively in air-sea coupled models. Ensemble prediction in coupled models seems more complex because of the 103 104 different time scales between the ocean and the atmosphere (Liu et al. 2013). An 105 initial error can also evolve on different time scales (Vannitsem 2017). In addition, 106 the feedback process between the coupled components makes the system highly 107 sensitive to errors (Zhang et al. 2005). Hence, important issues in ensemble 108 forecasting in coupled models which contain feedback processes at different time

109 scales remain to be explored.

110	Therefore, in this paper, we determine how to add appropriate ensemble initial
111	perturbations to a multiscale system, based on multiple initial perturbation methods.
112	The system is called the coupled Lorenz model, with a slow subsystem coupled with a
113	fast subsystem (Boffetta et al. 1998; Ding and Li 2012). The fast subsystem fluctuates
114	approximately 10 times faster than the slow subsystem, which is close to the relative
115	time-scale between the atmosphere and the ocean (Wang et al. 2002). Therefore, we
116	can assume the coupled Lorenz model as a toy coupled air-sea model.
117	The remainder of this paper is organized as follows. Section 2 introduces the
118	coupled Lorenz model and the algorithms to obtain the BVs, ETKFs and NLLVs.
119	Section 3 presents properties of RPs, BVs, ETKFs and NLLVs in the multiscale

system. Section 4 is a summary and discussion of our major findings. 120

#### 2. Model and methodology 121

#### 122 2.1. Coupled Lorenz model

The model used in this study is the coupled Lorenz model. It couples two simple 123 Lorenz63 model (Lorenz 1963), with different time scales. The first characterizes the 124 125 slow dynamics and the second characterizes the fast dynamics (Boffetta et al. 1998; Ding and Li 2012). It is governed by the equations 126

$$\begin{cases} \frac{dX_{1}^{(s)}}{dt} = \sigma\left(X_{2}^{(s)} - X_{1}^{(s)}\right), \\ \frac{dX_{2}^{(s)}}{dt} = \left(-X_{1}^{(s)}X_{3}^{(s)} + r_{s}X_{1}^{(s)} - X_{2}^{(s)}\right) - \varepsilon_{s}X_{1}^{(f)}X_{2}^{(f)}, \\ \frac{dX_{3}^{(s)}}{dt} = X_{1}^{(s)}X_{2}^{(s)} - bX_{3}^{(s)}, \\ \frac{dX_{1}^{(f)}}{dt} = c\sigma\left(X_{2}^{(f)} - X_{1}^{(f)}\right), \\ \frac{dX_{2}^{(f)}}{dt} = c\left(-X_{1}^{(f)}X_{3}^{(f)} + r_{f}X_{1}^{(f)} - X_{2}^{(f)}\right) + \varepsilon_{f}X_{1}^{(f)}X_{2}^{(s)}, \\ \frac{dX_{3}^{(f)}}{dt} = c\left(X_{1}^{(f)}X_{2}^{(f)} - bX_{3}^{(f)}\right), \end{cases}$$
(1)

128 where the superscripts (s) and (f) denote the slow dynamics and the fast dynamics, respectively. The physical parameters of the above equation are displayed in Table 1. 129 The relative time scale c is a constant set to 10, indicating that the fast dynamics 130 fluctuate approximately 10 times faster than the slow dynamics. It is near the relative 131 132 temporal scale of between ocean and the atmosphere, which is about 9 (Wang et al. 2002). The variation in the fast variables changes much faster than the variation in the 133 slow variables (Fig. 1). The uncoupled slow and fast Lorenz models (coupling 134 coefficients  $\varepsilon_s = 0$ ,  $\varepsilon_f = 0$ ) exhibit chaotic dynamics, with their Lyapunov exponents 135 greater than zero. Setting  $\varepsilon_s = 10^{-2}$ ,  $\varepsilon_f = 10$ , the maximal Lyapunov exponent in the 136 coupled Lorenz model has a value of 11.5, close to the value from uncoupled fast 137 138 Lorenz models (Boffetta et al. 1998) indicating that it is the error growth of the fast 139 system that determines the maximal Lyapunov exponent in the coupled Lorenz model. 140 The associated attractor of the coupled system seems interesting from the physical parameters given in Table 1. The two-dimensional projections of the attractor 141 142 are shown in Fig. 2. The fast dynamics appear to show a typical Lorenz model (Fig.

