<sup>1</sup> Predicting Observed and Hidden Extreme Events in Complex Nonlinear Dynamical

## <sup>2</sup> Systems with Partial Observations and Short Training Time Series

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Extreme events appear in many complex nonlinear dynamical systems. Predicting 11 extreme events has important scientific significance and large societal impacts. In 12 this paper, a new mathematical framework of building suitable nonlinear approxi-13 mate models is developed, which aims at predicting both the observed and hidden 14 extreme events in complex nonlinear dynamical systems for short-, medium- and 15 long-range forecasting using only short and partially observed training time series. 16 Different from many ad-hoc data-driven regression models, these new nonlinear mod-17 els take into account physically motivated processes and physics constraints. They 18 also allow efficient and accurate algorithms for parameter estimation, data assimila-19 tion and prediction. Cheap stochastic parameterizations, judicious linear feedback 20 control and suitable noise inflation strategies are incorporated into the new nonlin-21 ear modeling framework, which provide accurate predictions of both the observed 22 and hidden extreme events as well as the strongly non-Gaussian statistics in various 23 highly intermittent nonlinear dyad and triad models, including the Lorenz 63 model. 24 Then a stochastic mode reduction strategy is applied to a 21-dimensional nonlinear 25 paradigm model for topographic mean flow interaction. The resulting 5-dimensional 26 physics-constrained nonlinear approximate model is able to accurately predict the ex-27 treme events and the regime switching between zonally blocked and unblocked flow 28 patterns. Finally, incorporating judicious linear stochastic processes into a simple 29 nonlinear approximate model succeeds in learning certain complicated nonlinear ef-30 fects of a 6-dimensional low-order Charney-DeVore model with strong chaotic and 31 regime switching behavior. The simple nonlinear approximate model then allows 32 accurate online state estimation and the short- and medium-range forecasting of ex-33 treme events. 34

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Extreme events appear in many complex nonlinear dynamical systems. These 36 extreme events are associated with the sudden changes of states in the underly-37 ing complex systems and the occurrence of extreme events often results in large 38 social impact. Therefore, predicting extreme events has both scientific signifi-39 cance and practical implications. However, the big challanges of prdicting the 40 extreme events in complex nonlinear systems include the lack of understand-41 ing of physics, the huge computational cost in running the complex models 42 and data assimilation, as well as the availability of only short and partially ob-43 served training data. In this paper, a new mathematical framework of building 44 suitable nonlinear approximate models is developed, which aims at predicting 45 both the observed and hidden extreme events in complex nonlinear dynamical 46 systems for short-, medium- and long-range forecasting using only short and 47 partially observed training time series. This framework also allows efficient and 48 accurate data assimilation, parameter estimation and prediction algorithms. D-49 ifferent effective and practical strategies are incorporated into the framework to 50 develop suitable approximate models for predicting extreme events and other 51 non-Gaussian features in various complex turbulent dynamical systems. 52

## 53 I. INTRODUCTION

Extreme events appear in many complex nonlinear dynamical systems in geoscience, engineering, excitable media, neural science and material science<sup>1-8</sup>. Examples include oceanic rogue waves<sup>9,12</sup>, extreme weather and climate patterns<sup>10,11</sup> such as blocking events and turbulent tracers<sup>13–15</sup>, and bursting neurons<sup>16</sup>. These extreme events are associated with the sudden changes of states in the underlying complex systems and the occurrence of extreme events often results in large social impact. Therefore, predicting extreme events has both scientific significance and practical implications.

However, predicting the extreme events in complex nonlinear systems is quite challenging.
First, nature or the perfect model is never known in practice. Model error due to the lack of
the understanding of physics may prevent the skillful predictions of the extreme events<sup>1,17–19</sup>.
Second, even if the perfect model is known, the underlying nonlinear dynamics of nature
can be extremely complicated with strong non-Gaussian characteristics, multiscale features

and high dimensionality<sup>10,20,21</sup>. Thus, running the perfect model is usually computationally 66 unaffordable for real-time prediction. On the other hand, despite that coarse-graining the 67 numerical resolutions improves the computational efficiency, such a numerical approximation 68 often results in missing the key nonlinear interactions between different temporal and spatial 69 scales and brings about large errors, especially for extreme events. Third, it is important to 70 notice that only partial and noisy observations are available in many practical situations  $2^{2-24}$ . 71 which implies the states of the unobserved variables have to be estimated via online data 72 assimilation algorithms. Unfortunately, the existing data assimilation algorithms for general 73 complex nonlinear dynamical systems are either quite expensive (e.g., particle filter) or 74 involving intrinsic approximate errors due to the coarse-grained statistics (e.g., ensemble 75 Kalman filter)<sup>21,25–28</sup>. The assimilated states from the latter may also contain large biases 76 due to the fact that high order moments are important contributors to the extreme events. 77 Finally, the actual climate signal is often measured through time series. However, since the 78 high-resolution satellites and other refined measurements were not widely developed until 79 recent times, the available useful training data is very limited with about only 50 years in 80 many real applications. Thus, predicting extreme events using short and partially observed 81 training time series is another remarkably challenging task. 82

For the reasons given above, developing suitable approximate models for predicting ex-83 treme events is crucial in practice. These approximate models aim at capturing the key 84 nonlinear dynamical and non-Gaussian statistical features of nature. They also need to be 85 computationally tractable and allow efficient algorithms for online data assimilation, pa-86 rameter estimation and prediction. There have been some recent progress in the extreme 87 events prediction. For example, a new statistical dynamical model was developed to predict 88 extreme events and anomalous features in shallow water waves<sup>12</sup>. A suite of reduced-order 89 stochastic models was built, which succeeds in predicting the extreme events in complex 90 geophysical flows<sup>29</sup> and their long-term non-Gaussian features<sup>30</sup> as well as forecasting the 91 associated statistical responses and quantifying the uncertainty<sup>31</sup>. In addition, mode decom-92 position techniques were applied for probing the most unstable modes and building low-order 93 models for extreme events prediction $^{32,33}$ . 94

In this paper, a new mathematical framework of building suitable nonlinear approximate models is developed, which aims at predicting both the observed and hidden extreme events in complex nonlinear dynamical systems using only short and partially observed training

time series. The models belonging to this mathematical framework are highly nonlinear and 98 are able to capture many key non-Gaussian characteristics as observed in nature<sup>34</sup>. Unlike 99 traditional regression and other ad hoc models with prescribed basis functions or structures, 100 this framework contains a rich class of statistical dynamical models and is amenable to a 101 wide range of applications. One important feature of this nonlinear modeling framework is 102 that physically motivated processes and physics constraints<sup>35,36</sup> can be incorporated into the 103 models, which is fundamentally different from many purely data-driven statistical models 104 that have no clear physical meanings. Such a trait not only enables the models to take 105 into account both the dynamical and statistical information but also allows using only a 106 short training time series for model calibration. The latter is due to the (partially) iden-107 tified dynamical structures from some physics reasoning and physics constraints. Another 108 key advantage of this new framework is that despite the intrinsic nonlinearity, it allows 109 closed analytic formulae for assimilating the states of the unobserved variables<sup>37,38</sup>, which is 110 computationally efficient and accurate. This provides an extremely useful and practical ap-111 proach for predicting extreme events and other non-Gaussian features in complex nonlinear 112 dynamical systems. 113

Short-, medium- and long-range forecasting of extreme events all have practical significance<sup>10,39–41</sup>. 114 The efficient data assimilation scheme associated with the nonlinear models within the above 115 framework provides an accurate estimation of the initial values, which play a crucial role in 116 improving the short-term prediction skill. On the other hand, the focus of the long-term 117 prediction is on the statistics, which is calculated by making use of a long trajectory together 118 with the ergodic property of many complex turbulent systems<sup>1</sup>. In particular, reproducing 119 the statistical equilibrium non-Gaussian probability density function (PDF) with fat tails is 120 a good evidence of the successful prediction of extreme events, where the extreme events and 121 intermittency are the main contributors to the fat tails. The medium-range forecast aims at 122 recovering the transition behavior of the underlying dynamics. A skillful medium-range pre-123 diction requires both an accurate estimation of the initial values and a suitable description 124 of the time evolution of the approximate model, and is often a challenging task. Finally, 125 certain internal or external perturbations are able to kick the model variables outside the 126 attractor. Therefore, predicting the time evolution of the extreme events that start from a 127 state outside the attractor also has practical importance. It is worth remarking that many 128 purely data-driven or machine learning methods fail to predict extreme events even though 129

most of those methods show high skill in fitting the observed time series. For example, 130 as has been pointed out in some recent work<sup>42,43</sup>, even one of the most advanced neural 131 networks with long short-term memory<sup>44</sup> and the Gaussian process regression<sup>45</sup> suffer from 132 a finite time blowup issue when they are applied for predicting extreme events. Such a 133 pathological behavior can only be overcome by using hybrid strategies that combine these 134 methods with suitable models<sup>42</sup>. Note that these purely data-driven methods often demand 135 tremendous training data<sup>46,47</sup>, which is not practical in many scientific scenarios where only 136 short training time series are available. In addition, without suitable models, predicting 137 extreme events in the unobserved processes becomes extremely difficult. 138

This paper aims at incorporating practical strategies into the development of suitable 139 approximate models for predicting both the observed and hidden extreme events. These 140 approximate models belong to the new nonlinear modeling framework, which allows an ef-141 ficient and accurate data assimilation scheme and only short and partially observed time 142 series are needed for model calibration. The first effective strategy is to adopt simple s-143 to chastic parameterizations for approximating complicated hidden processes. Despite the 144 simple forms, the judicious applications of these stochastic parameterizations are neverthe-145 less able to capture the nonlinear interactions between the observed and hidden variables 146 and predict the associated extreme events. Such an idea has been successfully applied to 147 the stochastic parameterized extended Kalman filter (SPEKF) forecast models<sup>48,49</sup>, dynamic 148 stochastic superresolution of sparsely observed turbulent systems<sup>50,51</sup> and stochastic super-149 parameterization for geophysical turbulence<sup>52</sup>. The second strategy here is motivated from 150 control theory, which involves incorporating simple feedback control terms into the approx-151 imate models for model simplification. This simple feedback control strategy succeeds in 152 capturing the key nonlinear statistical interactions as well as the causal effects between 153 the observed and hidden variables, which are essential to accurately predicting the extreme 154 events in the hidden processes. Note that predicting the hidden extreme events is typical-155 ly a great challenge given only partial observations. The third strategy makes use of the 156 stochastic mode reduction technique 53-56, which allows a significant dimension reduction in 157 the approximate models for many multiscale turbulent dynamical systems while the reduced 158 order models retain the crucial nonlinear and non-Gaussian features. Applying this strategy, 159 the nonlinear effects of the unresolved fast modes in the motion of the resolved variables 160 are represented by effective damping and stochastic forcing. The resulting approximate 161

models naturally belong to the new nonlinear modeling framework that allows extremely 162 efficient data assimilation and prediction schemes. These approximate models also preserve 163 physics-constrained properties. Another extremely useful strategy is to incorporate simple 164 stochastic processes with additive noise and memory into the approximate models, which 165 aim at effectively describing certain complicated nonlinear components that are hard to 166 deal with in strongly nonlinear and chaotic dynamical systems. Due to the unique feature 167 of the new nonlinear modeling framework, it allows an efficient and accurate way of using 168 simple stochastic processes to learn these complex nonlinear components on the fly, which 169 greatly facilitates the short- and medium-range forecasts of both the observed and hidden 170 extreme events. Other approaches of building approximate predictive models that can be 171 incorporated into the new nonlinear framework developed here involve using the noise in-172 flation technique to effectively characterize the contributions from small-scale variables and 173 fast-wave averaging of the variables with rapid decaying<sup>57</sup>. 174

The rest of the paper is organized as follows. Section II describes the new nonlinear 175 mathematical framework for developing suitable approximate models. Section III contains 176 the efficient and accurate data assimilation, parameter estimation and prediction algorithms. 177 Both the path-wise and information measurements in quantifying the prediction skill are also 178 included in this section. Section IV illustrates the skill of predicting intermittent extreme 179 events using cheap stochastic parameterizations with significant model error. Section V 180 makes use of a nonlinear energy-conserving dyad model to show the success of applying 181 the simple feedback control strategy in facilitating the prediction of the hidden extreme 182 events. The effect of noise inflation in approximate models for predicting extreme events is 183 illustrated based on the chaotic Lorenz 63 model in Section VI. Section VII starts with a 184 21-dimensional nonlinear topographic mean flow interaction model with regime switching. 185 Stochastic mode reduction strategy is applied in a suitable way to develop an approximate 186 nonlinear model with only 5 dimensions, which is nevertheless able to predict the observed 187 and hidden extreme events as well as the regime switching between zonally blocked and 188 unblocked flow patterns with high accuracy. In Section VIII, it is shown that incorporating 189 judicious linear stochastic processes into a simple nonlinear approximate model succeeds in 190 learning certain complicated nonlinear effects of a 6-dimensional low-order chaotic Charney-191 DeVore model with strong chaotic and regime switching behavior. The resulting nonlinear 192 approximate model allows accurate online state estimation and the short- and medium-range 193

<sup>194</sup> forecasting of extreme events. The paper is concluded in Section IX.

# <sup>195</sup> II. A NONLINEAR MATHEMATICAL MODELING FRAMEWORK <sup>196</sup> WITH SOLVABLE CONDITIONAL STATISTICS

A nonlinear mathematical modeling framework is established in this section, which will be used to the development of suitable approximate models for predicting extreme events. The general form of the nonlinear models within this framework is the following<sup>38</sup>,

$$d\mathbf{u}_{\mathbf{I}} = [\mathbf{A}_0(t, \mathbf{u}_{\mathbf{I}}) + \mathbf{A}_1(t, \mathbf{u}_{\mathbf{I}})\mathbf{u}_{\mathbf{II}}]dt + \boldsymbol{\Sigma}_{\mathbf{I}}(t, \mathbf{u}_{\mathbf{I}})d\mathbf{W}_{\mathbf{I}}(t),$$
(1a)

$$d\mathbf{u}_{\mathbf{II}} = [\mathbf{a}_0(t, \mathbf{u}_{\mathbf{I}}) + \mathbf{a}_1(t, \mathbf{u}_{\mathbf{I}})\mathbf{u}_{\mathbf{II}}]dt + \boldsymbol{\Sigma}_{\mathbf{II}}(t, \mathbf{u}_{\mathbf{I}})d\mathbf{W}_{\mathbf{II}}(t),$$
(1b)

<sup>197</sup> where the state variables are written in the form  $\mathbf{u} = (\mathbf{u}_{\mathbf{I}}, \mathbf{u}_{\mathbf{II}})$  with both  $\mathbf{u}_{\mathbf{I}} \in \mathbb{R}^{N_{\mathbf{I}}}$  and <sup>198</sup>  $\mathbf{u}_{\mathbf{II}} \in \mathbb{R}^{N_{\mathbf{II}}}$  being multidimensional variables. In (1),  $\mathbf{A}_0, \mathbf{A}_1, \mathbf{a}_0, \mathbf{a}_1, \boldsymbol{\Sigma}_{\mathbf{I}}$  and  $\boldsymbol{\Sigma}_{\mathbf{II}}$  are vectors <sup>199</sup> and matrices that depend only on time t and the state variables  $\mathbf{u}_{\mathbf{I}}$ , and  $\mathbf{W}_{\mathbf{I}}(t)$  and  $\mathbf{W}_{\mathbf{II}}(t)$ <sup>200</sup> are independent Wiener processes. The systems in (1) are named as conditional Gaussian <sup>201</sup> systems due to the fact that once  $\mathbf{u}_{\mathbf{I}}(s)$  for  $s \leq t$  is given,  $\mathbf{u}_{\mathbf{II}}(t)$  conditioned on  $\mathbf{u}_{\mathbf{I}}(s)$ <sup>202</sup> becomes a Gaussian process with mean  $\mathbf{\bar{u}}_{\mathbf{II}}(t)$  and covariance  $\mathbf{R}_{\mathbf{II}}(t)$ , i.e.,

$$p(\mathbf{u}_{\mathbf{II}}(t)|\mathbf{u}_{\mathbf{I}}(s \le t)) \sim \mathcal{N}(\bar{\mathbf{u}}_{\mathbf{II}}(t), \mathbf{R}_{\mathbf{II}}(t)).$$
(2)

Despite the conditional Gaussianity, the coupled system (1) remains highly nonlinear and 203 is able to capture the non-Gaussian features as in nature. This conditional Gaussian nonlin-204 ear modeling framework includes many physics-constrained nonlinear stochastic models<sup>35,36</sup>, 205 large-scale dynamical models in turbulence, fluids and geophysical flows, as well as stochas-206 tically coupled reaction-diffusion models in neuroscience and ecology. See a recent work<sup>34</sup> 207 for a gallery of examples of the conditional Gaussian systems. Applications of the condition-208 al Gaussian systems to strongly nonlinear systems include developing low-order nonlinear 209 stochastic models for predicting the intermittent time series of the Madden-Julian oscilla-210 tion (MJO) and the monsoon intraseasonal variabilities<sup>58–60</sup>, filtering the stochastic skeleton 211 model for the MJO<sup>61</sup>, and recovering the turbulent ocean flows with noisy observations from 212 Lagrangian tracers<sup>62–64</sup>. Other studies that also fit into the conditional Gaussian framework 213 includes the cheap exactly solvable forecast models in dynamic stochastic superresolution of 214 sparsely observed turbulent systems<sup>50,51</sup>, stochastic superparameterization for geophysical 215 turbulence<sup>52</sup> and blended particle filters for large-dimensional chaotic systems<sup>65</sup>. 216

One important feature of the above conditional Gaussian nonlinear framework is that the conditional Gaussian distribution  $p(\mathbf{u}_{\mathbf{II}}(t)|\mathbf{u}_{\mathbf{I}}(s \leq t))$  in (2) has closed analytic form<sup>37</sup>,

$$d\overline{\mathbf{u}}_{\mathbf{II}}(t) = [\mathbf{a}_{0}(t, \mathbf{u}_{\mathbf{I}}) + \mathbf{a}_{1}(t, \mathbf{u}_{\mathbf{I}})\overline{\mathbf{u}}_{\mathbf{II}}]dt + (\mathbf{R}_{\mathbf{II}}\mathbf{A}_{1}^{*}(t, \mathbf{u}_{\mathbf{I}}))(\boldsymbol{\Sigma}_{\mathbf{I}}\boldsymbol{\Sigma}_{\mathbf{I}}^{*})^{-1}(t, \mathbf{u}_{\mathbf{I}}) \times [d\mathbf{u}_{\mathbf{I}} - (\mathbf{A}_{0}(t, \mathbf{u}_{\mathbf{I}}) + \mathbf{A}_{1}(t, \mathbf{u}_{\mathbf{I}})\overline{\mathbf{u}}_{\mathbf{II}})dt], \qquad (3a)$$
$$d\mathbf{R}_{\mathbf{II}}(t) = \left\{ \mathbf{a}_{1}(t, \mathbf{u}_{\mathbf{I}})\mathbf{R}_{\mathbf{II}} + \mathbf{R}_{\mathbf{II}}\mathbf{a}_{1}^{*}(t, \mathbf{u}_{\mathbf{I}}) + (\boldsymbol{\Sigma}_{\mathbf{II}}\boldsymbol{\Sigma}_{\mathbf{II}}^{*})(t, \mathbf{u}_{\mathbf{I}}) - (\mathbf{R}_{\mathbf{II}}\mathbf{A}_{1}^{*}(t, \mathbf{u}_{\mathbf{I}}))(\boldsymbol{\Sigma}_{\mathbf{I}}\boldsymbol{\Sigma}_{\mathbf{I}}^{*})^{-1}(t, \mathbf{u}_{\mathbf{I}})(\mathbf{R}_{\mathbf{II}}\mathbf{A}_{1}^{*}(t, \mathbf{u}_{\mathbf{I}}))^{*} \right\} dt. \qquad (3b)$$

It is natural to assume  $\mathbf{u}_{\mathbf{I}}$  contains the observed variables while  $\mathbf{u}_{\mathbf{II}}$  is a collection of the 217 unobserved ones. Therefore, the analytically solvable conditional statistics in (3) allows an 218 extremely efficient and accurate way of estimating the hidden states given the observations, 219 known as the data assimilation, which facilitates predictions. Note that in the data assimi-220 lation language the conditional mean and conditional covariance in (3) are also known as the 221 posterior mean and posterior covariance. In addition, the conditional Gaussian nonlinear 222 modeling framework (1) and its closed analytical form of the conditional statistics (3) offer a 223 statistical efficient and accurate way of solving the time evolution of the associated Fokker-224 Planck equation in high dimensions $^{66-68}$ , which also provides a powerful tool for carrying 225 out ensemble forecasts. 226

# III. DATA ASSIMILATION, PREDICTION, AND THE QUANTIFICATION OF PREDICTION SKILL

### <sup>229</sup> A. Data assimilation of the unobserved variables

Data assimilation (also known as state estimation or filtering)<sup>21,25–28</sup>, a procedure of estimating the states of the unobserved variables, is the precondition of predicting complex dynamical systems. In fact, data assimilation of the unobserved variables can also be regarded as the online "prediction" of these variables due to the fact that the recovered states of the unobserved variables are given by combining the information in the dynamics with the values of the observed variables.

