

Multiscale Data Assimilation and Prediction using Clustered Particle Filters

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Abstract

Multiscale data assimilation uses a coarse-resolution forecast model to increase the number of samples in the estimation of large-scale and long time behavior of high-dimensional complex systems along with noisy incomplete observations. A new class of multiscale particle filters, the multiscale clustered particle filter, is developed here as an effective multiscale data assimilation method for capturing non-Gaussian distributions and extreme events of high-dimensional turbulent systems using relatively few particles. The multiscale clustered particle combines the single-scale clustered particle filter with a general multiscale data assimilation framework that can handle mixed observations of both the resolved and unresolved scale components. To test the multiscale data assimilation method, we use a two-layer Lorenz system having 440 modes with important features of turbulent systems such as non-Gaussian statistics including fat-tails and intermittent extreme events. The effect of the observation model error is investigated and it is shown that the multiscale clustered particle filter captures non-Gaussian distributions using a small number of samples while an ensemble-based method fails to capture the correct distribution.

Keywords: data assimilation, filtering, Monte-Carlo, multiscale, clustered particle filter, non-Gaussian

1. Introduction

Data assimilation or filtering of turbulent systems is an important problem in many contemporary applications in science and engineering including real-time prediction of weather and climate as well as the spread of hazardous plumes of pollutants [1]. Data assimilation provides the best statistical estimate of the true signal by combining a numerical forecast model and noisy partial observations of the true signal. Although data assimilation is a well-developed discipline for low-dimensional dynamical systems [2], its application to turbulent systems is challenging due to the characteristics of turbulent systems. Turbulent systems are well-known for a high-dimensional phase space and a large dimensional space of instability with positive Lyapunov exponents [3]. Also turbulent systems show extreme events and non-Gaussian features such as skewed or fat-tailed distributions [4, 5] as observed in nature [6, 7].

21 Turbulent systems have a wide range of spatiotemporal scales in a high-dimensional
22 space and thus resolving all the active scales in a high-dimensional space is computa-
23 tionally prohibitive. Especially for ensemble-based data assimilation methods [8, 9], it
24 is important to use a sufficient number of ensemble to approximate the probability dis-
25 tribution of the system. However, due to the high computational costs to run a forecast
26 model resolving all the active scales of the system, the practical ensemble number is
27 limited and insufficient due to the high computational costs to run each forecast model,
28 which is called “curse of dimensionality” [10] or “curse of small ensemble size” [1].
29 Therefore, it is indispensable to use low-resolution or coarse-resolution forecast models
30 in data assimilation of turbulent systems to alleviate the curse of small ensemble size.
31 In [11], a cheap and robust coarse-resolution forecast model called stochastic superpa-
32 rameterization [12], which is 200 times cheaper than the full-resolution forecast model,
33 has been successfully applied for a two-layer quasigeostrophic baroclinic turbulent flows
34 with inhomogeneous statistics and zonal jets.

35 Another important issue in data assimilation of high-dimensional systems is catas-
36 trophic filter divergence [13, 14], which drives the filter forecast to machine infinity
37 although the system remains in a bounded set (see [15] for a rigorous mathematical
38 analysis of catastrophic filter divergence). The catastrophic filter divergence can occur
39 when observations are sparse, infrequent and of high-quality, which are typical in many
40 geophysical systems due to the vast area of the geophysical systems and expensive costs
41 to increase the number of observation points. In a recent study [16], it is shown that the
42 coarse-resolution forecast model, stochastic superparameterization, plays an important
43 role in preventing catastrophic filter divergence.

44 In the use of coarse-resolution forecast models for data assimilation of high-dimensional
45 systems, the imperfect coarse-resolution models lead to several model errors. The first
46 error is the forecast model error related to the numerical truncation error in modeling
47 the resolved large-scale dynamics and the error from unresolved sub-grid scale inter-
48 actions (see [17] for a study of the information barrier from the sub-grid scales). The
49 error due to imperfect models and insufficient ensemble size often yields underestima-
50 tion of the uncertainty in the forecast and thus the filter puts more confidence on the
51 forecast than the information given by observations, which is the standard filter diver-
52 gence. Covariance inflation [18, 19], which adds uncertainty in the forecast by inflating
53 the prior covariance, and localization [20], which calibrates the overestimated corre-
54 lations between observed and unobserved variables, are essential tools to remedy the
55 filter divergence. In a recent study [11], the effect of covariance inflation and stochastic
56 parameterization of the unresolved scales are investigated to remedy the standard filter
57 divergence and imperfect model errors.