143 2d-f), whereas the slow dynamics seems much more chaotic, losing the "butterfly"
144 appearance of the original Lorenz63 model (Fig. 2a-c).

145 2.2 Initial perturbation schemes

We use four methods to generate initial perturbations: RP, BV, ETKF and
NLLV. A brief description of the BV, NLLV and ETKF methods follows.

148 2.2.1 Computation of the BVs

149 The BV method is based on the rationale that any initial random errors in the 150 basic flow would evolve into the fastest growing directions (leading Lyapunov vectors) in the phase space (Feng et al. 2014; Toth and Kalnay 1993, 1997). The 151 generation of BVs is as described follows. At first, a group of small initial random 152 perturbations are added to the analysis state. After a period of integration (a breeding 153 154 cycle), the differences between the control and perturbed forecasts are rescaled to the 155 size of the initial perturbations and the rescaled difference fields will be added to the next analysis. After repeating the process for several breeding cycles, the perturbation 156 evolves into a fast-growing perturbation, and the BVs are generated. Following 157 158 mathematical language is to describe the repeated process:

$$\boldsymbol{x}_{p}(t_{i}) = \boldsymbol{x}_{c}(t_{i}) + \varepsilon_{0} \frac{\boldsymbol{p}}{\|\boldsymbol{p}\|}, \qquad (2)$$

159 where the  $x_c$  and  $x_p$  represent the control trajectory and perturbation trajectory, 160 respectively. The term  $\varepsilon_0 \frac{p}{\|p\|}$  represent the scaling, where  $\varepsilon_0$  is a scaling factor and

161 p is the difference between control forecast and perturbated forecast.

### 162 2.2.2 Computation of the NLLVs

163 NLLVs are a nonlinear extension of the Lyapunov vectors (LVs) similar to BVs (Feng et al. 2014; Hou et al. 2018). Compared to BVs, different NLLVs are 164 165 independent, and represent the fastest direction of error growth in different subspaces 166 of the phase space. The generation of NLLVs is introduced below (Feng et al. 2014; 167 Feng et al. 2016). As shown in Fig. 3, the leading NLLV (NLLV1), which is the 168 fastest growing direction, can be obtained via a breeding process similar to the 169 creation of a BV. In each breeding cycle, the rest of the NLLVs can be obtained via a 170 Gram-Schmidt reorthonormalization (GSR) process (Feng et al. 2014; Wolf et al. 1985). The evolved perturbations (grey dashed lines) are orthogonalized with the 171 leading NLLV (NLLVn are orthogonalized associated with NLLV1, NLLV2, 172 NLLV3, ..., NLLVn-1). The orthogonalized perturbations are then scaled back to the 173 initial size and enter the next breeding process. After multiple breeding cycles, the 174 NLLVs are produced. In this paper, the breeding cycle for generating BVs and 175 NLLVs is 0.05 time units (tus) and was repeated for 20 times. 176

177 2.2.3 Computation of the ETKFs

The ETKF method is initially introduced by Bishop et al. (2001). The method is derived from ensemble-based data assimilation theory, which is associated with the Kalman filtering (Wang and Bishop, 2003; Wei et al., 2006; Wu et al., 2015). Similar to the ensemble Kalman filter (EnKF), ETKF apply Kalman filtering to generate a sample analysis ensemble. However, the ETKF use the forecast error covariance

matrix only to estimate the analysis error covariance through a transformation matrix,
not updating the mean state (Wang and Bishop, 2003; Zhou et al., 2019). The
equation for the ETKF algorithm is as follows:

$$\boldsymbol{X}_{\mathrm{a}} = \boldsymbol{X}_{\mathrm{f}} \boldsymbol{T},\tag{3}$$

186 where  $X_a$  and  $X_f$  is denoted as the analysis perturbation and forecast perturbation 187 matrix and T is a transformation matrix. The detail computation process follows 188 Hunt et al. (2005). Localization is not used here. A multiplicative covariance inflation 189 factor (with a value of 1.3) is applied. The observation was produced by adding a 190 random perturbation (following standard Gaussian distribution) to true state. 191 Moreover, we use an ensemble size of 20, assimilated every 0.05 tus and the 192 performing time is over 1 tus.