Data assimilation of the unobserved variables plays an important role in short- and medium-range forecasts. This is because the ensemble prediction algorithm requires running the model forward with the given initial values for all the state variables. Since there is no

direct observations of the hidden or unresolved variables, assimilating their initial states 239 becomes a necessity part of the ensemble forecast. In practice, the data assimilation is often 240 required in an "online" form in the sense that the states of the unobserved variables need 241 to be estimated at each time instant as time evolves. Therefore, developing an efficient and 242 accurate data assimilation method is a crucial first step for predicting nonlinear complex 243 dynamical systems and the associated extreme events. However, the classical Kalman filter 244 or its continuous form Kalman-Bucy filter<sup>69–71</sup> works only for linear models. On the other 245 hand, for assimilating general complex nonlinear dynamical systems, the particle filter is 246 quite expensive and contains sampling error while the ensemble Kalman filter takes into 247 account only the first two moments which may end up with large biases for assimilating 248 extreme events. 249

The conditional Gaussian nonlinear modeling framework in Section II provides an efficient way of estimating the states of the highly non-Gaussian hidden variables  $\mathbf{u}_{II}(t)$  in the complex nonlinear dynamical systems given the observations up to the current time  $\mathbf{u}_{I}(s \leq t)$ . The closed analytic formula in (3) avoids numerical and sampling errors, and it results in an extremely efficient and accurate way of computing the optimal states of  $\mathbf{u}_{II}(t)$ .

#### <sup>255</sup> B. Short-, medium- and long-range forecasting

Prediction problems have been described by Lorenz as falling into two categories<sup>72,73</sup>. Problems that depend on the initial condition, such as short- to medium-range weather forecasting, are described as "predictions of the first kind", while problems for predicting the longer-term climatology, are referred to as "predictions of the second kind".

For short- and medium-range forecasts, the system starts from an initial time  $t_0$ , where 260 the initial values of the unobserved variables are determined by data assimilation. Then 261 an ensemble prediction algorithm is applied by running the model forward up to a given 262 time  $t_1$ . Typically,  $t_1$  is not quite far from  $t_0$  and therefore the system has not completely 263 lost its memory of the initial values. Therefore, a good state estimation of the initial values 264 via data assimilation plays an important role in providing an accurate short- and medium-265 range forecasting skill. The ensemble mean, which is the average value of all the ensemble 266 members, is often used as a predictor for the evolution of the trajectories and the ensemble 267 spread measures the uncertainty in the ensemble mean forecasts. The difference between 268

short- and medium-range forecasts is that the prediction skill at very short lead time largely depends on the accuracy of the initial values while both the dynamical structures and the initial values will be essential in predicting the model transition behavior in the medium range. Capturing the time evolution of the large bursts in intermittent time series with small uncertainty is the goal of short- and medium-range forecasts of the extreme events.

On the other hand, for the long-range forecast where  $t_1$  is much larger than  $t_0$ , the system 274 will lose its memory from the initial time and arrives at the statistical equilibrium state. In 275 such a scenario, the ensemble mean prediction provides no information beyond the mean of 276 the statistical equilibrium state. Therefore, the aim of the long-range forecast is to predict 277 the statistical behavior. In particular, reproducing the statistical equilibrium non-Gaussian 278 probability density function (PDF) with fat tails is a good evidence of successfully predicting 279 the extreme events, where the extreme events and intermittency are the main contributors 280 to the fat tails. 281

Note that different models may have the same characteristics for the long-term statistics 282 but they often have significantly different skill for short and medium range prediction as 283 well as the forced response. In a recent paper<sup>74</sup>, several instructive examples using both a 284 simple linear  $2 \times 2$  system and more complicated nonlinear models unambiguously illustrate 285 such a feature of predicting complex turbulent dynamical systems. It is also shown in the 286 paper<sup>74</sup> that in the presence of model error, developing suitable approximate models that 287 are skillful in one of the short-, medium- or long-range forecasting is already a quite difficult 288 task. In many cases, there exists an information barrier<sup>75</sup> that prevents the approximate 289 models predicting the exact statistics and capturing the perfect response. 290

It is worthwhile to mention that a grand challenge in contemporary climate, atmosphere, 291 and ocean science is to understand and predict intraseasonal variability for time scales from 292 30 to 60 days, which is longer than standard weather time scales of at most a week and 293 much shorter than the yearly time scales of short-term climate. Therefore, it belongs to the 294 medium-range forecasts. Von Neumann<sup>76</sup> called such problems at the intersection of weather 295 and climate the greatest challenge in future meteorology<sup>10,77</sup>. The Indian-Asian monsoon 296 and the MJO<sup>10,78–80</sup> are the most significant intraseasonal variability occurs in the tropical 297 areas. Notably, it is shown in the recent  $work^{58-60}$  that the nonlinear modeling framework 298 in Section II facilitates the development of effective low-order nonlinear stochastic models 299 for predicting the intermittent time series of the MJO and the monsoon as well as extending 300

<sup>301</sup> the predictability of these intraseasonal variabilities.

## 302 C. Prediction of the dynamical evolution towards to the attractor

The short-, medium-, and long-range forecasts discussed above typically assume the ini-303 tial values lie in the statistical equilibrium states. On the other hand, certain internal or 304 external perturbations are able to kick the model variables outside the attractor. Therefore, 305 predicting the time evolution of the extreme events that start from a state outside the at-306 tractor and its returning path to the statistical equilibrium state is another important issue. 307 Since most approximate models are calibrated using the training data from the attractor, 308 there is no guarantee that these approximate models are automatically able to predict the 300 relaxation towards the attractor. This results in a great challenge of predicting the extreme 310 events starting outside the attractor. Some instructive studies of the prediction and linear 311 response skill with the initial condition being off the attractor can be found in a recent 312  $paper^{74}$ . 313

#### <sup>314</sup> D. Calibration of the model through parameter estimation

One important issue before applying approximate models for predicting extreme events is 315 the model calibration through parameter estimation. The method adopted here follows the 316 algorithm in a recent work<sup>81</sup>. The main difficulty in estimating the parameters in general 317 nonlinear systems with only partial observations is that the closed form of the likelihood 318 function is typically unavailable. Therefore, data augmentation of trajectories associated 319 with the hidden variables is often  $applied^{82-85}$ , which then allows using the Markov Chain 320 Monte Carlo (MCMC) methods to sample the parameters and the hidden trajectories in 321 an alternative way for parameter estimation. Yet, since the hidden trajectories lie in an 322 infinitely dimensional space (or finite but large dimensional with the discrete approximation), 323 the data augmentation can be quite slow in many applications. 324

Here, in light of the closed analytic formulae (3) of the conditional Gaussian nonlinear approximate models (1), data assimilation can be incorporated into a classical MCMC algorithm to circumvent the most expensive part of the parameter estimation algorithm, namely sampling the unobserved trajectories using data augmentation. Specifically, in each iteration step k of the MCMC, we make use of the observed trajectories  $\mathbf{u}_{\mathbf{I}}$  and the current updated parameters  $\boldsymbol{\theta}^{(k)}$  to recover the unobserved trajectories of  $\mathbf{u}_{\mathbf{II}}$ , namely  $\mathbf{u}_{\mathbf{II}}^{mis,(k)}$  via data assimilation (3) in a deterministic and optimal way. Then  $\mathbf{u}_{\mathbf{II}}^{mis,(k)}$ ,  $\mathbf{u}_{\mathbf{I}}$  and  $\boldsymbol{\theta}^{(k)}$  are used together to compute the likelihood function

$$p(\mathbf{u}_{\mathbf{I}}|\boldsymbol{\theta}^{(k)}) = p(\mathbf{u}_{\mathbf{I}}|\boldsymbol{\theta}^{(k)};\mathbf{u}_{\mathbf{II}}^{mis,(k)}),$$

which will be used in the MCMC algorithm for updating the parameters in the k+1 iteration step. For a complete description of the algorithm, see<sup>81</sup> for details. The slight difference of the algorithm applied here compared to the original version in<sup>81</sup> is that an adaptive MCMC procedure<sup>86</sup> for choosing the proposal function is applied.

## 329 E. Quantifying the prediction skill

#### 330 1. Path-wise measurements

#### <sup>331</sup> The root-mean-square error (RMSE) and the pattern correlation (Corr).

The root-mean-square error (RMSE) and the pattern correlation (Corr) are the two pathwise measurements that have been widely applied to quantify the prediction skill<sup>21,87–91</sup>. Denote  $u_i$  the true signal and  $\hat{u}_i$  the prediction estimate, where  $i = 1, \ldots, n$  is an index in time. These measurements are given by

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n} (\hat{u}_i - u_i)^2}{n}},\tag{4}$$

$$\operatorname{Corr} = \frac{\sum_{i=1}^{n} (\hat{u}_i - \overline{\hat{u}}_i)(u_i - \overline{u}_i)}{\sqrt{\sum_{i=1}^{n} (\hat{u}_i - \overline{\hat{u}}_i)^2} \sqrt{\sum_{i=1}^{n} (u_i - \overline{u}_i)^2}},$$
(5)

where  $\overline{\hat{u}}_i$  and  $\overline{u}_i$  denote the mean of  $\hat{u}_i$  and  $u_i$  respectively.

In practice, the trajectory of the ensemble mean is often used as  $\hat{u}_i$  in measuring the RMSE and Corr. These two path-wise measurements are intuitive and easy to be applied. Typically, a prediction is said to be skillful if the RMSE is below one standard deviation of the true signal and the Corr is above the threshold Corr = 0.5.

Yet, we have to point out several potential issues in these measurements. First, since only the ensemble mean is used as the predictor, the predicted uncertainty which involves the ensemble spread (or the confidence interval of the ensemble mean prediction) is not involved in these path-wise measurements. Second, these path-wise measurements fail to quantify the skill of the long-term forecast, since the ensemble mean simply becomes the equilibrium mean state of the system. In addition, both the RMSE and Corr take into account only the information up to the second order statistics. Thus, they may lead to biased conclusions for predicting extreme events and non-Gaussian features. Nevertheless, due to the simple form, these path-wise measurements can still be applied to provide some useful information for the short- and medium-range forecasts.

#### <sup>347</sup> The temporal autocorrelation function (ACF).

Autocorrelation is the correlation of a signal with a delayed copy of itself, as a function of delay. For a zero mean and stationary random process u, the autocorrelation function (ACF) can be calculated as

$$ACF(t) = \lim_{T \to \infty} \frac{1}{T} \int_0^T \frac{u(t+\tau)u^*(\tau)}{\operatorname{Var}(u)} d\tau,$$
(6)

where  $\cdot^*$  denotes the complex conjugate. The ACF has been widely used to measure the 351 system memory. It also plays an important role in improving the linear response via the 352 fluctuation-dissipation theorem<sup>31,92</sup>. If the perfect model and the approximate model share 353 the similar ACFs, then the two systems usually have a similar dynamical behavior at least 354 up to the second order statistics. However, for nonlinear and chaotic systems, high order 355 statistics may play an important roles for extreme events. Therefore, the ACF can only be 356 regarded as a crude indicator of the overall predictability of the underlying system. As a 357 remark, the information theory is able to provide a rigorous and practical way to quantify 358 the error in the two ACFs associated with the perfect and approximate models by making 359 use of their spectral representations. See<sup>30,93</sup> for details. 360

## 361 2. Information measurements

Information theory provides a natural way to quantify the prediction skill and model error by measuring the lack of information. Different from the path-wise measurements, the information measurements assess the statistical behavior of the systems. The lack of information in one probability density q compared with another p is through the relative entropy  $\mathcal{P}(p,q)^{2,94-98}$ ,

$$\mathcal{P}(p,q) = \int p \log\left(\frac{p}{q}\right),\tag{7}$$

which is also known as the Kullback-Leibler divergence or information divergence<sup>99-101</sup>. Despite the lack of symmetry, the relative entropy has two attractive features. First,  $\mathcal{P}(p,q) \geq 0$ with equality if and only if p = q. Second,  $\mathcal{P}(p,q)$  is invariant under general nonlinear changes of variables.

## <sup>371</sup> Long-term prediction.

The long range forecast using the approximate model aims at capturing the non-Gaussian statistical equilibrium states of the truth, especially the fat tails that correspond to the extreme events. This is very different from the short- or medium-range forecasts, where the path-wise measurements of the ensemble mean are informative. In fact, the path-wise measurements completely fail to quantify the long range forecasting skill. Information theory, on the other hand, provides a natural quantification of the statistical prediction skill in the approximate model, which is given by

$$\mathcal{E}_{eq} = \mathcal{P}(p_{eq}, p_{eq}^M),\tag{8}$$

where  $p_{eq}$  and  $p_{eq}^{M}$  are the equilibrium PDFs of the perfect model and the approximate model, respectively. The information measurement in (8) is able to quantify the skill of the approximate model in capturing both the majority of the events represented by the mode of the PDF and the intermittent extreme events in the PDF tails. Note that minimizing the information score in (8) is also known as capturing the model fidelity<sup>94</sup> using approximate models.

#### <sup>385</sup> The short- and medium-range forecasts.

The information theory can also be applied to quantify the short- and medium-range forecasting skill. The fundamental difference between the information measurements and the path-wise ones is that the information measurements are able to take into account the predicted uncertainty. Denote  $p_t$  and  $p_t^M$  the PDFs of the time-dependent perfect and approximate models starting from the same initial time. Similar to (8), an information metric for quantifying the predicted model error as a function of time can be defined as

$$\mathcal{E}_t = \mathcal{P}(p_t, p_t^M). \tag{9}$$

<sup>392</sup> A suitable approximate model is expected to have a small model error throughout the time.

The information measurements can also be used to assess the predictability, also known as the internal prediction skill, of both the perfect and approximate models using the following matric<sup>74,102,103</sup>,

$$\mathcal{D}_t = \mathcal{P}(p_t, p_{eq}), \quad \text{and} \quad \mathcal{D}_t^M = \mathcal{P}(p_t^M, p_{eq}^M).$$
 (10)

<sup>396</sup> Clearly, the measurement in (10) quantifies the information provided by the initial condi-<sup>397</sup> tions about the future state of the system beyond the prior knowledge available through <sup>398</sup> equilibrium statistics. Obviously, both  $\mathcal{D}_t$  and  $\mathcal{D}_t^M$  will decay to zero eventually. Therefore, <sup>399</sup> the measurement in (10) can be regarded as an analog to the ACF but it takes into account <sup>400</sup> the entire predicted PDF rather than simply the path associated with the ensemble mean <sup>401</sup> prediction.

## IV. A SIMPLE MODEL WITH HIGHLY NON-GAUSSIAN BEHAVIOR IN THE HIDDEN PROCESS

Stochastic parameterizations are widely used in developing approximate models for com-404 plex dynamical systems with partial observations<sup>1,104–106</sup>. The idea of applying stochastic 405 parameterizations is to use simple stochastic processes to describe the complicated dynam-406 ics of the unobserved or unresolved scales such that the overall computational cost of the 407 approximate models is greatly reduced. One important practical issue is to develop suitable 408 stochastic parameterizations for the hidden processes such that the intermittent features 409 are captured and the approximate models with the stochastic parameterizations are able to 410 accurately predict the extreme events in the observed variables. 411

The goal of this section is to test the skill of a simple and efficient stochastic parameterization strategy in predicting intermittent non-Gaussian features and extreme events based on a low-order highly non-Gaussian test model given only a short period of training data with partial observations.

## <sup>416</sup> A. The perfect and approximate models

### 417 The perfect model.

The perfect test model here is given by a two-dimensional system where only a short

trajectory of one variable u is observed. The model reads,

$$du = \left(-\gamma u + F_u\right)dt + \sigma_u dW_u,\tag{11a}$$

$$d\gamma = (a_{\gamma}\gamma + b_{\gamma}\gamma^2 + c_{\gamma}\gamma^3 + f_{\gamma})dt + (A_{\gamma} + B_{\gamma}\gamma)dW_{\gamma,1} + \sigma_{\gamma}dW_{\gamma,2}.$$
 (11b)

In this model, the variable  $\gamma$  acts as a stochastic damping in the equation of u and the aver-418 aged value of  $\gamma$  over time needs to be positive to guarantee the mean stability of  $u^{107}$ . Once 419 the sign of  $\gamma$  switches from positive values to negative values,  $\gamma$  becomes anti-damping and 420 it leads to the intermittent events in u. On the other hand,  $\gamma$  is driven by a cubic nonlinear 421 equation with correlated additive and multiplicative noise. This cubic model is a canon-422 ical model for low frequency atmospheric variability<sup>108,109</sup>. This one-dimensional, normal 423 form has been applied in a regression strategy for data from a prototype atmosphere and 424 ocean model to build one-dimensional stochastic models for low-frequency patterns such as 425 the North Atlantic Oscillation and the leading principal component that has features of the 426 Arctic Oscillation. Given the non-Gaussian features and the potential physical explanations, 427 the low-order model (11) becomes a useful testbed for developing suitable stochastic param-428 eterization strategies of the hidden process that allows skillful prediction of the extreme 429 events in the observed variable. 430

### <sup>431</sup> The following parameters are taken in the perfect model,

$$F_{u} = 0.3, \qquad \sigma_{u} = 0.1, \qquad a_{\gamma} = -\frac{3}{8}, \qquad b_{\gamma} = 1, \qquad c_{\gamma} = -\frac{1}{2}, A_{\gamma} = 0, \qquad B_{\gamma} = \frac{1}{2\sqrt{2}}, \qquad f_{\gamma} = 0.1, \qquad \sigma_{\gamma} = \frac{1}{2\sqrt{2}}.$$
(12)

With these parameters, the model trajectories together with the equilibrium PDFs and ACFs are shown in Panels (a)–(c) of Figure 1. Note that the time series in Panel (a) only contains a length of 500 time units but the PDFs and ACFs in Panels (b)–(c) are computed based on the model simulation with a length of 10,000 units in order to minimize the sampling bias in showing these statistics.

In this dynamical regime, the time series of  $\gamma$  shows a stochastic switching behavior. Roughly speaking,  $\gamma$  has two statistical states. The averaged value in one state is slightly negative, corresponding to the intermittent phase of u, while another state of  $\gamma$  is positive, corresponding to the quiescent phase of u. The PDF of u, due to the intermittent extreme events, is highly skewed with an one-sided fat tail. On the other hand, the PDF of  $\gamma$  shows a bimodal behavior, which is also significantly non-Gaussian. The ACFs indicate that overall u has a longer memory than  $\gamma$ .

## <sup>444</sup> The approximate model.

The perfect model (11) here can be regarded as a paradigm model in many real applications, where the hidden variables are driven by some unknown complicated processes that interact with the observed variables in a highly nonlinear way. From a practical point of view, it is important to develop a simple and computationally tractable approximate model which is nevertheless able to capture the key nonlinear feedback from the unobserved variable  $\gamma$  to the observed variable u. The approximate model is expected to predict the extreme events of the observed process u.