58 The incorporation of a coarse-resolution forecast model for data assimilation of
59 high-dimensional systems has another model error, an observation model error. The
60 coarse-resolution forecast model provides predictions for only the resolved coarse scales.
61 However, the observation has mixed contributions from both the resolved and unre-
62 solved scales and thus there is an observation model error related to the contribution
63 of the unresolved or sub-grid scales to the observation. This error has been known as

64 "representation error" or "representative error" in the data assimilation community and
65 several approaches have been developed to analyze the representation error [21].

66 The general multiscale data assimilation framework in [22] addresses the issues
67 related to the use of coarse-resolution forecast models for data assimilation of high-
68 dimensional systems. The multiscale data assimilation framework provides the best
69 statistical estimate of the resolved coarse-scale dynamics using coarse-resolution fore-
70 cast models and mixed contributions from both the resolved and unresolved scales. The
71 general framework uses particle filtering for the low-dimensional resolved scales while
72 the unresolved scales are filtered using the standard Kalman filter formula and thus
73 it is also called multiscale particle filter (see [23] for multiscale data assimilation us-
74 ing the modified quasi-Gaussian closure model as a forecast model). From the general
75 multiscale data assimilation framework, a simpler version of multiscale data assimi-
76 lation method, an ensemble multiscale data assimilation method [24], can be derived
77 under the Gaussian assumption for the forecast and linear observations. The ensemble
78 multiscale data assimilation method treats the contribution of the unresolved scales to
79 the observations as representation errors. The ensemble method has been successfully
80 applied for several difficult problems including one-dimensional wave turbulence with
81 breaking solitons and shallow energy spectrum [24] and turbulence tracers advected by
82 baroclinic turbulent flows with inhomogeneous meridional structures [25]. Another data
83 assimilation method incorporating a coarse-resolution forecast model has been studied
84 and investigated in [26]. However, the observations in [26] depend only on the resolved
85 coarse scales while the general multiscale data assimilation framework can handle mixed
86 contributions from both the resolved and unresolved scales.

87 Despite the successful application of the multiscale particle filter [22] for the concep-
88 tual dynamical models for turbulence [27], which has energy-conserving nonlinear inter-
89 actions and mimics the interesting features of turbulent flows including non-Gaussian
90 statistics and extreme events, the application of the multiscale particle filter is limited
91 to low-dimensional resolved spaces. The problem is not from the multiscale data as-
92 similation algorithm but from the well-known inapplicability of the standard particle
93 filter for high-dimensional systems (in [28, 10], it is shown that the number of particles
94 increases exponentially with the dimension of the system). The multiscale ensemble
95 data assimilation method is a good workaround with successful results for several diffi-
96 cult test problems mentioned above. However, the method has a difficulty in capturing
97 non-Gaussian features, which are typical in turbulent systems [6, 7], using relatively few
98 samples as it assumes Gaussian prior and observation error statistics.

99 Recently a new class of particle filter, the clustered particle filter (CPF), has been
100 developed, which can be applied for high-dimensional systems effectively [29]. CPF cap-
101 tures the non-Gaussian features of high-dimensional systems using relatively few parti-
102 cles compared with the standard particle filter and is robust for sparse and high-quality
103 observations. The key features of CPF are coarse-grained localization through cluster-
104 ing of state variables depending on the observation network and particle adjustment
105 that translates forecast particles to prevent particle collapse. In this paper, we combine
106 the multiscale particle filter with CPF (which we call multiscale clustered particle filter

107 (MsCPF)) to apply the multiscale data assimilation framework for high-dimensional
 108 resolved spaces.

109 A preliminary result of the multiscale clustered particle filter applied for an one-
 110 dimensional wave turbulence model with Gaussian large-scale statistics is reported in
 111 [29]. To investigate several aspects of the multiscale data assimilation algorithm, in-
 112 cluding the effect of the observation model error (or representation error), we introduce
 113 an advective two-layer Lorenz-96 model as a test model, which contains both large- and
 114 small-scale advection to small-scale components. This model is a prototype model for
 115 slow-fast systems, which is typical, for example, in atmosphere where a slow advective
 116 vortical Rossby wave is coupled with fast inertia-gravity waves [30, 31]. The model has
 117 non-Gaussian statistics and extreme events represented by fat-tails and thus serves as
 118 a good test model for the multiscale data assimilation method.

119 The structure of this paper is as follows. In section 2, we briefly review the standard
 120 and clustered particle filters and describe the main algorithm, the multiscale clustered
 121 particle filter. In section 3, we propose a new test model with two different scales,
 122 advective two-layer Lorenz-96 model and discuss test regimes with non-Gaussian statis-
 123 tics and instability and provides linear stability analysis of the model as a guideline. In
 124 section 4, we show the data assimilation prediction experiments with a superior perfor-
 125 mance of MsCPF in capturing non-Gaussian statistics of the true signal, followed by
 126 discussions and conclusions in section 5.