193 Studies have shown that the ETKF can be used for generate ensemble 194 perturbations and have a better preformation on sampling the analysis uncertainties 195 than most ensemble generation schemes (Wei et al., 2006; Feng et al., 2016). One of 196 greatest qualities for ETKFs is that they are orthogonal in observation space (Wang 197 and Bishop, 2003; Wei et al., 2006; Feng et al., 2016).

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### 199 2.3 Experimental design

To make the performance of the evolution of the initial perturbations in a multiscale system as clear as possible, we undertook several ensemble forecasting experiments in the coupled Lorenz model, based on RP, BV, ETKF and NLLV 203 methods. The model is integrated by Fourth Order Runge-Kutta method with a time step of 0.005 tus in all experiments. The procedure for the ensemble forecasting 204 experiments is shown in Fig. 4. The first 10000 steps involve a spin up of the coupled 205 206 Lorenz model. After the spin up, we use a 200-step ensemble Kalman filter (EnKF) 207 data assimilation scheme (Evensen 2003, 2004) to create the initial analysis state. The 208 parameter set of EnKF assimilation procedure is same to the ETKF scheme. The 209 assimilation cycle is 0.05 tus, which is perfect to project to 6 hours window in real 210 world. Hence, 1 tus is assumed to be equal to 5 days in real world in this paper. At the 211 same time of assimilation process, the BV and NLLV perturbations are calculated based on the assimilated data as a basic flow. Then the ensemble perturbations created 212 by the RP, BV, ETKF and NLLV methods are added to the analysis state in pairs 213 (both positive and negative perturbations are added). The Ensemble perturbation 214 vectors are scaled to  $1 \times 10^{-2}$ . The integration from the analysis state is the control 215 forecast. And the perturbed forecasts are ensemble members. Increasing the number 216 of ensemble members, the prediction level of ensemble forecast which is drove by 217 BVs, NLLVs and ETKFs showed an improvement (not shown). Thus, the ensemble 218 219 size is 6 pairs in this paper (with positive and negative perturbations superimposed in 220 pairs). We run 10000 samples of the ensemble forecast (repeating the 221 assimilation/breeding processes and forecasting processes). The initial value of each sample has one step interval. The initial states of 10000 samples include a 222 representative range of coupled model states. 223

#### 224 2.4 Verification method

To evaluate the reliability of the ensemble predictions, a classical Brier score is
applied to assess the relative skill of the BV compared with that of NLLV and ETKF.
For any event \u03c6, the Brier score (Brier 1950) is computed as:

$$BS = \frac{1}{N} \sum_{i=1}^{N} (f_i - o_i)^2, \qquad (4)$$

where *N* is the number of samples,  $f_i$  denotes the probability of the *i*-th sample for event  $\phi$  prediction, and  $\theta_i$  denotes the probability of the *i*-th sample actually occurring for event  $\phi$  (which can take on values of only 0 or 1).

## **3. Results**

Before evaluating the quality of the ensemble predictions, the errors from the 232 control forecast are going to be investigated. We assume that the model is perfect, and 233 234 the true state is a long run of the model for each sample. As shown in Fig. 5, there exists a large difference between the control forecast and the true value. The evolution 235 of the control and true value show rapid fluctuating changes over the whole system 236 (Fig. 5a). When separating the coupled Lorenz system into a fast subsystem and a 237 238 slow subsystem, similar characteristics are found in the fast subsystem compared to 239 the whole system (Fig. 5b). However, these two time series in the slow subsystem 240 show slow fluctuating changes, and they show a significant distinction until 4 tus 241 (Fig. 5c). Given that there exists a relatively large difference between the control 242 forecast and the true state, we use the Lyapunov exponential form error growth rate to

measure the variation of forecast error for a control run. It is found that the initial error for analysis shows positive growth over time. The forecast error for a control run mainly comes from the fast subsystem. The variation in forecast error for the control run is different in the slow and fast subsystem, error growing much faster in fast subsystem than in slow subsystem (Fig. 5d). The equation for the Lyapunov exponential form error growth rate is as follows:

$$\lambda = \frac{1}{t - t_0} \ln \frac{\|\nabla x(t)\|}{\|\nabla x(t_0)\|},$$
(4)