One commonly used reduced order modeling strategy is to adopt a mean stochastic model (MSM) for the observed process u. The MSM makes use of the averaged value of  $\gamma$  as the damping term and the resulting system is

$$du = (-\hat{\gamma}u + F_u)dt + \sigma_u dW_u. \tag{13}$$

Since the mean stability is guaranteed in the original system, the constant  $\hat{\gamma}$  is positive. Thus, the MSM is a linear model with Gaussian statistics. It has been shown in<sup>22,107</sup> that the MSM is unable to capture the short-term rapid increment of the intermittent trajectory of *u* due to the lack of intermittent instability mechanism. Such a Gaussian model also fails to predict the long-term non-Gaussian PDF with skewness and fat tails.

Here, a new approximate model is developed using the stochastic parameterized equation technique<sup>48,49</sup>, the idea of which has been applied to the extended Kalman filters (known as the SPEKF-type model) and other prediction and data assimilation forecast models. The approximate model has the following form,

$$du = (-\gamma u + F_u)dt + \sigma_u dW_u, \tag{14a}$$

$$d\gamma = -d_{\gamma}(\gamma - \hat{\gamma})dt + \sigma_{\gamma}dW_{\gamma}.$$
(14b)

In (14), the nonlinear process  $\gamma$  with correlated additive and multiplicative noise in (11b) has been simplified to a linear process with only Gaussian additive noise. Nevertheless, the variable  $\gamma$  remains switching between positive and negative phases, representing damping and anti-damping effects as a feedback to u. Therefore, the variable  $\gamma$  is still able to trigger intermittent extreme events in u. One important feature is that the approximate model (14) belongs to the conditional Gaussian nonlinear framework as was described in Section II, which allows the effective algorithm (3) to solve the conditional statistics of the hidden variable  $\gamma$  given the observations from u. This greatly facilitates the data assimilation and predictions.

#### 469 B. Parameter estimation

Before applying the approximate model for prediction, the parameters  $(F_u, \sigma_u, d_\gamma, \hat{\gamma}, \sigma_\gamma)$ 470 in the approximate model (14) need to be estimated. The training time series only involves 471 the observed variable u and the training data has only a short period with 500 units as 472 shown in Panel (a) of Figure 1. Applying the parameter estimation algorithm described 473 in Section IIID, the results are shown in Figure 2. The trace plots associated with all the 474 parameters clearly indicate the convergence towards certain values with small uncertainties. 475 Notably, the estimation values of the two parameters  $\sigma_u$  and  $F_u$  in the observed process are 476 almost the same as the ones in the perfect model. The averaged values of the trace plots 477 from iteration k = 5000 to iteration k = 10000 are utilized as the estimated parameters in 478 the approximate model for prediction: 479

$$d_{\gamma} = 0.2545, \qquad \hat{\gamma} = 1.121, \qquad F_u = 0.2489, \qquad \sigma_{\gamma} = 0.4362, \qquad \sigma_u = 0.1008.$$
(15)

#### 480 C. Long-term prediction

With the estimated parameters, we begin with studying the long-term prediction using 481 the approximate model (14). As an analogy to Panels (a)-(c) in Figure 1 for the perfect 482 model, Panels (d)–(f) in Figure 1 show the trajectories, PDFs and ACFs of the approximate 483 model. Note that Panel (d) is simply a free run of the model. Therefore, there is no point-484 to-point correspondence between the trajectories shown in Panels (a) and (d) for the perfect 485 and approximate models. Nevertheless, it is easy to see that the trajectories from the perfect 486 and approximate models are qualitatively similar to each other, indicating the skill of the 487 approximate model in capturing the long-term dynamical and statistical behavior. Next, to 488 understand the quantitative similarity between the two models, the equilibrium PDFs and 489 the ACFs are compared. 490

Panels (c) and (f) show that both the ACFs of u and  $\gamma$  associated with the two models 491 are very similar to each other, indicating the success of the approximate model in capturing 492 the temporal information of the perfect system. On the other hand, as shown in Panels 493 (b) and (e), the PDF of u is also perfectly recovered by the approximate model, where 494 using the information distance (7) the difference between the PDFs associated with the 495 approximate and perfect models  $\mathcal{P}(p_{eq}(u), p_{eq}^M(u)) = 0.0345$  is a negligible value. The PDF 496 of  $\gamma$  is not perfectly recovered because the approximate model uses only a linear system with 497 additive noise for  $\gamma$ , which fails to capture the non-Gaussian PDF of  $\gamma$ . This is known as 498 the information barrier<sup>22</sup>. Nevertheless, the PDF of  $\gamma$  associated the approximate model is 499 nearly exact the same as the Gaussian fit of the bimodal distribution associated with the 500 truth. This in fact implies that the approximate model has reached its predictability limit 501 in predicting the long-term statistics of the hidden variable  $\gamma$ . 502

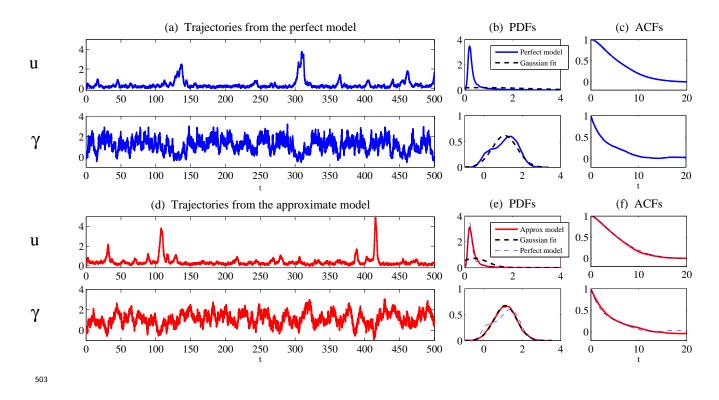


FIG. 1. Model trajectories, PDFs and ACFs of the perfect model (11) with parameters in (12). Top: u; Bottom:  $\gamma$ . Note that the PDFs and ACFs are computed based on the model simulation with a length of 10,000 units. But in panels (a) and (c) only time series with a length of 500 time units are shown. The black curves in the PDFs show the Gaussian fits.

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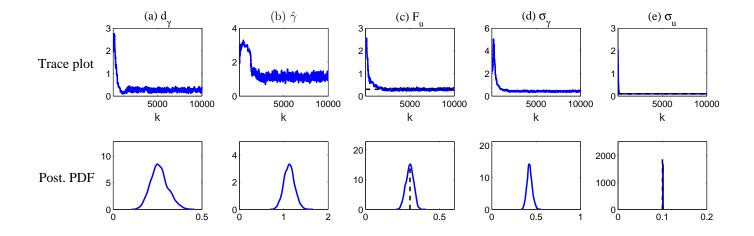


FIG. 2. Parameter estimation of the approximate model (14). Top: trace plot. Bottom: posterior PDFs of the parameters from the trace plot taking the values from k = 5000 to k = 10000. The black lines show the values of  $\sigma_u$  and  $F_u$  in the perfect model (11), serving as reference values.

#### 510 D. Data assimilation

One key feature of the approximate model (14) is that it belongs to the conditional Gaussian model family (1), which allows using the closed analytic formulae (3) to solve the the conditional distribution  $p(\gamma|u)$  for assimilating the unobserved variable  $\gamma$ . Note that the perfect model (11) is not a conditional Gaussian system and expensive particle methods have to be used in order to assimilate the unobserved variable  $\gamma$  even in this two-dimensional system. Therefore, the approximate model (14) is much more computationally efficient for state estimation, data assimilation and prediction.

Figure 3 shows the data assimilation results using the approximate model (14) as the 518 forecast model. It is clear that the  $\gamma$  values associated with the intermittent phase of u519 are recovered with both high accuracy and low uncertainty. The accurate recovery of the 520 hidden variable  $\gamma$  at the intermittent phase of u indicates its potential for predicting the 521 extreme events. On the other hand, assimilating the  $\gamma$  states corresponding to the quiescent 522 phase of u are recovered with high uncertainty. The posterior mean also fails to track the 523 fluctuations in the true trajectory. This is not surprising since the quiescent phases of u524 have weak amplitudes and therefore the noise-to-signal ratio is large. In fact, as long as the 525 hidden variable  $\gamma$  stays positive, playing the role as a damping, it has very weak influence 526 on the dynamics u at the quiescent phases. The assimilated values and uncertainties of  $\gamma$ 527 accurately reflect these features. 528

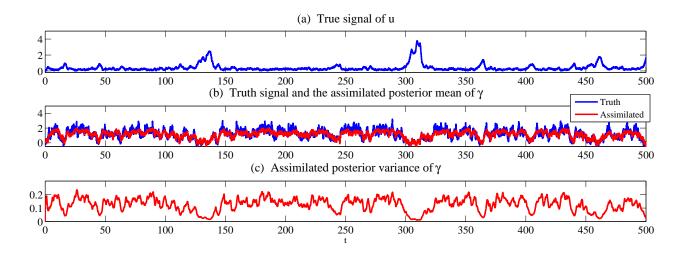


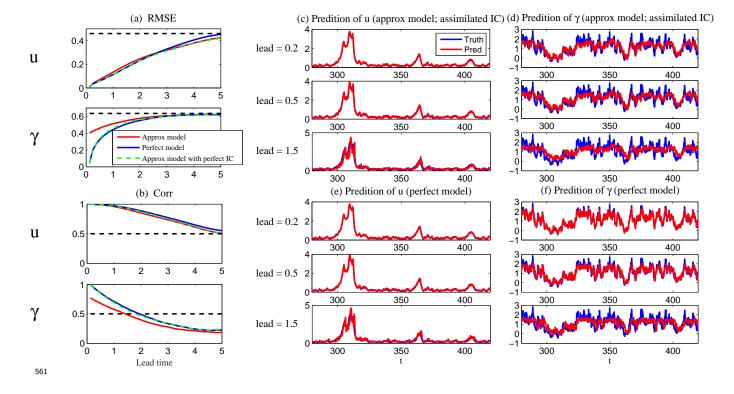
FIG. 3. Data assimilation of the hidden variable  $\gamma$  using the approximate model (14) as the forecast model. The true signal of the observed variable (panel (a)) is generated from (11). Panel (b) shows the true signal of  $\gamma$  from (11) and the assimilated (filtered) posterior mean of  $\gamma$  using the approximate forecast model (14). Panel (c) shows the posterior variance. The black dashed boxes indicates the events that will be studied for short-term prediction in the next subsections.

### 529 E. Short- and medium- range forecasts

To study the short- and medium-range forecast, we first show the RMSE and the Corr 530 between the predicted time series and the truth as a function of lead time. Here the ensemble 531 mean is used as the predicted time series. As illustrated in Panels (a)–(b) of Figure 4, 532 the approximate model with the assimilated initial conditions has an overall comparable 533 prediction skill as the perfect model prediction with the perfect initial conditions. The only 534 main difference lies in the very short term for predicting  $\gamma$ , where the prediction using the 535 approximate model with the assimilated initial conditions has a larger error. This is due 536 to the large uncertainty in the assimilated initial conditions at the quiescent phases. In 537 fact, if we adopt the approximate model as the forecast model but use the perfect initial 538 conditions (green curves), then the prediction skill is almost the same as using the perfect 539 model prediction. Note that the overall skillful prediction of u lasts up to 5 units while that 540 of  $\gamma$  is around 2 units. 541

Panels (c)–(d) and (e)–(f) of Figure 4 show the lead time prediction at 0.2, 0.5 and 1.5542 units using the approximate model with the assimilated initial conditions and the perfect 543 model with the perfect initial conditions, respectively. The prediction of u, especially the 544 extreme events, is quite accurate at all the three lead times for both the models. The 545 prediction of the negative phase of  $\gamma$  is also nearly perfect. The only difference between the 546 two models lies in predicting the positive phases of  $\gamma$ , where the approximate model cannot 547 provide an accurate prediction even at a very short lead time. This is due to the error and 548 the uncertainty in the assimilated initial conditions as was discussed above. On the other 549 hand, while the perfect model is able to predict the positive phase of  $\gamma$  (corresponding to the 550 quiescent phases of u) in a very short term, it is interesting to see that even with the perfect 551 model and perfect initial conditions, some significant errors already appear in predicting the 552 positive phases of  $\gamma$  at a lead time 0.5. At a lead time 1.5, the perfect model essentially gives 553 the same results as the approximate model, where an accurate prediction is found in both 554 u and the negative phase of  $\gamma$  while the model is not very skillful in predicting the positive 555 phase of  $\gamma$ . These facts indicate that when  $\gamma$  is positive it only has a weak influence on u 556 and therefore the system has an intrinsic weak dependence of  $\gamma$ . 557

To conclude, the approximate model has almost the same short- and medium-range forecasting skill as the perfect model, especially in predicting the extreme events in u and the



#### corresponding triggering phases in $\gamma$ .

FIG. 4. Short- and medium-range forecasts. Panels (a)–(b): RMS error and pattern correlation 562 between the predicted time series and the truth as a function of lead time. Red: prediction 563 using the approximate model (14), where the initial values of  $\gamma$  are obtained by data assimilation. 564 Dashed blue: prediction using the perfect model (11) with perfect initial conditions. Dashed green: 565 prediction using the approximate model (14) but with perfect initial conditions. Panels (c)-(d): 566 Ensemble mean prediction using the approximate model with assimilated initial condition (IC) at 567 lead times 0.2, 0.5 and 1.5. The blue curves show the truth while the red ones show the prediction. 568 Panels (e)–(f): Similar to (c)–(d) but using the perfect model and perfect initial condition. 569 570 571

### 572 F. Prediction with an initial value starting outside the attractor

Finally, we study the prediction skill of the approximate model if the initial value is out-573 side the attractor (the statistical equilibrium state). In Figure 5, we consider the situations 574 where either the initial value of u or that of  $\gamma$  is outside the attractor. It is clear that when 575 u(0) is outside the attractor while  $\gamma$  stays in the attractor (Panels (a) and (c)), the trajectory 576 of u releases to the attractor in a similar fashion using both the approximate model and 577 the perfect model. This is because there is no approximation in the observed process u and 578 the time evolution of  $\gamma$  at the attractor has already been shown to be accurately described 579 using the approximate model. On the other hand, if  $\gamma$  starts from a value that is outside the 580 attractor (Panels (b) and (d)), then the approximate model in capturing the relaxation of  $\gamma$ 581 towards the attractor may contain errors. In fact, when  $\gamma$  starts from a large value as shown 582 in Panel (b), the cubic damping plays an important role in strongly pushing the system 583 towards the attractor. Starting from a large value of  $\gamma$ , the impact of the cubic damping is 584 much stronger than that at the attractor and therefore the approximate model with a linear 585 damping in  $\gamma$  fails to capture this feature. Nevertheless, if u stays on the attractor, then as 586 long as  $\gamma$  is positive it has only a weak influence on the observed variable u. Therefore, the 587 overall dynamics of u can still be described quite well using the approximate model. 58

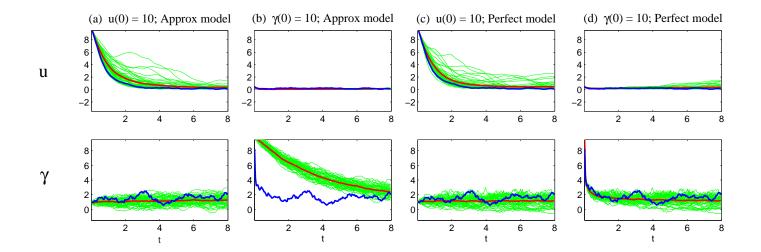


FIG. 5. Ensemble predictions with the initial values starting outside the attractor. Panels (a) and (c): u(0) = 10 starts from a value that is off the attractor.  $\gamma(0) = 1$  is inside the attractor. Panels (b) and (d): u(0) = 0.5 starts from a value that is inside the attractor.  $\gamma(0) = 10$  is off the attractor. Here Panels (a)–(b) show the results using the approximate model while Panels (c)–(d) show those using the perfect model. In all the panels, blue curves show the truth and red curves show the ensemble mean which is the average value of 50 ensembles showing in green color.

## <sup>590</sup> V. A DYAD MODEL WITH ENERGY-CONSERVING NONLINEAR <sup>591</sup> INTERACTION

<sup>592</sup> The nonlinear test model in the previous section involves only an one-way influence from <sup>593</sup>  $\gamma$  to u. Yet, in many applications, the observed variables and the unobserved ones have <sup>594</sup> mutual interactions, which are also often though energy-conserving nonlinear terms<sup>35,36</sup>. <sup>595</sup> Therefore, it is important to understand different strategies in building approximate models <sup>596</sup> to predict the extreme events and other non-Gaussian behavior in such kind of the systems. <sup>597</sup> In this section, a simple but judicious feedback control strategy is adopted to facilitate the <sup>598</sup> prediction of the hidden extreme events in an energy-conserving nonlinear dyad model.

## 599 A. The models

## 600 The perfect model.

601 Consider a nonlinear dyad model with energy-conserving nonlinear interaction,

$$dv = \left(-d_v v - cu^2\right) dt + \sigma_v dW_v,$$
  

$$du = \left((-d_u + cv)u + F_u\right) dt + \sigma_u dW_u.$$
(16)

Again only partial observations are available in this nonlinear dyad model, where v is the 602 observed variable while u is unobserved. This low-order nonlinear model can be regarded 603 as a toy model of complex turbulent flows. For example, v can be treated as one of the 604 Fourier modes associated with the large-scale observed variables while u is associated with 605 the hidden mechanism that drives v. If u represents unresolved or small-scale variables, then 606 its statistics can be highly non-Gaussian. Here, v plays the role of the stochastic damping 607 in the process of u such that intermittent extreme events appear in the trajectory of u. 608 Note that this model is very different from the SPEKF-type of the model described in the 600 previous section. In fact, in the dyad model (16), the variable u also provides a nonlinear 610 feedback to v via  $-cu^2$  such that the total energy in the nonlinear terms of the coupled 611 system is conserved, which is known as the physics constraint  $^{35,36}$ . 612

Below, the nonlinear dyad model (16) is used as the perfect model. The focus of this section is to predict the extreme events in the unobserved process u. To this end, the <sup>615</sup> following parameters are taken in the nonlinear dyad model (16),

$$F_u = 1,$$
  $d_u = 0.8,$   $d_v = 0.8,$   $\sigma_u = 0.2,$   $\sigma_v = 2,$   $c = 1.2.$  (17)

As shown in Panels (a)–(c) of Figure 6, the nearly Gaussian observed variable v switches between positive and negative states, which leads to the intermittency in the hidden process u. The non-zero forcing  $F_u = 1$  makes the signal of u stay almost within the positive values and the PDF of u is skewed with an one-side fat tail. Note that the amplitude of this forcing term provides different dynamical behavior of the model. In the last part of this section, the prediction skill in different dynamical regimes with various values of  $F_u$  will be reported.

#### <sup>622</sup> The approximate model.

Again, a suitable approximate model is able to predict the extreme events and other 623 important non-Gaussian features of the perfect model. Meanwhile, the approximate model 624 is expected to be computationally efficient for data assimilation and prediction. Due to 625 the closed analytic formulae of the conditional Gaussian models in assimilating the unob-626 served variables, we now aim at developing a suitable approximate model that belongs to 627 the conditional Gaussian framework. Note that by observing v, the perfect model (16) is 628 not a conditional Gaussian nonlinear system. One starting idea for building an approximate 629 model is to apply a bare truncation strategy, which ignores the quadratic feedback term  $-u^2$ 630 in the process of v in (16). This is actually a commonly used strategy in developing approx-631 imate models for many complicated systems in practice, where some nonlinear terms are 632 dropped. However, this strategy does not work for studying the extreme events with partial 633 observations. In fact, without this feedback term, the variable u is completely decoupled 634 from the process of v. In other words, given only the observations in v, the processes and 635 the parameters of u are not even identifiable. What is more, using the same parameters as 636 in (17), such an approximate model suffers from a finite-time blowup of the signals<sup>35,110</sup>. 637

The failure of the bare truncation model is due to the complete ignorance of the nonlinear feedback term from u to v. This nonlinear feedback not only provides the observability of u in the v process but also offers the important causal effects between the two processes. Therefore, a suitable approximate model is supposed to take into account such an interaction <sup>642</sup> between the two processes. To this end, the following approximate model is adopted,

$$dv = \left(-d_v v - cu\right) dt + \sigma_v dW_v,$$
  

$$du = \left((-d_u + cv)u + F_u\right) dt + \sigma_u dW_u.$$
(18)

This approximate model uses a linear feedback -cu to approximate the nonlinear interaction  $-cu^2$  in the original dyad model. This simplification can be regarded as using a linear control term to retain the mutual dependence of u and v. It also allows the approximate model to belong to the conditional Gaussian framework that facilitates efficient data assimilation and prediction algorithms.