where  $t_0$  is the initial time,  $\|\nabla x(t)\|$  denotes the error size in the  $L_2$  norm at time t. 249 Studies have proved that the ensemble forecast improves the quality of the 250 control forecast (Ndione et al. 2020; Toth and Kalnay 1997). Running an ensemble of 251 forecasts from adding perturbations to initial conditions, the ensemble mean can 252 improve the prediction by filtering out unpredictable components, and the spread 253 among the forecasts can provide a probability prediction (Toth and Kalnay 1993). In 254 order to explore appropriate ensemble initial perturbations configuration in a 255 multiscale system, many ensemble forecast experiments are conducted in this part, 256 with multiple perturbation methods (RP, BV, ETKF and NLLV). The root-mean-257 square error (RMSE) for the ensemble mean and the ensemble spread are used to 258 259 measure the forecast skill from the experiments. For a "perfect ensemble", the 260 ensemble spread will be close to the RMSE of the ensemble mean for all forecast 261 times (Buckingham et al. 2010; Magnusson et al. 2008; Palmer et al. 2006).

262 Additionally, considering different error growth in the fast subsystem and slow subsystem, we shall discuss them separately. In Fig. 6, the mean RMSE (solid lines) 263 264 and ensemble spread (dashed lines) are plotted for the control (black), RP (red), BV 265 (blue), ETKF (purple) and NLLV (green) after adding perturbations to all variables. 266 The RMSE is oscillating at short lead time. It is possible that the RMSE oscillation at 267 short lead- time relate our temporal scale, which is similar to diurnal cycling. In the first 0.5 tus, the RMSE for the NLLV, ETKF, BV, and RP ensembles are similar to 268 269 that of the control run. This is mainly because positive and negative perturbations 270 superimposed on the control run cancel each other out at the initial time (errors grow linearly at the initial time (Ding and Li 2007)). Soon after, regardless of the 271 perturbation method, the ensemble forecast can effectively reduce forecast errors from 272 the control run in general. In the RMSE for the ensemble mean, the results from 273 NLLVs are the lowest, followed by ETKFs, BVs, RPs, and the control forecast. 274 Among them, NLLVs and ETKFs have nearly the same forecast ability. These two 275 276 methods have obviously better predictive skill than BVs in the two main periods: 0.5-2 tus and 4.5-8 tus (smaller RMSE for ensemble mean and bigger ensemble spread) 277 (Fig. 6a). During the period 0.5-2 tus, the better predictive skill of NLLVs and 278 279 ETKFs over the whole system is reflected mainly in the reduction in forecast errors in 280 fast subsystem (Fig. 6b). And it is reflected in the reduction in forecast errors in slow subsystem during the period 4.5–8 tus (Fig. 6c). 281

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Now we wonder whether to add perturbations to different variables of this

283 system can achieve improvements from BVs to ETKF and NLLVs. Good ensemble perturbations should reflect the initial uncertainty of analysis (Toth and Kalnay 1993). 284 Different perturbation methods have different ability in capturing the initial 285 286 uncertainties. Owing to different error growth for initial perturbations in fast and slow 287 subsystem (Fig. 5d), the prediction skill for different perturbation methods may differ 288 when adding different timescale perturbations. Here, three error-addition schemes are 289 used in this study: adding perturbations to both fast and slow variables, adding 290 perturbations only to fast variables, and adding perturbations only to slow variables. It 291 is shown that whether adding perturbations to fast variables or to slow variables contributes to an improvement in the forecasting skill for fast variables due to the 292 293 feedback process between the coupled components (Fig. 7). When adding perturbations only to fast variables, the ensemble skills of all perturbation methods are 294 improved in the prediction of fast variables after 0.4 tus (Fig. 7b). However, when 295 adding perturbations only to slow variables, only NLLVs and ETKFs can improve the 296 prediction skill of fast variables during the period 0.4-0.8 tus (Fig. 7c). In other 297 words, only better independent perturbations superimposed on the slow subsystem 298 299 can improve the forecasting skill of the fast subsystem.

The ensemble forecast of slow variables behaves differently with fast variables. The advantages of the ensemble forecast over the control forecast become apparent up to 4 tus (Fig. 8). When adding perturbations only to fast variables, the forecasting skills of BVs, ETKFs and NLLVs are equivalent (Fig. 8b). However, when adding 304 perturbations only to slow variables, large differences are shown between the BVs 305 with NLLVs and ETKFs, indicating that more independent perturbations have better 306 prediction skill for the slow subsystem (Fig. 8c). Because of the feedback process 307 between the coupled components, perturbations to both fast variables and slow 308 variables contribute to an improvement in the forecasting skill for slow variables.