#### 648 B. Parameter estimation

For the parameter estimation of the approximate model (18), we make use of a short training data of v with only 500 time units as shown in Panel (a) of Figure 6. The parameter estimation algorithm is run for K = 15000 steps and the averaged values from the trace plots between k = 5000 to k = 15000 is used as the estimated parameters,

$$d_v = 0.9234,$$
  $d_u = 0.6672,$   $c = 1.8249,$   $F_u = 0.6041,$   
 $\sigma_u = 0.0527,$   $\sigma_v = 2.0203.$  (19)

It is useful to compare the estimated parameter values in the approximate model (19) with those in the perfect model (17). This helps understand the dynamical properties of the approximate model.

The feedback parameter c in the approximate model (17) is increased. This is due to 656 the fact that  $cu^2$  in the perfect model is replaced by cu in the approximate model while 657 the amplitude of u in the perfect model is often larger than 1 especially in the intermittent 658 phases. Therefore, the coefficient c has to be increased in order to retain the amplitude of 659 the feedback from u to v. On the other hand, according to the second equation in (18), due 660 to the increase of c, the amplitude of u will increase as well especially for the intermittent 661 phase. Therefore, the forcing  $F_u$  in the approximate model is decreased in order to retain 662 the amplitude of the observed variable u as in the perfect model. 663

#### 664 C. Long-term prediction

<sup>665</sup> With the estimated parameters in hand, we first compare the long range forecasts between <sup>666</sup> the perfect dyad model (16) and the approximate model with the linear feedback (18).

In Panels (d)–(f) of Figure 6, the trajectories, the PDFs and the ACFs associated with the approximate model are shown, where for a fair comparison of the time series, the same random number seeds are used. The recovered trajectory of the observed variable v using the approximate model with the linear feedback term almost perfectly matches that of the truth (with Corr = 0.998 and RMSE = 0.011).

Now let us focus on the hidden intermittent variable u. Comparing the second and the 672 fourth rows of Figure 6, it is clear that the approximate model with the linear feedback 673 (18) is skillful in generating the intermittent extreme events in u. In fact, the pattern 674 correlation between the two time series in these two rows is 0.93, which also indicates that 675 the approximate model is able to capture the timing of the occurrence of extreme events. 676 Yet, there are two main errors in the approximate model. First, the amplitudes of the 677 intermittent events seem to be slightly overestimated. This is easy to understand because in 678 order to reach the same observed trajectory v, the linear feedback requires a larger u in the 679 approximate model than the quadratic nonlinear feedback in the perfect model. Second, the 680 quiescent events also seem to be slightly underestimated in the approximate model. This 681 results in the fact that the peak of the associated PDF is closer to zero than that of the true 682 signal. The model error 683

$$\mathcal{E}_{eq} = \mathcal{P}(p_{eq}, p_{eq}^M) = 0.46, \tag{20}$$

which, although is non-negligible, comes largely from the quiescent events. The PDFs of u associated with both the perfect and approximate models are skewed with an one-sided fat tail. Therefore, the long range behavior of the approximate model in capturing the information in the tail that corresponds to the extreme events remains similar to that of the perfect model.

Another conclusion drawn from Figure 6 is that the ACFs of u and v associated with both the perfect model and the approximate model are very similar to each other, decaying to zero after one time unit.

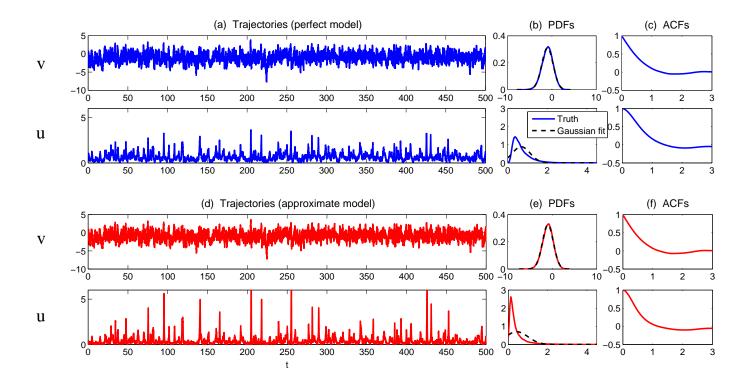


FIG. 6. Panels (a)–(c): Time series, PDFs and ACFs of the dyad model (16) with the parameters in (17). Panels (d)–(f): those of the approximate model (17) with the estimated parameters in (19).

#### <sup>693</sup> D. Data assimilation, Short- and medium-range forecasts

Given the observation in v, the assimilated u is shown in Figure 7. Overall, the assimilated signal of the hidden variable u and the truth have a very good match in terms of the patterns. Yet, due to the intrinsic model error as discussed above, the quiescent and intermittent phases are slightly underestimated and overestimated, respectively.

Panels (a)–(b) of Figure 8 show the RMSE and the Corr between the true signal and the 698 ensemble mean predictions as a function of lead time. Except at the very short lead time, 699 where the data assimilation results in some uncertainties in the initial values, the approxi-700 mate model essentially gives the same prediction skill as the perfect model in terms of the 701 RMSE and the Corr. This indicates the overall skillful prediction using the approximate 702 model. Note that since our focus is the extreme events in the hidden process, some extra 703 information beyond the RMSE and Corr needs to be explored. In Panels (c)-(d), a compar-704 ison of the medium range forecasts and the forecast PDFs at lead time t = 0.6 is shown. It 705 is clear that the approximate model is more skillful in capturing the extreme events and the 706 fat tail of the predicted PDF than the perfect model. This is not surprising. In fact, it is 707 well known that the amplitude of the ensemble mean prediction decays as time evolves. On 708 the other hand, the slight overestimation of the amplitude of u in the approximate model 709 compensates the underestimation of the amplitudes in the ensemble mean forecast, which is 710 crucial in predicting extreme events at the medium range. 711

Figure 9 shows four case studies of the time evolution of the predicted PDFs starting 712 from different initial phases. The predictions of v using both the perfect model and the 713 approximate model are overall similar to each other. Note that more ensemble members in 714 the prediction using the approximate model are actually able to forecast the extreme events 715 than the perfect model. This feature is quite useful for medium-range forecast, especially 716 when the starting time is an onset phase of the extreme events in u (Cases 1 and 2). In 717 addition, even with some errors in the initial condition due to the data assimilation (Case 718 4), the approximate model is still able to capture the time evolution of extreme events. 719

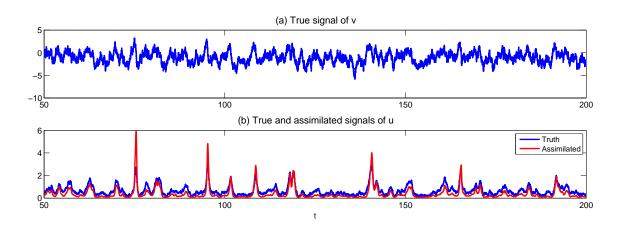


FIG. 7. Panel (a): the true signal of v from the perfect dyad model (16). Panel (b): the true signal of u from the perfect dyad model (16) and assimilated signals of u using the approximate model (18).

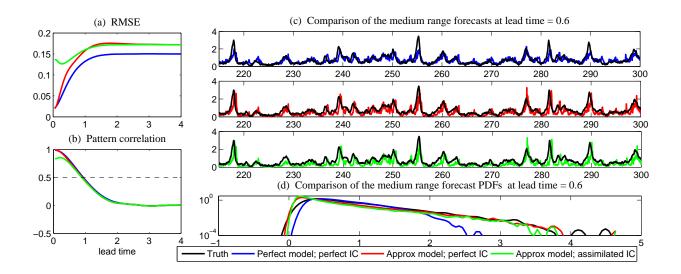


FIG. 8. Short- and medium-range forecasts based on the ensemble mean forecast. Panel (a)–(b): RMSE and Corr between the true signal and the prediction ones as a function of lead time. Blue: perfect model prediction with the perfect initial condition. Red: approximate model prediction with perfect initial condition. Green: approximate model prediction with assimilated initial conditions. Panel (c): comparison of the medium range forecasts at lead time t = 0.6. Panel (d): comparison of the medium range forecast PDFs at lead time t = 0.6.

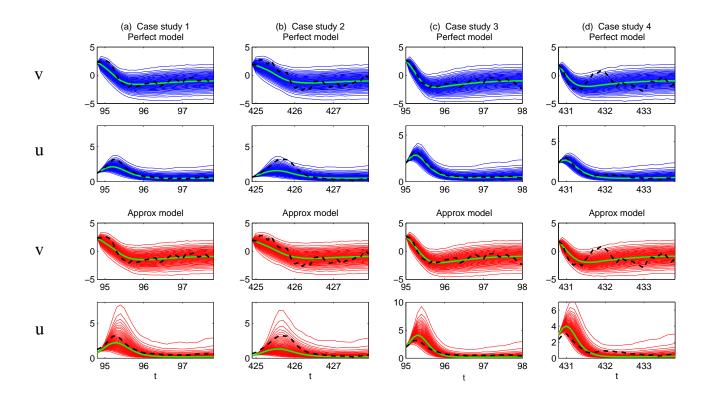


FIG. 9. Case studies. Time evolution of the predicted PDFs starting from different initial phases. Each PDF is shown with 50 thin curves, which represent the 1st, 3nd, 5th, ..., 97th and 99th percentiles of the of the PDF. The green curve represents the mode of the PDF since the PDF is non-Gaussian. The black dashed curve is the true signal. Columns (a)–(b): starting from an onset phase of extreme events. Columns (c)–(d): starting from a mature phase of extreme events.

#### <sup>720</sup> E. Prediction with an initial value starting outside the attractor

In this subsection, we compare the predictions when the initial values are outside the attractor. According to Figure 6, the attractor of u contains values that are positive but almost always stay below u = 4. Thus, we consider the following two situations: A). the hidden variable u starting from a negative value, and B). the hidden variable u starting from a large positive value.

#### <sup>726</sup> A. The hidden variable u starting from a negative value.

In Panels (a)–(f) of Figure 10, we show the prediction where u starts from a negative 727 value u(0) < 0. Here, v always starts from its equilibrium mean value v(0) = -0.9584. 728 In Panels (a)–(b), u(0) = -0.2 is slightly negative. The approximate model behaves in a 729 similar way as the perfect model, where after a short term, the trajectory will arrive at the 730 attractor. However, when u(0) = -0.5 as shown in Panels (c)–(d), some of the ensemble 731 members in the approximate model blows up in finite time (around t = 1.5). See the second 732 row of Panel (d). Such a behavior becomes even worse when u(0) is decreased to u(0) = -0.8733 as shown in Panels (e)-(f), where quite a few ensemble members blow up in a short finite 734 time (around t = 0.5 to t = 1.5). Panel (g) of Figure 10 shows the percentage of the events 735 that blow up as a function of the initial value u(0). As expected, with the decrease of u(0), 736 the number of blowup events increases. 737

Now we look at both the perfect and approximate models (16) and (18) to understand the 738 mechanism that leads to such a finite time blowup issue in the approximate model. First, 739 when u and v are at the attractor, u stays in positive values. When the amplitude of u740 increases due to a negative value of v, both the linear and nonlinear feedback in (16) and 741 (18) will push v back to a negative value and the consequence is that v will strongly damp 742 u and decreases the amplitude of u. However, when u is negative, the nonlinear feedback 743  $-cu^2$  and the linear feedback -cu will play completely different roles since  $-cu^2 < 0$  while 744 -cu > 0. The dynamical property of the perfect dyad model (16) remains unchanged. But 745 the blowup issue appears in the approximate model (18). In fact, once u is negative, the 746 linear feedback will make v become positive. As a result, the positive anti-damping of v747 will further increase the amplitude of u, which makes u blow up in a short time. When the 748 initial value u(0) has a small amplitude (e.g., u(0) = -0.2), the forcing  $F_u = 1 > 0$  may be 749 able to overcome the anti-damping in the short term and push the solution to the attractor. 750

<sup>751</sup> But if the amplitude of u(0) is large, then the role of  $F_u$  is weaker than the anti-damping <sup>752</sup> from v, and the solution has a much higher chance to blow up.

# 753 B. the hidden variable u starting from a large positive value.

Now we let the hidden variable u start from a large positive value and study how the solution adjusts to the attractor. See Panels (h)–(k) in Figure 10.

First, with a moderately large initial condition u(0) = 5 as shown in Panels (h)–(i), the hidden variable u using the approximate model releases to the attractor in almost the same way as that using the perfect model. The trajectories of v are slightly different, but since v is always very negative, the strong damping of v makes the trajectories of u in the two models have very similar behavior.

Next, we increase the initial condition to u(0) = 10. Then we first notice a more significant 761 different in the predicted trajectory of v, where in a short term t = 0.2 the true trajectory 762 and the perfect model prediction can reach v = -8 while the approximate model only allows 763 v = -3. This is due to the model error in the feedback terms. In fact, when u is large,  $-cu^2$ 764 in the perfect model will be much larger than -cu in the approximate model. This leads to 765 the large error in v. As a result, the damping in the approximate model then becomes much 766 weaker compared with the perfect model. Therefore, u releases slower in the approximate 767 model (see the second row of Panel (k)). Notably, the ensemble prediction in the second 768 row of Panel (k) seems not to be too far from the truth (black dashed curve). But the truth 769 is outside 99 percentile of the prediction (the most bottom red curve) when t is between 770 t = 0.1 and t = 0.5. 771

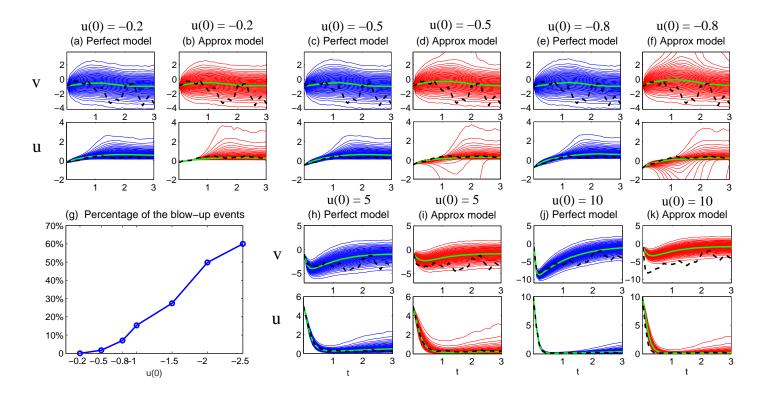


FIG. 10. Prediction of the dyad model with initial values being outside the attractor. Panels (a)-(f) and (h)-(k): Time evolution of the predicted PDFs starting from different initial phases. Each PDF is shown with 50 thin curves, which represent the 1st, 3nd, 5th, ..., 97th and 99th percentiles of the of the PDF. The green curve represents the mode of the PDF since the PDF is non-Gaussian. The black dashed curve is the true signal. In Panels (a)-(f), the hidden variable u starting from a negative value. In panels (h)-(k), the hidden variable u starting from a large positive value. Panel (g) shows the percentage of the events that blow up as a function of the initial value u(0).

# 772 F. Dynamical regimes with different $F_u$

So far, we have focused on the regime with  $F_u = 1$ . In this subsection, the role of  $F_u$ will be explored and dynamical regimes with different  $F_u$  will be studied for predicting the hidden extreme events.

In Panel (a) of Figure 11, the trajectories of u from the perfect model (16) with different  $F_u$  are shown. Here, the same random number seeds are used in generating these time series for a fair comparison.

# 779 **Regime I:** $0.7 \le F_u$ .

When  $F_u$  is sufficiently large, the approximate model with the linear feedback (18) is a suitable model for predicting the hidden extreme events.

782 **Regime II:**  $0 \le F_u < 0.3$ .

When  $F_u$  approaches zero, the intermittent events in u can have both signs. As was 783 discussed in Section VE, when u is negative, the linear feedback -cu in (18) will play a 784 significant different role compared with the nonlinear feedback  $-cu^2$  in the perfect model 785 (16). In fact, the linear feedback -cu becomes positive and make v to be positive. Then 786 the anti-damping of v in the process of u leads to the finite time blowup. Therefore, we 787 conclude that using the approximate model (18) with a linear feedback to predict the hidden 788 extreme events in u requires that the forcing  $F_u$  in the perfect dyad model cannot be too 789 small. If the forcing  $F_u$  in the perfect dyad model is too small, then the approximate model 790 does not have a mechanism to recover the intermittent events in u when u is negative. A 791 new approximate model that has skill in capturing the extreme events with both signs needs 792 to be developed. 793

794 **Regime III:**  $0.3 \le F_u < 0.5$ .

<sup>795</sup> When  $F_u \ge 0.3$ , the intermittent events in the true signal of u only occur in the positive <sup>796</sup> phase. However, the true trajectory of u still goes below 0 quite frequently (with small <sup>797</sup> amplitudes). Panel (c) of Figure 11 shows the data assimilation of u using the approximate <sup>798</sup> model with the linear feedback (18), where the parameters are re-estimated based on the <sup>799</sup> observed signal of v in  $F_u = 0.3$  regime. One important result is that the assimilated state <sup>800</sup> of u can occasionally become quite negative! In fact, as is shown in Panels (b)–(c), before <sup>801</sup> the assimilated u goes to a negative value, the signal of v is large and positive while u is <sup>802</sup> nearly zero. Therefore, when the trajectory of u becomes slightly negative in the true signal, <sup>803</sup> the anti-damping v will amplify the negative phase of u. Since the positive forcing  $F_u = 0.3$ <sup>804</sup> here is pretty weak, this forcing is unable to push u back to the attractor with positive <sup>805</sup> values immediately and therefore the assimilated state of u will stay in the negative phase <sup>806</sup> for a while. According to the discussions in Section V E, if the prediction starts with a large <sup>807</sup> negative value of u, then even for a short term, the prediction using the approximate model <sup>808</sup> may suffer from a short-term blowup<sup>110</sup>.

# 809 Regime IV: $0.5 \le F_u < 0.7$ .

Now the data assimilation results using the approximate model (18) provides the state 810 of u that is always positive. Thus, there will be no issue in data assimilation. However, as 811 shown in Panels (d)-(f) of Figure 11, the approximate model can still suffer from a long (but 812 finite) time blow up issue. This is again related to the insufficient strength of  $F_u$ . In fact, 813 the trajectory of u still has some chances to become slightly negative and the corresponding 814 values of v at these time instants are usually large. Therefore, the anti-damping v and the 815 forcing  $F_u$  in the process of u compete with each other. If the strength of forcing is not 816 strong enough, then for some events, the anti-damping can result in the blowup issue of 817  $u^{110}$ . 818

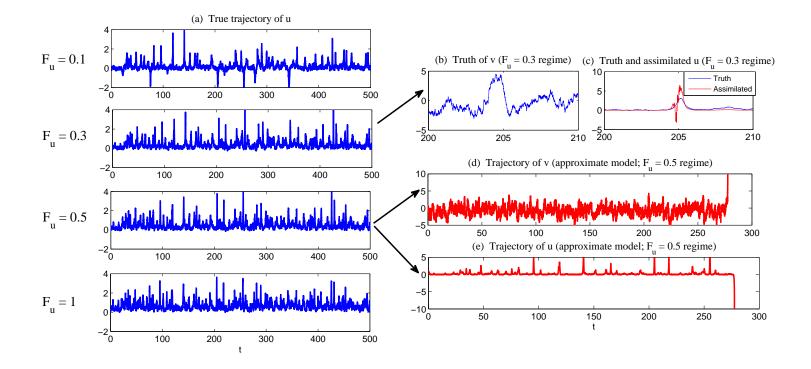


FIG. 11. Dynamical regimes with different  $F_u$ . Panel (a): trajectories of u from the perfect model (16) with different  $F_u$  are shown. Here, the same random number seeds are used in generating these time series for a fair comparison. Panel (b): True signal of v in  $F_u = 0.3$  regime from the perfect model. Panel (d): True signal of u in  $F_u = 0.3$  regime from the perfect model (blue) and the assimilated posterior mean using the approximate model. Panels (e) and (f): trajectories of the approximate model with the estimated parameters from the observed true signal of v in  $F_u = 0.5$ regime.