309 In general, the ensemble forecast shows a different performance in different time-scale systems. After a while the ensemble forecast starts to show better 310 311 prediction skill than the control run. The advantages of the ensemble forecast become 312 apparent after a very short period of time in a fast subsystem, but after a relatively long period of time in the slow subsystem. The reason for this difference is associated 313 with the different error growths of different time-scale systems. In fast dynamics, 314 errors from the analysis state grow quickly, whereas they will grow relatively slowly 315 316 in slow dynamics. Besides, adding perturbations to both fast variables and slow variables contributes to an improvement in the forecasting skill for fast variables and 317 slow variables, indicating that uncertainty in both fast and slow variables plays a role 318 in the prediction of fast variables and slow variables. When adding perturbations to 319 slow variables, it seems that independent perturbations (NLLVs and ETKFs) perform 320 321 much better than the other types (BVs or RPs) in the prediction of both fast variables 322 and slow variables. This is probably mainly because highly independent perturbations can better capture initial uncertainty information. Additionally, NLLVs seems to win 323 ETKFs by a narrow margin (Fig. 6-8). To further confirm this, we conduct an 324

independent samples t-test with RMSE of 10000 samples for the ETKF method and
NLLV method. The RMSE data is from the experiments same as in Fig. 6a. The mean
RMSE from NLLV is less than that from ETKF (with a difference of -0.1429),
exceeding the 90% confidence level (with a probability value of 0.0812; not shown).
Therefore, of the two independent perturbations, NLLV is better than ETKFs.

330 Other evidence also shows that the independent perturbations (NLLVs) show better forecasting quality than BVs. Figure 9 provides the distribution of RMSE and 331 332 ensemble spread from 10000 samples for NLLV and BV predictions. At the 333 beginning of the ensemble forecast, the forecast errors for both NLLVs and BVs are concentrated mainly around the diagonal, indicating that the forecasting skill of 334 NLLVs is roughly equal to that of BVs (Fig. 9a). The number of samples with a 335 prediction error by NLLVs less than that by BVs increase over time, reaching 58% of 336 total samples at 6 tus (Fig. 9b). The number of samples with an ensemble spread by 337 NLLVs is greater than that by BVs at any time (Fig. 9d-f). It is concluded that 338 compared to BVs, NLLVs tend to have smaller RMSE for the ensemble mean and 339 bigger ensemble spread, indicating a better ensemble prediction performance. 340

The Brier score (BS) is commonly used in evaluating the quality of probabilistic forecasts generated by ensembles (Stephenson et al. 2008). We choose the event  $\phi_1$ (for  $X_3^{(f)}$  is the climatological mean to the distance of one standard deviation) (Fig. 10a) and event  $\phi_2$  (for  $X_3^{(s)}$  is the climatological mean to the distance of one standard deviation) (Fig. 10b) to calculate the basic BS from the average of 10000 samples. The smaller the value of BS, the better the forecasting skill of the ensemble forecast.
As shown in Fig. 10, the NLLVs are more skillful than the BVs or RPs and their
performance are similar to ETKFs.

349 The other verification method used was the Talagrand diagram (also called a 350 rank histograms), which can characterize the reliability of an ensemble forecast 351 (Candille and Talagrand 2010; Talagrand et al. 1997). For a reliable ensemble forecasting system, the observation must fall with equal probability into any of the 352 N+1 intervals divided by the N ensemble forecast values (Talagrand et al. 1997). 353 354 Considering an ensemble forecasting system with N members, the predicted value of  $X_3^{(s)}$  can be defined as  $P_{i,j}$ , where *i* denote the *i*-th sample, and *j* denotes the *j*-th 355 ensemble member. For each sample, we count the number of members whose 356 predicted values are smaller than the true values, represented as n, which can take on 357 values of only 0 - N. Then, we count the number of samples (for all samples of S, 358 we run 10000 samples of the ensemble forecast) under each n, defined by  $S_n$ . The 359 ideal frequency of  $S_n$  is S/(N+1), for which we expect the true value to have equal 360 probability in the N+1 intervals. We calculate the relative frequency 361  $P_n = \frac{S_n}{S/(N+1)}$ . The distribution of  $P_n$  is plotted in Fig. 11. It shows that both the 362 363 NLLV, ETKF and BV ensembles are under-dispersive. But the results for NLLVs show a flatter histogram, indicating the greater reliability of the NLLV ensemble 364 system. The stability of the NLLV and the ETKF ensemble system is comparable. 365 The results from BS and the Talagrand diagram are based on the ensemble experiment 366

367 which adds perturbations to both fast and slow variables and we choose  $X_3^{(f)}$  and 368  $X_3^{(s)}$  to analyze. Similar results can be obtained from other error-addition schemes and 369 variables (not shown). These results prove the better performance of NLLVs and 370 ETKFs than BVs in the ensemble prediction.