# 819 VI. THE LORENZ 63 MODEL

In many applications with chaotic or turbulent phenomena, due to the incomplete knowl-820 edge of the underlying dynamics, noise inflation is often incorporated into the dynamical 821 processes<sup>21,104,111</sup>. The enhanced noise plays the role of parameterizing small-scale fluctua-822 tions, which helps increase the variability of the system and has a potential of improving 823 the data assimilation and prediction skill. Yet, it has not been well understood the effect of 824 noise inflation in the extreme events prediction. Therefore, in this and the next two sections 825 (Section VII and Section VIII), noise inflation will be incorporated into the dynamical sys-826 tems for testing the ensemble prediction skill of the observed and hidden extreme events as 827 well as other non-Gaussian characteristics. The difference between the studies in these three 828 sections is as follows. In Section VII and Section VIII, the noise inflation will be combined 829 with various effective and practical strategies for developing effective and simple approxi-830 mate models for improving the prediction of the extreme events resulting from complicated 831 turbulent dynamical systems with regime switching. In this section, the chaotic Lorenz 63 832 model is used as a testbed to understand the skill of the extreme events predictions, where 833 the inflated noise acts as the only source of the model error. 834

# <sup>835</sup> A. The perfect and approximate models

The model considered in this section is the Lorenz  $63 \mod^{72}$ . It is a simplified mathe-836 matical model for atmospheric convection with chaotic behavior. The equations relate the 837 properties of a two-dimensional fluid layer uniformly warmed from below and cooled from 838 above. In particular, the equations describe the rate of change of three quantities with 839 respect to time: x is proportional to the rate of convection, y to the horizontal tempera-840 ture variation, and z to the vertical temperature variation. The constants  $\sigma$ ,  $\rho$ , and  $\beta$  are 841 system parameters proportional to the Prandtl number, Rayleigh number, and certain phys-842 ical dimensions of the layer itself<sup>112</sup>. The Lorenz 63 model is also widely used as simplified 843 models for lasers, dynamos, thermosyphons, electric circuits, chemical reactions and forward 844  $osmosis^{113-119}$ 845

Here, we study a slightly different version of the original Lorenz 63 model by adding a small noise into the x process. We also assume that only a short trajectory of x is observed

as the training data while y and z are the unobserved variables. The model reads:

$$dx = \sigma(y - x)dt + \sigma_x dW_x, \qquad (21a)$$

$$dy = (x(\rho - z) - y)dt, \qquad (21b)$$

$$dz = (xy - \beta z)dt, \tag{21c}$$

The small noise here can be regarded as the observational or measurement uncertainty. It also helps prevent the singularity in the data assimilation formula in (3), which requires a non-zero noise in the observational process. Nevertheless, with a small noise coefficient, the dynamical behavior of the model in (21) remains almost the same as the original noise-free Lorenz 63 model. Below, we always take  $\sigma_x = 1$ , which is a sufficiently small value. The other parameters that are used to generate the true signals of (21) are

$$\sigma = 10, \qquad \rho = 28, \qquad \beta = 8/3.$$
 (22)

These are the classical choices of the Lorenz 63 model. Figure 12 shows the trajectories, PDFs and phase plots of the Lorenz 63 model (21), where the butterfly profile in the phase plots and the chaotic features in the model trajectories are clearly demonstrated. Notably, there are quite a few extreme events that appear in all the three components due to the fact that one of the Lyapunov exponents of the Lorenz 63 system is positive. These extreme events occur when the system states switch between the two branches of the "butterfly wings".

The short trajectory of x in Panel (a) of Figure 12 with only 50 units will be used as the observed training data for the approximate models below.

#### <sup>861</sup> The approximate models.

Below, we aim at understanding the model error that comes from the noise inflation. To this end, it is natural to propose the following approximate model,

$$dx = \sigma(y - x)dt + \sigma_x dW_x,$$
  

$$dy = (x(\rho - z) - y)dt + \sigma_y dW_y,$$
  

$$dz = (xy - \beta z)dt + \sigma_z dW_z,$$
  
(23)

where the noise coefficients  $\sigma_y$  and  $\sigma_z$  are given and fixed empirically, which account for the noise inflation in the hidden variables. Note that here the deterministic parts in the perfect model (21) and the approximate model (23) are the same, which is not always the case in

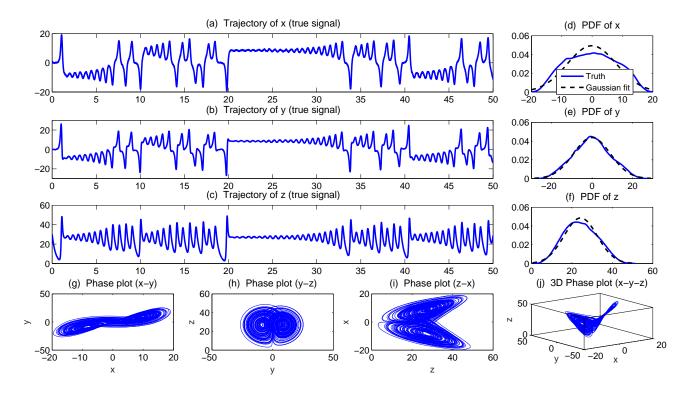


FIG. 12. Trajectories (Panels (a)–(c)), PDFs (Panels (d)–(f)) and the phase plots (Panels (g)–(j)) of the noisy Lorenz 63 model (21) with parameters in (22) and a small noise coefficient  $\sigma_x = 1$ .

real applications where noise inflation is often used to compensate other model errors and simplifications. Nevertheless, the setup here allows us to understand the model error that comes purely from the noise inflation and its effect on the prediction skill.

The noise coefficient  $\sigma_x$  will be estimated from the parameter estimation algorithm. Note that since  $\sigma_x$  is associated with the quadratic variation of the continuously observed training data, a prescribed value with inflation may lead to pathological behavior of the parameter estimation. Depending on the level of noise inflation, we consider the following three approximate models,

Approximate model I.Small noise inflation:
$$\sigma_y = \sigma_z = 1$$
,Approximate model II.Moderate noise inflation: $\sigma_y = \sigma_z = 3$ ,(24)Approximate model III.Large noise inflation: $\sigma_y = \sigma_z = 5$ .

#### 875 B. Parameter estimation

In the approximate models, there are four parameters to be estimated:  $\rho, \sigma, \beta$  and  $\sigma_x$ . Here the parameter estimation algorithm as described in Section III D is run up to K = 15000steps and the averaged values of the trace plots from k = 5000 to k = 15000 are used as the estimated parameters, which are:

Approx model I:	$\rho = 27.48,$	$\sigma = 10.34,$	$\beta = 2.70,$	$\sigma_x = 1.03,$	
Approx model II:	$\rho = 31.04,$	$\sigma = 9.051,$	$\beta = 2.33,$	$\sigma_x = 1.06,$	(25)
Approx model III:	$\rho = 34.17,$	$\sigma = 7.525,$	$\beta = 2.20,$	$\sigma_x = 1.08.$	

Note that due to the model error from noise inflation, the estimated parameters in the approximate models are not exactly the same as those in the perfect model. In particular, with the increase of the noise coefficients  $\sigma_y$  and  $\sigma_z$ , the estimated parameter  $\rho$  and  $\sigma$  seem to be more different compared with the one in the perfect model in order to compensate the model error.

## 885 C. Data assimilation

Figure 13 shows the data assimilation results using the approximate model (23) with the estimated parameters, where the true signal of the observed variable x is generated using the perfect model (21).

In the approximate model I, due to the small model error in the inflated noise coefficients, 880 the assimilated values of y and z are nearly perfect and the uncertainty reflected by the 890 posterior variance in both variables is small. In the approximate model II, the assimilated 891 values of y are still quite accurate but those of z show some errors where the mean state of 892 z has a slight shift towards the positive value. Such a bias in the assimilated posterior mean 893 state is possibly due to the fact that the noise  $\sigma_y$  leads to the change of the mean value of 894 xy in z process since x and y are highly correlated. On the other hand, x and z are not so 895 closely correlated, and therefore the mean value of xz that contributes to the mean state of 896 y is hardly polluted by the noise. Finally, in the approximate model III, where the inflated 897 noise coefficients are large, there are some non-negligible errors in the assimilated states of 898 z and the associated uncertainty increases as well. Nevertheless, despite such a mean state 899 shift, the overall patterns and amplitudes of z are assimilated quite well. 900

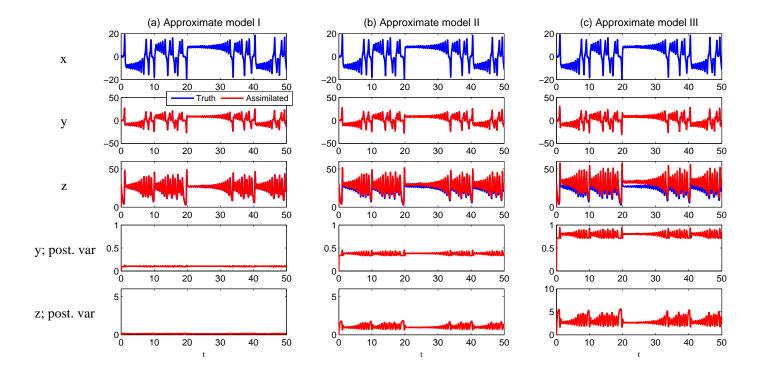


FIG. 13. Data assimilation using the approximate model (23) with different noise inflation levels (24). The first row shows the true trajectory of x. The second and third rows show the true signals of y and z as well as the posterior mean estimations from data assimilation (red). The fourth and fifth rows show the posterior variance of y and z, respectively.

#### <sup>902</sup> D. Long-range forecast

To quantify the long-range forecast skill, the comparison of the equilibrium PDFs and the ACFs between the perfect model and approximate models is shown in Figure 14.

First, all the three approximate models are able to capture the equilibrium non-Gaussian PDFs of both x and y with high accuracy, where the information model error in the equilibrium PDF  $\mathcal{P}(p_{eq}, p_{eq}^M) \leq 0.05$  is tiny even using the approximate model III. For the variable z using the approximate model III, the error is slightly larger  $\mathcal{P}(p_{eq}, p_{eq}^M) = 0.28$  but is still acceptable. Such a model error is due to the fact that the PDF associated with z using the approximate model has a mean shift compared with the truth, which has already been seen in the data assimilation results.

Next, the approximate models and the perfect model overall share quite similar ACFs, indicating similar time evolution behavior (at least up to the second order statistics in time). In particular, the direct relaxation of the ACFs of x, y and the oscillated relaxation of that of z are both captured by the approximate models. The only non-negligible difference appears in the ACF of z when the noise inflation level is large, i.e., in approximate model III, where the approximate model has a slightly faster decaying ACF.

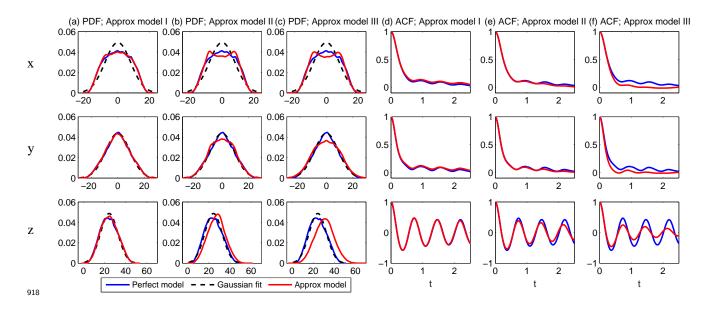


FIG. 14. Comparison of the PDFs and the ACFs of the perfect model and the approximate model.

## 920 E. Short- and medium-range forecasts

To study the short- and medium-range forecasts, we show in Figure 15 three skill scores 921 of the predictions as a function of lead time. Two of them, namely the RMSE and the Corr, 922 are the classical path-wise measurements while the third one is an information criterion, that 923 is, the relative entropy (7) between the PDF of the predicted time series and that of the 924 truth. In order to distinguish the errors due to the noise inflation and the initial uncertainty 925 with data assimilation, we show the predictions using the approximate model with either 926 assimilated initial conditions (ICs) or with perfect initial conditions. All the predictions 927 here are based on the ensemble mean, which is the average of 50 ensemble members. 928

Columns (a)–(b) and Columns (d)–(e) show the RMSE and Corr of the predictions using 929 the approximate models I and II, respectively. These path-wise measurements indicate that 930 the skillful predictions of the approximate models regardless of using perfect or assimilated 931 initial conditions are up to nearly 3 time units. However, the conclusion based on these 932 path-wise measurements can be misleading in this strongly chaotic system. In Columns 933 (g)-(h), the relative entropy has a significant increase as the lead time, especially using the 934 approximate model II. This implies certain non-negligible errors are not captured by the 935 two path-wise measurements. To see such errors, the ensemble mean prediction using the 936 approximate models (green) and the truth (blue) at lead time t = 1 are compared in Figure 937 16. Both the trajectories and the PDFs are shown in order to compare the path-wise and the 938 information measurements. Note that only the Gaussian fits of the PDFs are shown here for 939 the purpose of comparing the variance in the truth and the predicted PDFs which reflects 940 the skill of capturing the amplitudes especially those of the extreme events. In Column 941 (b) of Figure 16, it is shown that although the patterns of the predicted signal are quite 942 consistent with the truth, the amplitudes of all the extreme events are underestimated to 943 some extent. Thus, the predicted PDF has a narrower shape compared with the truth. Such 944 a phenomenon becomes more significant in Column (c) of Figure 16 where the approximate 945 model III is used. At lead time t = 1, despite that Corr  $\approx 0.8$  for x and y and Corr  $\approx 0.5$ 946 for z remain skillful, the large values of the relative entropy clearly indicate the discrepancy 947 between the predicted PDF and the truth, which is due to the fact that the amplitudes 948 of the extreme evens are severely underestimated. These facts conclude the importance of 940 using the information criterion in quantifying the model error in the PDFs in addition to 950

<sup>951</sup> the path-wise measurements.

Figure 17 includes a case study of the ensemble prediction for short- and medium range 952 forecasts using approximate models I and III starting from t = 16.5. First, the ensemble 953 mean (green) using the approximate model I is skillful up to 2.5 units of the lead time 954 while that using the approximate model III has a much shorter skillful prediction. These 955 are consistent with the results shown in Figure 16. Next, the uncertainty of the prediction 956 is reflected in the ensemble spread. It is clear that in the perfect model prediction the 957 ensembles do not spread out until t = 19 while those in the approximate models start 958 spreading out around t = 17. This is obviously due to the fact that the noise level is 959 higher in the approximate models. Using approximate model I, despite some members 960 give false prediction due to the intrinsic chaotic behavior, most of the ensemble members 961 are still able to follow the true trajectories, which also results in the skillful ensemble mean 962 prediction. However, using the approximate model III, both the large noise inflation and the 963 initial uncertainty due to the data assimilation lead to a quick divergence of the ensembles. 964 The ensemble spread is able to tell the uncertainty but the ensembles reach the attractor 965 much faster than those using the perfect model and therefore the ensemble mean using the 966 approximate model losses its skill. 968

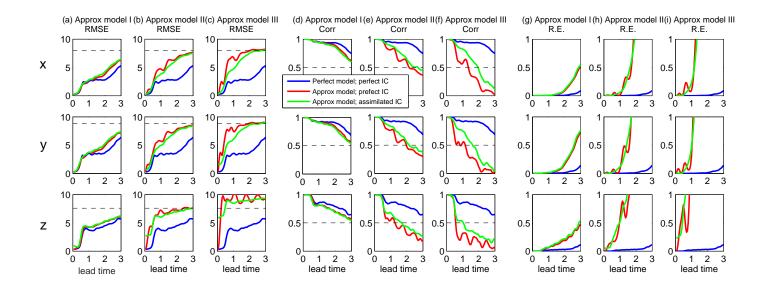


FIG. 15. RMSE (Panels (a)–(c)), Corr (Panels (d)–(f)) and relative entropy (R.E.; Panels (g)–(i)) as a function of lead time for short- and medium-range forecasts using the perfect model (21) (blue) and the three approximate models (23)–(24) with perfect initial conditions (red) and assimilated initial conditions (green). The prediction here is based on the ensemble mean. The dashed black lines in the RMSE panels show one standard deviation of the true signal and those in the Corr panels show the Corr = 0.5 threshold.

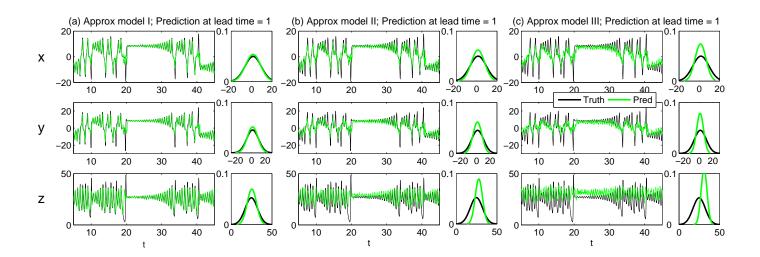


FIG. 16. Comparison of the ensemble mean prediction using the approximate models and the assimilated initial conditions (green) with the truth (blue) at lead time t = 1. In each panel, both the trajectories and the Gaussian fits of the PDFs are shown.

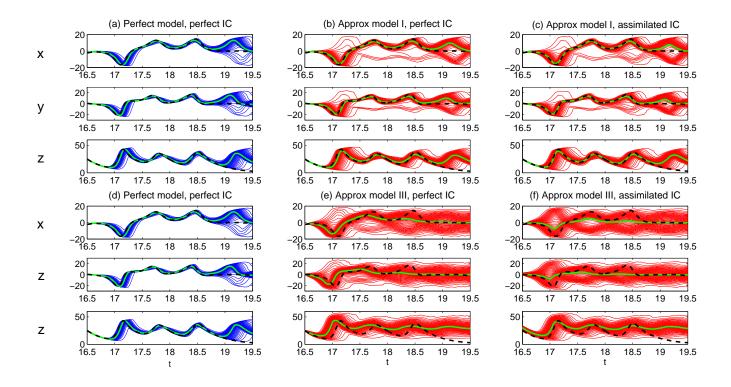


FIG. 17. Case studies of the ensemble forecasts. Panels (a)–(c): a case study using the approximate model I. Panels (d)–(f): the same case study using the approximate model III. Each subpanel shows the time evolution of the prediction, as represented by the time dependent PDF of the ensemble forecast. Note that each PDF is shown with 50 thin curves, which represent the 1st, 3nd, 5th, ..., 97th and 99th percentiles of the of the PDF. The green curve represents the mode of the PDF since the PDF is non-Gaussian. The black dashed curve is the true signal.

## <sup>969</sup> F. Prediction with an initial value starting outside the attractor

Panels (a)–(f) and Panels (g)–(l) in Figure 18 show the prediction where the initial values of the observed variables x(0) = 150 and those of the unobserved ones y(0) = z(0) = 150are outside the attractor, respectively.

The skill of capturing the transition behavior of the approximate models depends on the 973 model error in the noise inflation. The approximate model I behaves almost the same as the 974 perfect model due to its small noise inflation. The approximate model II is able to capture 975 the transition behavior in short and medium ranges if the initial values of y and z are off 976 the attractor. However, it fails to predict the two hidden variables after a very short period 977 if the initial value of x is off the attractor. On the other hand, the approximate model 978 III, which has the largest noise inflation coefficients, only has skillful prediction for a short 979 period no matter which variable starts from a value that is outside the attractor. 980

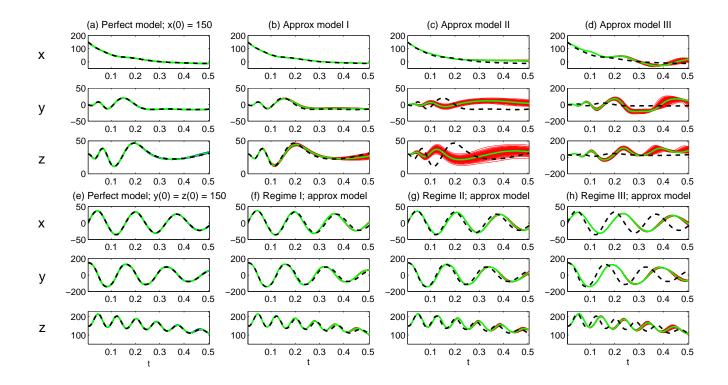


FIG. 18. Prediction with an initial value starting outside the attractor. Panels (a)–(d): Prediction where x starts at x = 150, which is a value that is off the attractor. Panels (e)–(h): Prediction where both y and z start at y = z = 150, which are values that are off the attractor. Each PDF is shown with 50 thin curves (blue for the perfect model and red for the approximate model), which represent the 1st, 3nd, 5th, ..., 97th and 99th percentiles of the of the PDF. The green curve represents the mode of the PDF since the PDF is non-Gaussian. The black dashed curve is the true signal.

# 981 VII. A PARADIGM MODELS FOR TOPOGRAPHIC MEAN FLOW 982 INTERACTION WITH REGIME SWITCHING BEHAVIOR

Regime switching between multiple metastable states is a key feature in many nonlinear 983 turbulent dynamical systems<sup>120–122</sup>. One example is the atmospheric flow regimes, which rep-984 resent the recurrence of certain flow structures despite the intrinsic chaotic behavior of the 985 underlying system. The existence of persistent or recurrent weather patterns<sup>123</sup> with block-986 ings is one of the most pronounced illustrations of synoptic-scale circulation regimes<sup>124,125</sup> 987 while different circulation regimes and their switching were also found in planetary-scale 988 patterns<sup>126,127</sup>. The metastable states have their unique dynamical behavior and the regime 989 switching often triggers extreme events and other important nonlinear phenomena. Notably, 990 the regimes can appear even though the observed data have a nearly Gaussian probability 991 distribution<sup>122,128,129</sup>. Due to the highly complex nature of these regimes and their switching 992 behavior as well as only the availability of the partial observations, it is important to develop 993 suitable approximate models for capturing both the dynamical and statistical features of the 994 regime switching and for predicting the associated extreme events. In this section, we con-995 centrate on the development of nonlinear low-order models to achieve the above tasks, where 996 the topographic effect is regarded as the result of random structures from either atmosphere 997 or ocean in intermediate and small scale. 998

# 999 A. The perfect model

Consider the barotropic quasi-geostrophic equations<sup>2</sup>,

$$\frac{\partial q}{\partial t} + \nabla^{\perp}\psi \cdot \nabla q + u(t)\frac{\partial q}{\partial x} + \beta \frac{\partial \psi}{\partial x} = 0, \qquad (26a)$$

$$q = \Delta \psi + h, \tag{26b}$$

$$\frac{du}{dt} = \int h \frac{\partial \psi}{\partial x}.$$
(26c)

This is an ideal model to study the complex nonlinear interaction of the large-scale and the small-scale flow and the role of the topography. The model exhibits a regime switching behavior with blocked and unblocked zonal flow structure despite that the associated PDF of the zonal flow has only a single modal. The study of this model for understanding its mathematical properties, developing reduced order models and uncertainty quantification can be found in a series of papers<sup>2,36,53,130,131</sup>. In particular, rigorous statistical bounds in
quantifying the uncertainty for the ensemble prediction of barotropic flow over topography
has been shown in a recent paper<sup>132</sup>.

In this model, the small-scale flow is given in terms of the stream function  $\psi$ , and q is the 1008 small-scale potential vorticity. The large-scale velocity field only has the zonal component 1009 u(t), and the topography is given by the function h = h(x, y). The parameter  $\beta > 0$  is the 1010 contribution from the beta-plane effect. Both the small-scale potential vorticity q and the 1011 small-scale stream function  $\psi$ , as well as the topography h, are assumed to be  $2\pi$ -periodic 1012 functions in both variables x and y with zero average. The large-scale velocity u(t) is strongly 1013 coupled with the small-scale flow through equation (26c), where the bar across the integral 1014 sign indicates that the integral has been normalized by the area of the domain of integration. 1015 Below, we consider a special situation to the full nonlinear system, which inherits the 1016 nonlinear coupling of the small-scale flow with the large-scale mean flow via topographic 1017 stress. The model is named as the *layered topographic equations*. Here the topography is 1018 layered in the fixed direction  $\vec{l} = (l_x, l_y)$ . We assume that both  $\psi$  and q only depend on 1019  $\xi = \vec{l} \cdot \vec{x}$  with  $\vec{x} = (x, y)$ . One key feature of the layered topographic equations is that 1020 the small-scale nonlinear term in (26a),  $\nabla \psi \cdot \nabla^{\perp} q$ , is identically zero. Nevertheless, the 1021 nonlinear coupling due to topographic stress remains and is responsible for much of the 1022 complex behavior. Without loss of generality we can always rescale the system with  $l_x \neq 0$ 1023 to align to a special case with  $\vec{l} = (1, 0)$ . 1024

In such a situation, the Fourier expansion of  $\psi$  and h are given by

$$\psi(x, y, t) = \sum_{k \neq 0} \psi_k(t) e^{ik\vec{l}\cdot\vec{x}},$$

$$h(x, y) = \sum_{k \neq 0} h_k e^{ik\vec{l}\cdot\vec{x}},$$
(27)

where we have assumed that the topography has zero mean with respect to spatial average, that is  $h_0 = 0$ . Substituting the ansatz (27) into (26) and adding stochastic forcing and damping, we arrive at the layered topographic equations in Fourier form,

$$\frac{d\psi_k}{dt} = -d_k\psi_k + ikl_x\left(\frac{\beta}{k^2|\vec{l}|^2} - u\right)\psi_k + i\frac{kl_x}{k^2|\vec{l}|^2}h_ku + \sigma_k\dot{W}_k,$$

$$\frac{du}{dt} = -d_uu - il_x\sum_{k\neq 0}kh_k\psi_k^* + \sigma_u\dot{W}_u,$$
(28)

where \* denotes the complex conjugate. In (28),  $\psi_k, k = 1, 2, ..., \Lambda$  are the stream functions and u is the large-scale zonal velocity.

In the study here, we adopt  $\Lambda = 10$  and therefore in total there are 21 modes in the model (28), where 1 mode u represents the large-scale zonal flow. The other 20 modes are for the small-scale stream functions with  $k = \pm 1, \ldots, \pm 10$ , which based on the layered topographic functions determine the meridional flows. We assign the following function for the topography,

$$h(x) = H_1\Big(\cos(x) + \sin(x)\Big) + H_2\Big(\cos(2x) + \sin(2x)\Big) - \frac{i}{2}\sum_{3\le k\le\Lambda} \frac{e^{i(kx+\theta_k)}}{k^p} + c.c., \quad (29)$$

where  $H_1$  and  $H_2$  are associated with the leading two Fourier modes  $k = \pm 1, \pm 2$  while the remaining part in (29) represents the amplitudes of the topography for other Fourier modes. Here  $\theta_k$  are random phase and p is a power that controls the effects of the small-scale topography. The topography plays an important role in altering the stream functions. With a simple manipulation, it is easy to show that the topographic functions associated with the first two Fourier modes are

$$h_1 = H_1/2 - H_1/2i$$
, and  $h_2 = H_2/2 - H_2/2i$ . (30)

The other  $h_k$  can also be written explicitly using (29). The following parameters are adopted in the study here. The beta-plane effect is  $\beta = 2$ . The coefficients of the topography are  $H_1 = 1$  and  $H_2 = 1/2$ . The damping coefficients are chosen as

$$d_k = d_u = 0.0125,\tag{31}$$

which represents a time scale of relaxation time of roughly 80 time units. Such a choice allows a relatively slow (but not infinitely slow) mixing of the system. With different choices of the stochastic noise, the system can also have fast mixing rate. Finally, the stochastic noise coefficients are chosen as follows,

$$\sigma_u = \sigma_1 = \sigma_2 = \frac{1}{20\sqrt{2}}, \qquad \sigma_k = \frac{1}{20\sqrt{2}} \frac{1}{k^p}, \qquad \text{for } p = 3, \dots, \Lambda.$$
 (32)

#### <sup>1049</sup> Dynamical regimes.

Two dynamical regimes will be studied below, which correspond to different values of pwith p = 1 and p = 0.5. Note that the "dynamical regimes" here should not be confused with the "regime switching". The latter stands for the switching of the model variables
between different values or states within a given dynamical regime.

Figure 19 shows the time series of the zonal flow u, its associated PDFs and ACFs as well as the accumulated energy in the small-scale stream functions. Here, the accumulated energy  $E[\psi_{1:s}]$  is defined as

$$E[\psi_{1:s}] = \sum_{k=1}^{s} |\psi_k|^2.$$
(33)

In the regime with p = 1, the trajectory of the zonal velocity u switches between roughly 1057 two different states and it stays in each state for a while before switching to the other 1058 (see Panel (a)). One state with positive u corresponding to the eastward zonal flow contain 1059 extreme events. Despite the nearly "two-state" time series, the associated PDF of u is single 1060 modal and is slightly skewed where a single (positive) side fat tail correspond to extreme 1061 events for the eastward zonal flow. Note that the regime (state) switching behavior with 1062 such a single modal distribution has been systematically studied in<sup>122</sup>. Despite the single 1063 modal distribution, the ACF is highly different from a Gaussian model with exponential 1064 decay. In fact, the ACF here first experiences a sharp decrease to ACF = 0.5 and then it 1065 decays slowly with almost a linear decaying rate to zero. The total decaying time is about 1066 60 time units. On the other hand, regarding the small-scale stream functions  $\psi_k$ , the leading 1067 two modes contain about 84% of the total energy. The ACF associated with  $\psi_1$  has a strong 1068 oscillation with a long memory while that associated with  $\psi_2$  only has a weak oscillation. 1069 For modes  $\psi_k$  with  $k \geq 3$ , the ACFs decay quite fast. 1070

<sup>1071</sup> Next, in p = 0.5 regime, the trajectory of the zonal velocity u has a relatively strong <sup>1072</sup> mixing rate. The direction of the zonal velocity alternates between eastward and westward <sup>1073</sup> quite frequently. Despite the Gaussian statistics, the dynamical regime is still chaotic. The <sup>1074</sup> ACF associated with u now behaves in a very different way, where it oscillates and decays <sup>1075</sup> quickly to zero. The leading two modes of the small-scale stream functions  $\psi_1$  and  $\psi_2$  contain <sup>1076</sup> about 61% of the total energy, and the ACFs associated with  $\psi_k$  with  $k \ge 3$  now decay more <sup>1077</sup> slowly compared with those in p = 1 regime.

<sup>1078</sup> Notably, in both regimes, the total flow field alternatives between zonally blocked and <sup>1079</sup> unblocked patterns as shown in Panels (j)–(k) and (u)–(v). Recall in (27) the topographic <sup>1080</sup> effect is imposed on the layered modes with  $\vec{l} = (1, 0)$ . This implies that the contributions <sup>1081</sup> of all the small-scale stream functions  $\psi_k$  are on the meridional flows while the zonal flow is driven by the large-scale zonal mode u. As a consequence, when the total flow field is zonally blocked, the large scale zonal velocity u = 0 and the total energy lies in the smallscale stream functions (see Panels (j) and (u)). Similarly, when the zonal flow becomes dominant, its kinetic energy accounts for a large portion of the total energy (see Panels (k) and (v)). Therefore, the regime switching not only alters the flow patterns but also adjusts the energy contributions in the total flow field.

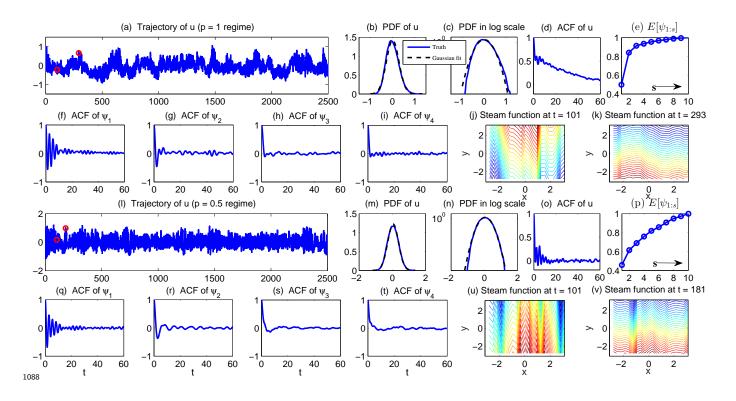


FIG. 19. Dynamical regimes of the layered topographic model (28). Panels (a)–(k): regime with p = 1. Panels (a)–(d) show the time series, PDF, PDF in logarithm scale and the ACF of u. Panel (e) shows the accumulated energy  $E[\psi_{1:s}]$  defined in (33). Panels (f)–(i) show the ACFs of the first four stream functions. Panels (j)–(k) show the total streamline at two different time instants marked in red dots in Panel (a). At these two time instants, the model shows the blocked and unblocked zonal flow structure, respectively. Panels (l)–(v) are similar to (a)–(k) but for regime with p = 0.5.

### 1096 B. The approximate model

Recall that the perfect model (28) has a 21-degree of freedom. The approximate model developed here has a much simpler form, which includes only the zonal flow u and the leading two Fourier wavenumbers (with  $k = \pm 1$  and  $\pm 2$ ).

The motivation of such a choice of the approximate model comes from the rapid decay 1100 of the ACFs associated with the small-scale stream functions. In fact, as shown in Figure 1101 19, the stream functions  $\psi_k$  with  $k = 3, \ldots, 10$  decorrelate very fast while  $\psi_1$  has a much 1102 longer relaxation time and  $\psi_2$  also has some memory. Therefore, it is natural to retain the 1103 dynamics of the leading two modes and incorporate the effects of the small- and fast-scale 1104 modes using extra damping and stochastic forcing in the approximate model. This follows 1105 the basic idea of the stochastic mode reduction strategy 53-56, though the manipulation here 1106 is less sophisticated. It is also important to notice that the extra stochastic noise added into 1107 the approximate model is crucial since the energy in modes  $\psi_k$  for  $k = 3, \ldots, 10$  as shown 1108 in Panels (e) and (p) of Figure 19 is non-negligible. Without these extra stochastic noise, 1109 the total variance will be underestimated, which will severely affect the prediction skill of 1110 the extreme events in the system. 1111

<sup>1112</sup> For the simplicity of notation, we make a change of variables,

$$\psi_1 = \frac{1}{2\sqrt{2}} \Big( (v_2 - v_1) - (v_2 + v_1)i \Big), \quad \text{and} \quad \psi_2 = \frac{1}{2\sqrt{2}} \Big( (v_4 - v_3) - (v_4 + v_3)i \Big).$$
 (34)

and therefore the 5-mode approximate model is given by,

$$\frac{du}{dt} = \omega_1 v_1 + 2\omega_3 v_3 - d_u u + \sigma_u \dot{W}_u, 
\frac{dv_1}{dt} = -\beta v_2 + v_2 u - 2\omega_1 u - d_{v_1} v_1 + \sigma_1 \dot{W}_1, 
\frac{dv_2}{dt} = \beta v_1 - v_1 u - d_{v_2} v_2 + \sigma_2 \dot{W}_2, 
\frac{dv_3}{dt} = -\frac{\beta}{2} v_4 + 2v_4 u - \omega_3 u - d_{v_3} v_3 + \sigma_3 \dot{W}_3, 
\frac{dv_4}{dt} = \frac{\beta}{2} v_3 - 2v_3 u - d_{v_4} v_4 + \sigma_4 \dot{W}_4,$$
(35)

where  $\omega_1 = H_1/\sqrt{2}$  and  $\omega_3 = H_2/\sqrt{2}$ . In (35), all the variables  $u, v_1, v_2, v_3$  and  $v_4$  are real. The damping and stochastic forcing here are different from the perfect model since they now also include some effects from the smaller scale modes of the perfect model that are ignored here. Notably, the approximate model (35) satisfies the physics constraint, where the total energy in the nonlinear terms is conserved<sup>35,36</sup>.

#### <sup>1119</sup> C. Parameter estimation, data assimilation and long-term prediction skill

The system in (35) is a nonlinear system. In practice, the observational data of the leading 1120 a few stream functions can be obtained. Therefore, we assume here the observational time 1121 series of  $\psi_1$  and  $\psi_2$  are available. As in many real applications of atmosphere and ocean, the 1122 observational training data is very limited. Here only the short period as shown in Panel 1123 (a) or Panel (l) of Figure 19 is used for model calibration. On the other hand, we assume 1124 that there is no observations for the zonal flow u. Recall that u plays an important role in 1125 transferring energy with the small-scale stream functions in a nonlinear way and altering the 1126 system between zonally blocked and unblocked patterns. Thus, for predicting the extreme 1127 events in the system, assimilating the unobserved zonal flow u becomes necessary. Note 1128 that despite the intrinsic nonlinearity in the coupled system (35), the system belongs to the 1129 conditional Gaussian framework as was discussed in Section II, which allows an efficient way 1130 of implementing parameter estimation and data assimilation. 1131

#### <sup>1132</sup> Parameter estimation.

Applying the parameter estimation algorithm described in Section III D, we arrive at the following estimated parameters in the approximate model (35),

Regime 
$$p = 1$$
: $d_u = 0.0132$ , $d_v = 0.0187$ , $\sigma_u = 0.0515$ , $\sigma_v = 0.0501$ , $\omega_1 = 0.7035$ , $\omega_3 = 0.3508$ , $\beta = 1.9954$ ,Regime  $p = 0.5$ : $d_u = 0.1417$ , $d_v = 0.0205$ , $\sigma_u = 0.1450$ , $\sigma_v = 0.0504$ , $\omega_1 = 0.6712$ , $\omega_3 = 0.3485$ , $\beta = 1.9963$ ,

(36)

where we have assumed all the damping coefficients in the  $v_i$  equations are the same and all equal to  $d_v$ . Similar assumption is used for the stochastic forcing coefficients in the  $v_i$ equations which all equal to  $\sigma_v$ .

For the estimated parameters, those with clear physical meanings, for example  $\beta$ ,  $\omega_1$  and  $\omega_3$ , are quite close to the truth. The other parameters, mainly the stochastic forcing and damping coefficients, are different from those in the perfect model. Note in particular that the noise coefficients in the approximate model are larger than those in the perfect model. Such a judicious model error with noise inflation compensates the error in the approximate model due to the ignorance of the small-scale stream functions  $\psi_k$  from  $k = \pm 3$  to  $\pm 10$ .

#### 1144 Data assimilation.

Using the approximate model (35) as the forecast model for data assimilation of the 1145 zonal flow u, the assimilated values are almost the same as the truth (figures not shown 1146 here) with a pattern correlation between the truth and the posterior mean states being 0.98 1147 and 0.95 in p = 1 and p = 0.5 regimes, respectively. In addition, the amplitudes of the 1148 assimilated states and the truth are also comparable with each other, implying the success 1149 of assimilating the extreme events. These results indicate the skill of using the approximate 1150 model in real-time state estimation of the unobserved process and accurately recovering the 1151 overall flow structure. 1152

#### <sup>1153</sup> Long-range forecast.

Figure 20 shows the long-term forecast results. Panels (a)–(b) present model trajectories 1154 of  $\psi_1, \psi_2$  and u simulated from the perfect model (28) and the approximate model (35) 1155 in p = 1 regime. These are simply a free run of each model and therefore we do not 1156 expect point-to-point correspondence between the two simulations due to the randomness. 1157 Nevertheless, these trajectories indicate that the qualitative features from both the models 1158 are similar. In particular, the approximate model succeeds in recovering the regime switching 1159 behavior in u. In Panels (c)–(d), the ACFs and PDFs associated with both the models are 1160 illustrated. The approximate model is quite skillful in capturing the strong oscillation, weak 1161 oscillation and the slowly but non-exponential decay in the ACFs associated with  $\psi_1, \psi_2$  and 1162 u respectively. The approximate model also succeeds in recovering the PDFs of all the three 1163 variables, especially the variance which is important for predicting the extreme events in 1164 short- and medium-range, as will be discussed in the next subsection. Similar conclusions 1165 can be made in p = 0.5 regime. The only slight error lies in tracing the fast decay ACF of 1166 u in the approximate model. But the equilibrium PDFs and the ACFs associated with  $\psi_1$ 1167 and  $\psi_2$  are recovered with high accuracy. 1168

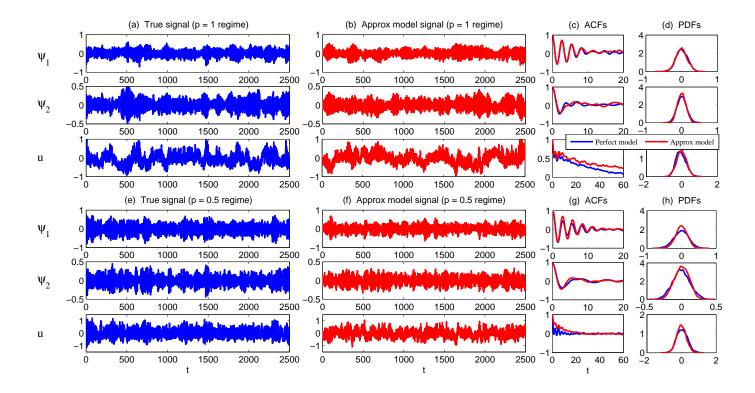


FIG. 20. Long-range forecasts of the layered topographic model. Panels (a)–(d): trajectories of the perfect model, trajectories of the approximate model, ACFs and PDFs in p = 1 regime. Panels (e)–(h): similar but for p = 0.5 regime.