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4.

## Summary and discussion

372 It is still a huge challenge for ensemble prediction in multiscale systems 373 (Vannitsem and Duan 2020). One important issue is how to generate appropriate perturbations for different time-scale variables. This issue has been addressed here by 374 considering different time-scale initial perturbations in the prediction of different 375 time-scale variables. Besides, the selection of ensemble generation schemes is very 376 377 important. The NLLV method has been proved to have many advantages in ensemble forecasting (Feng et al. 2014; Feng et al. 2016; Hou et al. 2018). Therefore, we have 378 explored how to add appropriate ensemble initial perturbations to a multiscale system, 379 based on multiple initial perturbation methods. The results are as below. 380

Compared to the control forecast, the ensemble forecast can effectively reduce forecasting errors in the coupled model. Due to different error growth in different time-scale systems, the advantages of an ensemble forecast become apparent after a very short period of time in a fast subsystem, but after a relatively long period of time in a slow subsystem. After adding perturbations separately to a fast subsystem and a slow subsystem, we found that, as a result of coupled dynamic processes, whether adding perturbations to fast variables or to slow variables contributes to an

388	improvement in the forecasting skill for fast variables and slow variables. In terms of
389	initial perturbation methods, it is evident that independent perturbations (NLLVs and
390	ETKFs) are relatively superior to the other kinds (BVs or RPs). The two of them had
391	nearly equivalent prediction skill, and NLLVs won by a narrow margin. The ensemble
392	forecasting system based on NLLVs or ETKFs is of higher quality than that based on
393	BVs. In particular, when adding perturbations to slow variables, the highly
394	independent perturbations (NLLVs and ETKFs) can capture initial uncertainty
395	information quickly, giving them better prediction skill in the coupled system.
396	We may deduce that in a coupled ocean-atmosphere model, for the prediction of
397	fast-scale variables (e.g. atmospheric variables), the ensemble forecast works on
398	reducing the errors from the control forecast after a short period of time. However, for
399	slow-scale variables (e.g. oceanic variables), the ensemble forecast may be effective
400	in improving the medium and long-term forecasts. Considering air-sea coupling,
401	adding perturbations to oceanic variables will contribute to an improvement in the
402	forecasting skill for atmospheric variables and adding perturbations to atmospheric
403	variables can also improve the forecasting skill for oceanic variables. For the
404	prediction of atmospheric and oceanic variables, when adding perturbations to
405	oceanic variables, independent perturbations may perform better in the ensemble
406	forecast. These results may have important implications for the development of
407	ensemble forecasts of the coupled model in the future.

408 In general, NLLVs and ETKFs have a better performance than BVs and RPs in a

409 coupled model. The computations of ETKFs require much computing resources.
410 Fortunately, ETKF perturbations can be a byproduct from the data assimilation.
411 Compared to ETKFs, NLLVs are completed independent (orthogonal) and easy to
412 calculate. Both NLLVs and ETKFs are expected to have a wide potential application
413 in coupled models.

414 Nevertheless, since we obtained these results through a toy model, further research is however necessary to expand these results to realistic air-sea coupled 415 416 models. Our research team have tried applying NLLVs in the Weather Research and 417 Forecasting (WRF) model. It is expected that NLLVs will have a good performance in realistic air-sea coupled models. Besides, Vannitsem and Duan (2020) discovered that 418 the fastest backward Lyapunov vectors are not the most suitable for initializing a 419 multiscale ensemble forecasting system. So how to choose the appropriate NLLV 420 421 modes in a multiscale ensemble forecasting system may be an important issue. Both 422 will be addressed in the near future.