## <sup>1169</sup> D. Short- and medium-range forecast

With the approximate model and the assimilated initial conditions of u, the ensemble forecast is applied to study the short- and medium-range forecasts.

Figure 21 shows the RMSE and Corr in the ensemble mean forecast as a function of the 1172 lead time. As comparison, the prediction using the perfect model is also included (blue). The 1173 approximate model has essentially the same skill as the perfect model in predicting all the 1174 three variables  $\psi_1, \psi_2$  and u. The useful prediction based on these path-wise measurements 1175 as well as the information criterion for comparing the predicted amplitudes (not shown here) 1176 in p = 1 regime is about 5 units for all the three variables and that in p = 0.5 regime is 1177 3.5, 2.5 and 1 units for  $\psi_1, \psi_2$  and u, respectively. Figure 22 shows the predicted trajectories 1178 at lead time 1, 2 and 3 units. The prediction of the extreme events up to 3 lead time units 1179 in p = 1 is quite accurate in terms of both the predicted patterns and the amplitudes. The 1180 p = 0.5 regime has a shorter range of useful predictions, but the overall skill up to 1 unit 1181 for both quiescent and extreme events are significant. 1182

Some case studies are included in Figure 23. In Panels (a)–(c), the ensemble prediction 1183 starts from t = 300, 1390 and 1460, respectively, and each prediction is run for 30 units 1184 forward. Although the overall skillful prediction in p = 1 regime as shown in Figure 21 is 1185 5 units, the three events in Panels (a)-(c) of Figure 23 indicate that the useful prediction 1186 depends on the initial phase and the follow-up structure of the signal. Despite the intrinsic 1187 chaotic behavior, the useful prediction in case study 1 reaches 12 units, where all the extreme 1188 events within this time interval are captured accurately by the approximate model. On the 1189 other hand, the prediction in case study 2 is completely unskillful due to the fact that u has 1190 no internal oscillation structure for this particular event while the long-term trend cannot 1191 be captured by the ensemble mean forecast. Case study 3 shows a skillful prediction up 1192 to 6 units where again the extreme events within this time interval are captured with high 1193 accuracy. 1194

Panels (d)–(e) in Figure 23 compare the predicted stream functions using the approximate model with the truth in the case study 1 from Panel (a) at lead times 1.5 and 6.3, where the truth is generated from the perfect 21-mode model. The true values of the large-scale zonal flow at these two time instants are u = 0.727 and u = -0.03, respectively. The approximate model is quite skillful in predicting the overall flow patterns. In particular, the predictions

succeed in capturing the regime switching phenomenon with a zonally unblocked structure 1200 at t = 301.5 and a zonally blocked structure at t = 306.3. There are some small errors in the 1201 prediction. For example, in Panel (d) the true signal at x = 0.8 has a sudden increase in the 1202 meridional velocity while it is missed in the prediction using the 5-mode approximate model. 1203 This meridional velocity is actually triggered by the modes  $\psi_k, k = 3, 4, \ldots$ , which are not 1204 included approximate model. Therefore, even if  $u, \psi_1$  and  $\psi_2$  are predicted almost perfectly, 1205 which is the case here, there can be a small intrinsic barrier in recovering the original field 1206 because of the simplification of the model by dropping the smaller scale modes. 1207

Similar conclusions are reached for p = 0.5 regime, as can be see in Panels (f)–(j) in Figure 23, despite that the useful prediction becomes shorter due to the more intrinsic turbulent behavior in this regime.

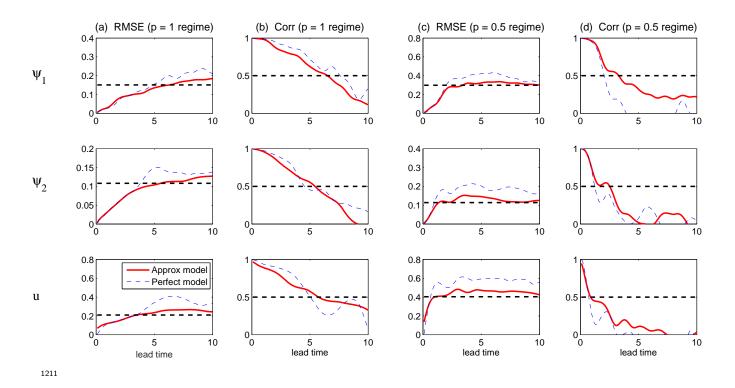


FIG. 21. Short- and medium-range forecasts of the layered topographic model. Panels (a)–(b) show the RMSE and Corr as a function of the lead time in p = 1 regime. Panels (c)–(d) show those in p = 0.5 regime. The black dashed lines in the RMSE panels show the standard deviation of the true signal and those in the Corr panels show the Corr= 0.5 threshold.

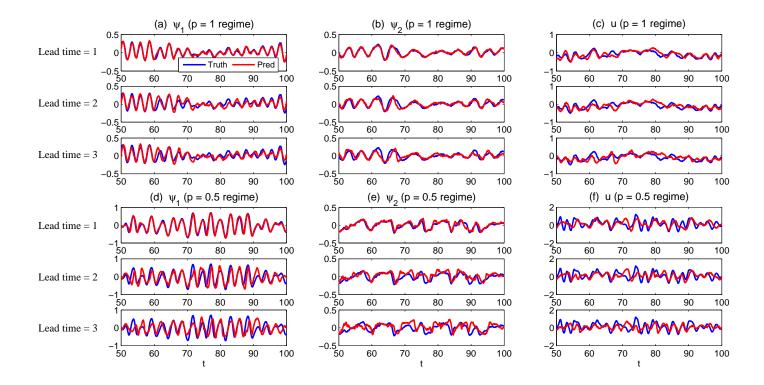


FIG. 22. The truth and the ensemble mean prediction at three different lead times 1, 2 and 3 using the approximate model with assimilated initial conditions of u. Panels (a)–(c): p = 1 regime. Panels (d)–(f): p = 0.5 regime.

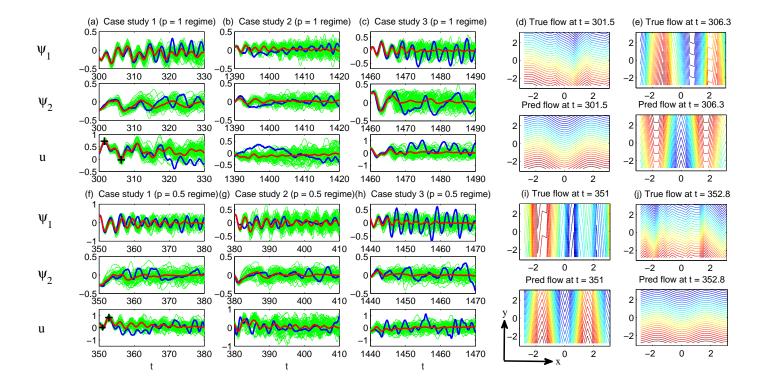


FIG. 23. Case studies of the ensemble prediction. Panels (a)–(e): p = 1 regime. Panels (f)–(j): p = 0.5 regime. In each subpanel of (a)–(c) and (f)–(h) the blue curve shows the truth and the red one shows the ensemble mean forecasts which is averaged over 50 ensemble members in green. Panels (d)–(e) compare the truth and the predicted overall streamlines in p = 1 regime at t = 301.5and t = 306.3 (marked in black '+' in Panel (a)), where the starting time is t = 300. Panels (i)–(j) compare the truth and the predicted overall streamlines in p = 0.5 regime at t = 351 and t = 352.8(marked in black '+' in Panel (f)), where the starting time is t = 350.

#### 1218 E. Prediction with an initial value starting outside the attractor

Finally, we study the prediction skill of the approximate model, which starts from a value that is outside the attractor. In the three columns of Figure 24, we show the ensemble predictions in p = 1 regime by letting the initial value of  $u, \psi_1$  and  $\psi_2$  be outside the attractor, respectively. It is not difficult to tell that the true trajectories starting from values outside the attractor behave in a very different way from those inside the attractor.

When u(0) is outside the attractor (Column (a)), the ensemble mean prediction using 1224 the approximate model is accurate up to 3 units. The ensemble spread is very skillful in 1225 capturing the envelope of the true signals as time evolves. When  $\psi_1(0)$  is outside the attractor 1226 (Column (b)). The useful ensemble mean prediction using the approximate model is about 1227 10 units. The extreme events within this 10-unit interval in the zonal velocity are accurately 1228 captured. Again, the ensemble spread clearly and accurately indicates the amplitudes in the 1229 true signal. When  $\psi_2(0)$  is outside the attractor (Column (c)). The skillful ensemble mean 1230 prediction using the approximate model extends to 20 units! Note that within the first 10 1231 units, the ensemble spread is very narrow, indicating the high confidence in the ensemble 1232 mean prediction, including all the extreme events. 1233

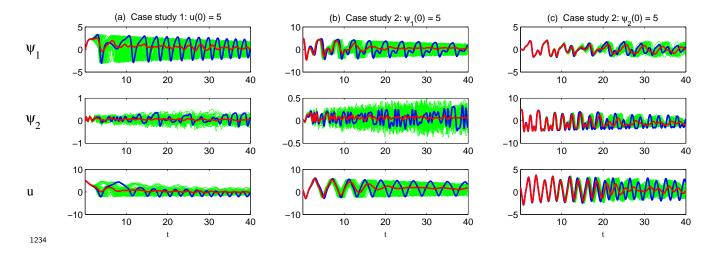


FIG. 24. Prediction using the approximate model starting from a point that is outside the attractor. Column (a) shows that when generating the true signal from the prefect model, the initial value of  $\psi_1$  is outside the attractor. Columns (b) and (c) show that the initial value of  $\phi_2$  and u are outside the attractor respectively. Again, the blue curve is the true and the red curve is the ensemble mean prediction with the 50 ensemble members shown in green. Here p = 1.

# VIII. A 6-DIMENSIONAL LOW-ORDER MODEL MIMICKING THE CHARNEY-DEVORE (CDV) MODEL

#### 1242 A. The perfect model and its properties

Charney and DeVore (CDV) made an fundamental contribution for the regime switching 1243 behavior of the atmosphere<sup>120</sup>. In this section, a 6-dimensional low-order model that mimics 1244 the dynamical behavior of the CDV model is used as the perfect model. Despite the regime 1245 switching behavior, this model has distinct mathematical structures and physical mecha-1246 nisms compared with the one studied in the previous section. It also possesses some unique 1247 features, as will be discussed at the end of this subsection, that provide a very tough test 1248 for predicting the extreme events and the transition behavior. The goal here is to design 1249 suitable and efficient strategies of developing an approximate model that is able to predict 1250 the extreme events and other non-Gaussian features in such a model. 1251

This 6-dimensional low-order model is obtained by a Galerkin projection and truncation of the barotropic vorticity equation on a  $\beta$ -plane channel<sup>133,134</sup>. The barotropic vorticity equation is the following,

$$\frac{\partial}{\partial t}\nabla^2\psi = -J(\psi, \nabla^2\psi + f + \gamma h) - C\nabla^2(\psi - \psi^*), \qquad (37)$$

where the domain of longitude and latitude (x, y) are given by  $[0, 2\pi] \times [0, \pi b]$ . The parameter b = 2B/L determines the ratio between the dimensional zonal length L and the meridional width B of the channel. The stream function  $\psi$  is periodic in x. The meridional boundaries y = 0 and  $y = \pi$  have the conditions  $\partial \psi / \partial x = 0$  and  $\int_0^{2\pi} (\partial \psi / \partial y) dx = 0$ . The Coriolis parameter f generates the beta effect in model. Orography enters with h, the orographic height, and is scaled with  $\gamma$ . J is the Jacobi operator and the damping coefficient C is the newtonian relaxation to the streamfunction profile  $\psi^*$ , which represents the forcing associated with the two zonal modes as will be discussed shortly. Next, the barotropic vorticity equation (37) is projected on a set of basis functions which are eigenfunctions of the Laplace operator  $\nabla^2$ ,

$$\phi_{0m}(y) = \sqrt{2}\cos(my/b), \qquad \phi_{nm}(x,y) = \sqrt{2}e^{inx}\sin(my/b),$$

The 6-dimensional model is obtained by truncating the expansion of the stream function and the topographic height after |n| = 1 and m = 2. Then the time-dependent complex variables of the stream functions  $\psi_{01}, \psi_{02}, \psi_{\pm 11}, \psi_{\pm 12}$  are transformed to real variables:

$$\begin{aligned} x_1 &= \frac{1}{b}\psi_{01}, \qquad x_2 &= \frac{1}{b\sqrt{2}}(\psi_{11} + \psi_{-11}), \qquad x_3 &= \frac{i}{b\sqrt{2}}(\psi_{11} - \psi_{-11}), \\ x_4 &= \frac{1}{b}\psi_{02}, \qquad x_5 &= \frac{1}{b\sqrt{2}}(\psi_{12} + \psi_{-12}), \qquad x_6 &= \frac{i}{b\sqrt{2}}(\psi_{12} - \psi_{-12}), \end{aligned}$$

while the topography h is chosen to have only the (1,1) wave profile,

$$h(x, y) = \cos(x)\sin(y/b).$$

These manipulations lead to a 6-dimensional ODE model, where  $x_1, x_4$  represent the zonal flow,  $x_2, x_3$  are the topographic Rossby waves and  $x_5, x_6$  are the Rossby waves.

In the study here, extra small noise is added to this model, which allows some effects from the small-scale modes to enter into this low-order model. The noisy version of the 6-dimensional CDV model reads,

$$dx_{1} = \left(\gamma_{1}^{*}x_{3} - C(x_{1} - x_{1}^{*})\right)dt + \sigma_{1}dW_{1},$$

$$dx_{4} = \left(\gamma_{2}^{*}x_{6} - C(x_{4} - x_{4}^{*}) + \epsilon(x_{2}x_{6} - x_{3}x_{5})\right)dt + \sigma_{4}dW_{4},$$

$$dx_{2} = \left(-(\alpha_{1}x_{1} - \beta_{1})x_{3} - Cx_{2} - \delta_{1}x_{4}x_{6}\right)dt + \sigma_{2}dW_{2},$$

$$dx_{3} = \left((\alpha_{1}x_{1} - \beta_{1})x_{2} - \gamma_{1}x_{1} - Cx_{3} + \delta_{1}x_{4}x_{5}\right)dt + \sigma_{3}dW_{3},$$

$$dx_{5} = \left(-(\alpha_{2}x_{1} - \beta_{2})x_{6} - Cx_{5} - \delta_{2}x_{4}x_{3}\right)dt + \sigma_{5}dW_{5},$$

$$dx_{6} = \left((\alpha_{2}x_{1} - \beta_{2})x_{5} - \gamma_{2}x_{4} - Cx_{6} + \delta_{2}x_{4}x_{2}\right)dt + \sigma_{6}dW_{6}.$$
(38)

Here the terms multiplied by  $\alpha_i$  model the advection of the waves by the zonal flow. The  $\beta_i$  terms are due to the Coriolis force; the  $\gamma$  terms are generated by the topography. The C terms are the Newtonian damping to the zonal profile  $x^* = (x_1^*, 0, 0, x_4^*, 0, 0)$ . The  $\delta$ and  $\epsilon$ -terms describe the nonlinear triad interaction between the zonal (0, 2) mode and the (1, 1) and (1, 2) waves. This triad is responsible for the possibility of barotropic instability of the (0, 2) mode. Note that the model is scaled such that 1 time unit in the model roughly corresponds to 1 day.

Following<sup>133,134</sup>, the following parameter values are taken: C = 0.1, corresponding to a damping time of 10 days;  $\beta = 1.25$ , corresponding to a channel centered around a latitude of 45°; b = 0.5, the north-south extent of the channel is 25% of its east-west extent; and  $x_1^* = 0.95$  and  $x_4^* = -0.76095$ . These parameters allow a combination of topographic and barotropic instabilities. The noise coefficients added here are  $\sigma_1 = ... = \sigma_6 = 0.005$ . Such <sup>1272</sup> a choice of the noise coefficients allow the dynamical behavior of this stochastic model to <sup>1273</sup> remain similar to its deterministic version as was studied in<sup>133,134</sup>.

Note that  $x_1$  and  $x_4$  associated with  $\psi_{01}$  and  $\psi_{02}$  describe the zonal flows, and the forcing  $x_1^*$  and  $x_4^*$  are only imposed on these modes. Therefore, it is natural to assume  $x_1$  and  $x_4$ are the observed variables while  $x_2, x_3, x_5$  and  $x_6$  are unobserved. The goal is to predict the extreme events in the system given only short trajectories of  $x_1$  and  $x_4$ .

# 1278 Model properties.

Panels (a)–(c) of Figure 25 show the chaotic trajectories, non-Gaussian PDFs and the 1279 ACFs of the model (38). It is easy to tell from the model trajectories that this model 1280 has multiple equilibria, which is confirmed by the phase plot  $(x_1, x_4)$  in Panel (d) (two 1281 stable equilibria; top left and bottom right). The spatial patterns associated with these two 1282 equilibria are quite different with each other, as shown in Panels (e) and (f) for two sample 1283 events corresponding to the time instants marked in red in Panel (a) that lie near these two 1284 equilibria. The streamlines shown in Panel (e) corresponds to an equilibria with largely zonal 1285 character with strong zonal jets while that in Panel (f) is dominated by topographically 1286 effects with vortices and meander jets. When the blocking events happen,  $x_1$  reaches its 1287 maximum while  $x_4$  lies in its minimum value. 1288

Panel (b) shows the equilibrium PDFs of all the 6 model variables. The profiles of these PDFs are quite different:  $x_1$  and  $x_3$  have weakly bimodal distributions;  $x_2, x_4$  and  $x_6$  are highly skewed with an one-sided fat tail towards the negative side; and  $x_5$  is skewed with a fat tail towards the positive side. Panel (c) illustrates the ACFs, which imply multiple decorrelation time scales of the system, where  $x_1, x_3$  and  $x_4$  has a much longer memory than  $x_2, x_5$  and  $x_6$ .

One very interesting and important feature of this model (or more precisely its determinis-1295 tic version) is that projecting this 6-dimensional model to its leading 5 Empirical Orthogonal 1296 Functions (EOFs) explains 99.5% of the variance. However, such a 5-dimensional projected 1297 dynamics completely misses the dynamical features in the original model, where the multiple 1298 equilibria disappears and the 5-dimensional model cannot reproduce regime transitions<sup>134</sup>. 1299 Therefore, this 6-dimensional model provides a very useful and tough testbed for developing 1300 suitable approximate models in predicting the transition behavior and extreme events in 1301 highly chaotic systems. 1302

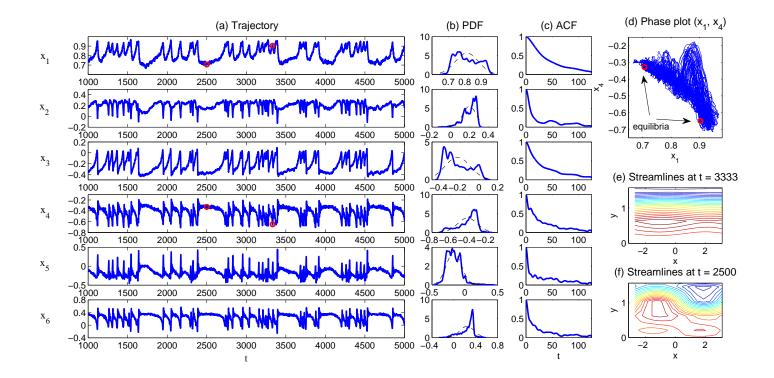


FIG. 25. Panels (a)–(c): Model trajectories, PDFs and ACFs of the 6-D CDV model (38). The black dashed lines in column (b) show the Gaussian fits of the PDFs. Panel (d): Phase plot of  $(x_1, x_4)$ . Panels (e)–(f): Streamlines at t = 3333 and t = 2500, corresponding to the time instants marked in red dots in Panel (a).