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Parameter	Description	Value
σ	Prandtl number	10
b	Physical dimensions of the layer	8/3
С	Relative time scale	10
ľs	Rayleigh number of the	28
$r_{f}$	Rayleigh number of the	45
$\mathcal{E}_{s}$	fast dynamics Coupling coefficient of the	10 <sup>-2</sup>
	slow dynamics	10
${\cal E}_f$	fast dynamics	10

**Table 1.** Physical parameters used in the coupled Lorenz model



598 FIG. 1. Time evolution of variables for the coupled Lorenz model: (a) slow variables







602 FIG. 2. Projections of the coupled Lorenz model on three two-dimensional planes:

603 (a)–(c) for the slow variables, and (d)–(f) for the fast variables.







FIG. 3. Schematic diagram of the generation of NLLVs [adapted from Hou et al. (2018)]. The creation of NLLV1 is similar to the creation of BV. To acquire the NLLV2, a pair of RPs is initially added to the analysis state. The evolved perturbations (grey dashed line) are orthogonalized with the NLLV1 (blue dashed line) to produce the NLLV2 (green dashed line) using a Gram–Schmidt reorthonormalization (GSR) procedure. Similarly, NLLVn are orthogonalized with NLLV1, NLLV2, NLLV3, ..., NLLVn-1.



614 FIG. 4. Illustration of the initialization and forecasting procedure. Numbers represent

615 the integration steps, and 1 step = 0.005tus.





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FIG. 5. (a)–(c) Evolution of control forecasts (light blue) against true state (light red) as a function of lead time, for (a) the whole system, (b) the fast subsystem, and (c) the slow subsystem (in the  $L_2$  norm). (d) Mean growth rate in the form of Lyapunov exponent (value \*100) of 10000 samples as a function of lead time from the coupled Lorenz model for the control run (the whole system (light purple), the fast subsystem (light orange), and the slow subsystem (light blue)).



FIG. 6. Mean RMSE (solid lines) and ensemble spread (dashed lines) of 10000
samples as a function of lead time for the control run (black), RP method (red), BV
method (blue), ETKF method (purple), and NLLV method (green) after adding
perturbations to all variables. (a) the whole system, (b) the fast subsystem, and (c) the
slow subsystem.



FIG. 7. Mean RMSE (solid lines) and ensemble spread (dashed lines) of 10000 samples in the fast subsystem as a function of lead time for the control run (black), random perturbation method (red), BV method (blue), ETKF method (purple), and NLLV method (green) after adding perturbations to different variables: (a) adding perturbations to both fast variables and slow variables, (b) adding perturbations only to fast variables, and (c) adding perturbations only to slow variables.



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FIG. 8. Mean RMSE (solid lines) and ensemble spread (dashed lines) of 10000 samples in the slow subsystem as a function of lead time for the control run (black), random perturbation method (red), BV method (blue), ETKF method (purple), and NLLV method (green) after adding perturbations to different variables: (a) adding perturbations to both fast variables and slow variables, (b) adding perturbations only to fast variables, and (c) adding perturbations only to slow variables.



647 FIG. 9. (a)–(c) RMSE of 10000 samples based on NLLV and BV methods at (a) 3 tus, (b) 6 tus, (c) 9 tus in the slow subsystem. The upper right-hand corner indicates the 648 ratio of samples where RMSE for the NLLV method is smaller than the RMSE for the 649 BV method in (a)-(c). (d)-(f) The same as (a)-(c), but for an ensemble spread of 650 651 10000 samples. The upper right-hand corner indicates the ratio of samples where the 652 ensemble spread for the NLLV method is larger than it is for the BV method in (d)-653 (f). (a)–(f) are based on the experiments which add perturbations to both fast and slow variables. 654





FIG. 10. (a) Basic Brier score (BS) for the event  $\phi_1$  ( $\phi_1$ : where  $X_3^{(f)}$  is the climatological mean to the distance of one standard deviation) of ensemble forecasts based on NLLVs (green line), ETKFs (purple line), BVs (blue line) and RPs (red line) as a function of lead time. (b) The same as (a), but for event  $\phi_2$  ( $\phi_2$ : where  $X_3^{(s)}$  is the climatological mean to the distance of one standard deviation) 



FIG. 11. The histogram of the Talagrand distribution for different member intervals. The horizontal dashed lines denote the expected probability. Ensemble forecasts based on (a) BVs, (b) NLLVs and ETKFs at 2 tus. (a)–(c) are based on the experiment which add perturbations to both fast and slow variables and predicts the variable  $X_3^{(f)}$ . (d)-(f) The same as (a)-(c), but at 6 tus and predicted variable is  $X_3^{(s)}$ .

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