#### 1303 B. The approximate model

Our goal here is to develop a suitable approximate model for describing and predicting 1304 the key features of the 6-dimensional low-order CDV model (38). Recall that the conditional 1305 Gaussian nonlinear models in Section II allow an efficient and accurate data assimilation al-1306 gorithm, which facilitates effective predictions. Therefore, it is natural to develop a suitable 1307 approximate model that belongs to the conditional Gaussian nonlinear modeling framework. 1308 Note that by observing  $x_1$  and  $x_4$ , the 6-dimensional CDV model (38) is not a conditional 1309 Gaussian model due to the nonlinear coupling term  $\epsilon(x_2x_6 - x_3x_5)$ . In fact, the topographic 1310 Rossby waves  $x_2, x_3$  and the Rossby waves  $x_5, x_6$  interact with each other through the above 1311 nonlinear coupled term. Only in the absence of the Rossby waves  $x_5, x_6$ , the coupled sys-1312 tem  $x_1, \ldots, x_4$  is a conditional Gaussian system. Therefore, suitable strategies need to be 1313 developed to cope with this nonlinear term in the approximate model. 1314

#### <sup>1315</sup> Strategy 1: A bare truncation model.

The simplest way to deal with this nonlinear term is to build a bare truncation model, where the nonlinear term  $\epsilon(x_2x_6 - x_3x_5)$  is completely dropped. However, this bare truncation model suffers from finite time blowup issue. In fact, the blowup occurs very quickly and even for a very short lead time (much shorter than the decorrelation time), the predicted values have a large chance to go to infinity.

# <sup>1321</sup> Strategy 2: A nonlinear approximate model with linear feedback terms.

Another straightforward idea is to replace the quadratic term  $\epsilon(x_2x_6 - x_3x_5)$  by a combination of four linear terms  $c_1x_2 + c_2x_6 - c_3x_3 - c_4x_5$ . This approximation is better than the bare truncation model in the sense that the system will not blow up in a very short term. However, the predicted trajectories from this model still have a high probability to blow up in a finite time. In addition, the skillful prediction only lasts for very short time even if the predicted amplitude remains finite within that range.

# <sup>1328</sup> Strategy 3: An approximate model with a stochastic forcing term.

Instead of using a deterministic and linear way to parameterize the nonlinear quadratic term, a new strategy is developed here, which involves using a simple stochastic forcing process  $b_1$  to describe the effect of the quadratic term  $\epsilon(x_2x_6 - x_3x_5)$ . The approximate 1332 model reads,

$$dx_{1} = \left(\gamma_{1}^{*}x_{3} - C(x_{1} - x_{1}^{*})\right)dt + \sigma_{1}dW_{1},$$

$$dx_{4} = \left(\gamma_{2}^{*}x_{6} - C(x_{4} - x_{4}^{*}) + b_{1}\right)dt + \sigma_{4}dW_{4},$$

$$dx_{2} = \left(-(\alpha_{1}x_{1} - \beta_{1})x_{3} - Cx_{2} - \delta_{1}x_{4}x_{6}\right)dt + \sigma_{2}dW_{2},$$

$$dx_{3} = \left((\alpha_{1}x_{1} - \beta_{1})x_{2} - \gamma_{1}x_{1} - Cx_{3} + \delta_{1}x_{4}x_{5}\right)dt + \sigma_{3}dW_{3},$$

$$dx_{5} = \left(-(\alpha_{2}x_{1} - \beta_{2})x_{6} - Cx_{5} - \delta_{2}x_{4}x_{3}\right)dt + \sigma_{5}dW_{5},$$

$$dx_{6} = \left((\alpha_{2}x_{1} - \beta_{2})x_{5} - \gamma_{2}x_{4} - Cx_{6} + \delta_{2}x_{4}x_{2}\right)dt + \sigma_{6}dW_{6},$$

$$db_{1} = \left(-d_{b}b_{1} + \sigma_{b}b_{2} + f_{b}\right)dt + \sigma_{b}dW_{b},$$

$$db_{2} = \left(-d_{b}b_{2} - \sigma_{b}b_{1} + f_{b}\right)dt + \sigma_{b}dW_{b}.$$
(39)

This is motivated by the SPEKF model<sup>48,49</sup>, where a stochastic forcing is able to automati-1333 cally learn the missing information on the fly via online data assimilation. Here, we adopt the 1334 simplest possible choice — a stochastic forcing  $b_1$  driven by a Gaussian process. Note that 1335 two new processes  $b_1$  and  $b_2$  are actually incorporated into the approximate model. They to-1336 gether form a linear stochastic oscillator while only  $b_1$  gives feedback to the  $x_4$  process. The 1337 reason to impose an "oscillated" forcing is that all the variables  $x_i$  have chaotic oscillator 1338 structures and so does the nonlinear term  $\epsilon(x_2x_6 - x_3x_5)$ . As will be seen below, with this 1339 cheap stochastic strategy, the approximate model is able to avoid finite time blowup issue 1340 and it provides surprisingly skillful predictions in both short and medium ranges. Notably, 1341 treating  $b_1$  and  $b_2$  as the extra unobserved variables, the resulting 8-dimensional nonlin-1342 ear system in (39) is a conditional Gaussian nonlinear model, where only  $x_1$  and  $x_2$  have 1343 observations. The estimated parameters are given by: 1344

$$F_b = 0.0081, \qquad \omega_b = 0.6815, \qquad d_b = 0.1339, \qquad \sigma_b = 0.01326.$$
 (40)

Below the focus will be on the data assimilation and prediction skill using the approximate model in (39).

# 1347 C. Data assimilation

<sup>1348</sup> Since the approximate model with the stochastic forcing (39) is a conditional Gaussian <sup>1349</sup> system, the data assimilation algorithm (3) provides an efficient state estimation of both the unobserved variables  $x_2, x_3, x_5, x_6$  and the stochastic forcing  $b_1, b_2$ , which are shown in Figure 26 (in red color). As comparison, we also show the truth of the unobserved variables  $x_2, x_3, x_5, x_6$  (in blue color). It is clear that the data assimilation with the help of such a stochastic forcing term provides very accurate estimation of the hidden variables  $x_2, x_3, x_5, x_6$ , where the pattern correlation of the assimilated and the true signals is higher than 0.95 for all the variables.

Another striking result is presented in Panels (c) and (d) of Figure 26, where a comparison between the assimilated state of the stochastic forcing  $b_1$  and the nonlinear term  $\epsilon(x_2x_6 - x_3x_5)$  computed from the perfect model is illustrated. It is clear that the stochastic forcing  $b_1$  almost perfectly recovers the nonlinear feedback, especially at the time instants that the nonlinear feedback is intermittent. This is a very important feature because it guarantees that the stochastic forcing is able to, at least for a short term, play the role of the nonlinear feedback term in prediction.

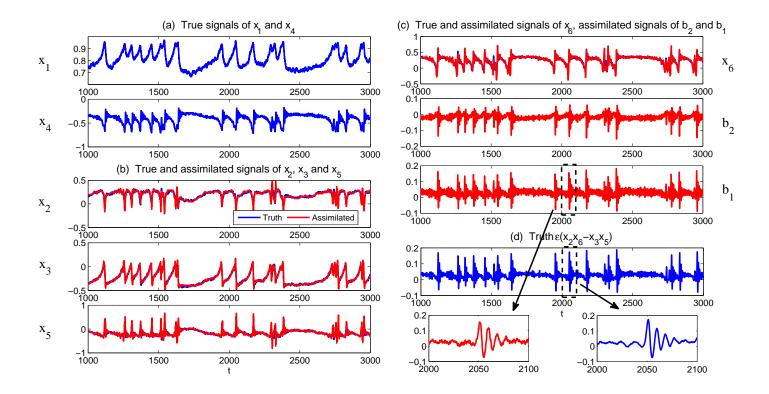


FIG. 26. Data assimilation of the 6-D CDV model using the approximate model (39). Panel (a): the true signals of  $x_1$  and  $x_4$ . Panels (b)–(c) the true and the assimilated posterior mean of  $x_2, x_3, x_5$  and  $x_6$ , and the assimilated stochastic forcing  $b_2$  and  $b_1$ . Panel (d): the true value of the nonlinear term  $\epsilon(x_2x_6 - x_3x_5)$ . A zoomed-in period of  $b_1$  and the nonlinear term is also shown for comparison.

### 1363 D. Predictions

#### 1364 Short- and medium-range forecasts.

Our focus now is on the short- and medium-range forecasts. In Figure 27, the prediction skill in terms of the RMSE and Corr as a function of lead time is presented. The blue curves show the predictions using the perfect model with the perfect initial conditions; the red curves show those using the approximate model (39) with the perfect initial conditions; and the green curves show those using the approximate model (39) and the assimilated initial conditions. The ensemble mean is used here for computing the RMSE and Corr.

Despite that the prediction using the approximate model (39) is less skillful than that 1371 using the perfect model as the increase of lead time, it is clear that the useful prediction for all 1372 the variables using the approximate model (39) is still at least 8 units. For some variables 1373 such as  $x_3$  the useful prediction is 16 days and for  $x_1$  it is much longer. In addition, 1374 the approximate model (39) using the assimilated initial conditions has nearly the same 1375 prediction skill as that using the perfect initial conditions, which verifies the accuracy in the 1376 assimilated states. These results imply that the approximate model is a suitable model for 1377 both short- and medium-range forecasts of such an extremely tough test model. 1378

Figures 28–29 include two case studies of the prediction tests. The ensemble mean pre-1379 diction shown in Figure 28 is extremely accurate for both short and medium ranges. On the 1380 other hand, although the ensemble mean prediction in Figure 29 has a slight phase shift, 1381 which results in the deterioration of the pattern correlation, the overall prediction using the 1382 approximate model remains skillful. From these figures, it is clear that most of the extreme 1383 events take around 8 units to develop from the onset phase to the peak, which is within the 1384 skillful prediction range of the approximate model (39). Therefore, the approximate model 1385 is able to predict the entire development phase of the extreme events. On the other hand, 1386 starting from the peak of an extreme event, the approximate model succeeds in predicting 1387 the returning path to the quiescent state. In addition to the ensemble mean, the ensemble 1388 envelope also plays an important role in the prediction here. In fact, despite a slight phase 1389 shift in the ensemble mean prediction in Figure 29, the ensemble envelope clearly predicts 1390 the correct overall time evolution trends of the truth. Admittedly, the ensemble spread 1391 using the approximate model with the assimilated initial condition is larger than the pre-1392 diction with the perfect initial condition, which is mainly due to the initial uncertainty in 1393

assimilating the hidden variables and the uncertainty introduced from the stochastic forcing.
Nevertheless, the correct trends are still unambiguously predicted by the ensemble members
in both short and medium terms.

### <sup>1397</sup> Long range forecast.

The approximate model (39) fails to reproduce the same long-term equilibrium PDFs as 1398 the truth. This is not surprising since the stochastic forcing for the long range forecast loses 1390 its memory of the initial condition and essentially becomes a constant. Its contribution to 1400 the system is then quite different from the original nonlinear term  $\epsilon(x_2x_5 - x_3x_6)$ , which 1401 evolves in time. Note that the study in the previous work<sup>74</sup> has already illustrated that in 1402 the presence of model error it is extremely difficult to develop suitable approximate models 1403 that are able to simultaneously have both short and long range forecast skill. Nevertheless, 1404 the approximate model (39) is still able to provide some useful information for the long-1405 range forecasts. First, the approximate model (39) avoids finite-time blowup issue and 1406 its equilibrium PDFs contain non-Gaussian features, which already outweighs many other 1407 approximation strategies, such as bare truncation and linear approximations, for describing 1408 strongly chaotic systems. Second, the ACFs of  $x_1, x_2$  and  $x_3$  from the approximate model 1409 (39) are quite similar to the truth and the errors in the ACFs of  $x_4, x_5$  and  $x_6$  are also only 1410 moderate. These features in the ACFs together with the accurate data assimilation results 1411 actually guarantee the skillful short- and medium-range forecasts. 1412

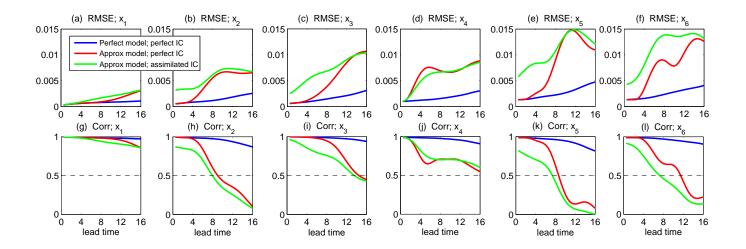


FIG. 27. Short- and medium-range forecasts using the perfect model and the approximate model (39). Top and bottom rows show the RMSE and Corr and a function of lead time. The blue curves show the predictions using the perfect model with the perfect initial conditions; the red curves show those using the approximate model (39) model with the perfect initial conditions; and the green curves show those using the approximate model (39) and the assimilated initial conditions. The ensemble mean is used here for computing the RMSE and Corr with the truth.

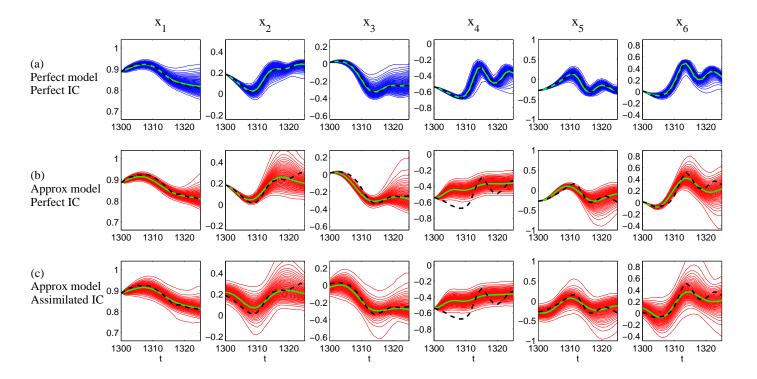


FIG. 28. Case study. Prediction starting from t = 1300. Note that each PDF is shown with 50 thin curves (blue for the perfect model and red for the approximate model), which represent the 1st, 3nd, 5th, ..., 97th and 99th percentiles of the of the PDF. The green curve represents the mode of the PDF since the PDF is non-Gaussian. The black dashed curve is the true signal.

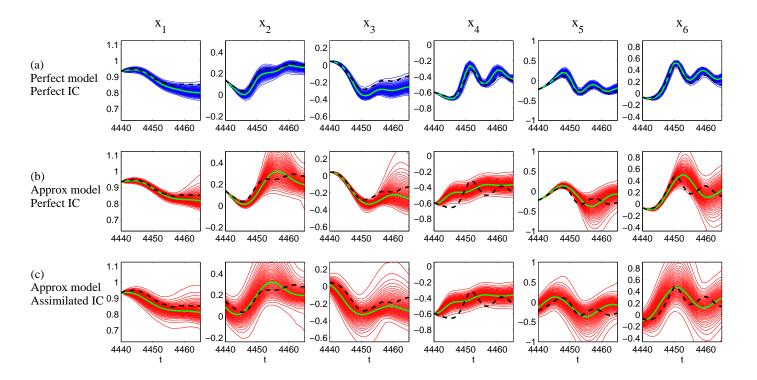


FIG. 29. Case study. Prediction starting from t = 4440.

# 1413 IX. CONCLUSION

Extreme events appear in many complex nonlinear dynamical systems. Predicting ex-1414 treme events has both scientific significance and practical implications. The main difficulties 1415 in predicting the extreme events include the lack of a complete understanding of physics, 1416 the unaffordable computational cost of running the complex dynamical systems and the 1417 errors in data assimilation or state estimation. Notably, in many practical situations, only 1418 partially observed time series are available for model calibration and the training period is 1419 often very short. All these facts result in great challenges and lead to the failure of many 1420 purely data-driven methods in the extreme events prediction. 1421

In this paper, a new mathematical framework of building suitable nonlinear approximate 1422 models is developed, which aims at predicting both the observed and hidden extreme events 1423 in complex nonlinear dynamical systems using only short and partially observed training 1424 time series. The models belonging to this mathematical framework are highly nonlinear and 1425 are able to capture many key non-Gaussian characteristics as observed in nature. Physically 1426 motivated processes and physics constraints can be incorporated into the models, which make 1427 this framework fundamentally different from many purely data-driven statistical models that 1428 have no clear physical meanings. Such a feature also allows using only a short training time 1429 series for model calibration. In addition, this modeling framework provides closed analytic 1430 formulae for assimilating the states of the unobserved variables, which is computationally 1431 efficient and accurate. The details of this modeling framework is shown in Section II. Section 1432 III contains the efficient and accurate data assimilation, parameter estimation and prediction 1433 algorithms as well as the details of using both the path-wise and information measurements 1434 in quantifying the prediction skill. Different effective and practical strategies of developing 1435 suitable approximate models for predicting extreme events and other non-Gaussian features 1436 in various complex turbulent dynamical systems are illustrated in Section IV to Section 1437 VIII. 1438

In Section IV, the skill of applying a cheap stochastic parameterization to approximate the complicated dynamical behavior in the hidden process is explored. This simple and efficient stochastic parameterization is able to recover the nonlinear feedback from the unresolved variable to the observed one. Notably, the nonlinear approximate model with such a cheap stochastic parameterization has nearly the same skill in predicting the extreme events at

all short, medium and long ranges. Section V makes use of a nonlinear dyad model to 1444 show the success of applying a simple feedback control strategy in the approximate model 1445 to facilitate the prediction of the hidden extreme events, which is a great challenge given 1446 only partial observations. In Section VI, the Lorenz 63 model is used as a simple test model 1447 for predicting extreme events in the intrinsic chaotic models. The goal for testing this 1448 model is to understand the model error due to the noise inflation in affecting the extreme 1449 events prediction, where the noise inflation is a typical strategy of developing approximate 1450 models in many real applications. It is shown that a moderate noise inflation retains the 1451 skill of the extreme events prediction at all short, medium and long ranges. Next, regime 1452 switching between multiple metastable states is a key feature in many nonlinear turbulent 1453 dynamical systems. Section VII starts with a 21-dimensional nonlinear topographic mean 1454 flow interaction model with regime switching. A simplified version of the stochastic mode 1455 reduction strategy is applied in a suitable way to develop an approximate physics-constrained 1456 nonlinear model with only 5 dimensions. The 5-dimensional physics-constrained nonlinear 1457 model has a significant skill in predicting both the observed and hidden extreme events as 1458 well as other non-Gaussian features, nearly the same as the perfect model prediction. It 1459 also succeeds in predicting the regime switching between the zonally blocked and unblocked 1460 patterns with high accuracy. In Section VIII, a 6-dimensional low-order Charney-DeVore 1461 (CDV) model is used as a testbed for predicting extreme events. This model is highly 1462 nonlinear and has strong chaotic features. The leading 5 EOFs contain more than 99.5%1463 of the explained variance but they completely miss the nonlinear dynamical features and 1464 the regime switching behavior. Therefore, this 6-dimensional model is an extremely tough 1465 test model for predicting the intrinsic nonlinear transitions and extreme events. It is shown 1466 that a simple but judicious linear stochastic process with additive noise and memory has 1467 a significant skill in learning certain complicated nonlinear effects of this model on the fly. 1468 The resulting approximate nonlinear model by incorporating such a simple stochastic process 1469 allows efficient and accurate data assimilation. It succeeds in predicting both the observed 1470 and hidden extreme events in short and medium terms. 1471

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