127 2. Multiscale Clustered Particle Filter

128 In this section, we explain a mathematical setup and introduce notation to describe
 129 the main algorithm, the multiscale clustered particle filter. After introducing the basic
 130 setup, we briefly review the standard particle filter [2] and the clustered particle filter
 131 [29], which are important to derive and understand the multiscale clustered particle
 132 filter algorithm.

133 Throughout this paper, we consider the data assimilation of the true signal $\mathbf{u} \in \mathbb{R}^N$
 134 at a discrete time (or observation time) $n\Delta T, n \in \mathbb{N}$, where ΔT is the observation
 135 interval, whose dynamics is given by a nonlinear map ψ

$$\mathbf{u}^{n+1} = \psi(\mathbf{u}^n). \quad (1)$$

136 As we are concerned with high-dimensional systems with turbulent behavior, the dimen-
 137 sion of the system, N , is assumed to be large $N \gg 1$, and ψ has chaotic characteristics
 138 such as a large dimensional space of instability with positive Lyapunov exponents. As
 139 the system is difficult to estimate and predict due to the chaotic behavior, we use ob-
 140 servations $\mathbf{v} = \{v_1, \dots, v_{N_o}\} \in \mathbb{R}^{N_o}, N_o \leq N$, which are available at each observation
 141 time. We assume that the observation operator, $\mathbf{H} : \mathbb{R}^N \rightarrow \mathbb{R}^{N_o}$ is local, that is, each
 142 observation variable y_j , depends on only the corresponding state variable at the same
 143 location

$$\mathbf{v} = \mathbf{H}(\mathbf{u}) + \xi = (h(x_{i_1}) + \xi_1, h(x_{i_2}) + \xi_2, \dots, h(x_{i_{N_o}}) + \xi_{N_o}) \quad (2)$$

144 where ξ_j is I.I.D. Gaussian with mean zero and variance r_o . In real applications, a full
 145 recovery of the true state from observations is impossible due to incomplete observations;
 146 the observations are noisy and sparse, i.e., the number of observation N_o is smaller than
 147 the dimension of the full state N for high-dimensional systems $N \gg 1$, along with
 148 the nonlinear dependence of the observation on the true signal. Thus the goal of data
 149 assimilation is to provide the best statistical estimate combining the forecast PDF from
 150 a numerical prediction model and incomplete partial observations.

151 The standard particle filter [2] is a well-developed discipline for filtering low-dimensional
 152 non-Gaussian systems using different weights for different samples (or particles) to ef-
 153 fectively represent the PDF of the system. Using K particles and scalar particle weights
 154 $\{w_k \geq 0, k = 1, 2, \dots, K\}$, the standard particle filter approximates a probability density
 155 using the following form of PDF

$$p(\mathbf{u}) = \sum_k^K w_k \delta(\mathbf{u} - \mathbf{u}_k), \quad (3)$$

156 where δ is the Dirac delta function. In comparison with the standard Monte-Carlo
 157 or ensemble-based method, which uses the same weight $\frac{1}{K}$ for each sample, the stan-
 158 dard particle filter can represent non-Gaussian distributions more efficiently using non-
 159 constant particle weights for each sample. The standard particle filter shows robust
 160 performance in many applications in science and engineering [2]. However, its appli-
 161 cations are limited to low-dimensional systems as the number of particles increases
 162 exponentially with the dimension of the system [28, 10]; in the application of the stan-
 163 dard particle filter for high-dimensional systems, the standard particle filter suffers from
 164 particle collapse where only a small fraction of particles have the most weights while
 165 the rest of the particles have nearly zero weights.

166 *2.1. Clustered particle filter*

167 There are several attempts to overcome the limitation of the standard particle filter
 168 in the application for high-dimensional systems including the method that solves an
 169 optimal transport problem for the transition before the posteior to avoid the random
 170 sampling aspects of the standard particle filter [32], hybrid ensemble transform particle
 171 filter [33], and the localized particle filter [34]. Recently a new class of particle filter,
 172 clustered particle filter (CPF), has been proposed and it shows robust filtering per-
 173 formance with successful application for difficult test regimes, sparse and high-quality
 174 observation networks, in [29]. CPF also does not need ad-hoc tuning parameters.

175 *Coarse-grained localization*

176 The main features of the clustered particle filter are coarse-grained localization and
 177 particle adjustment, which enable the method to use relatively few particles to cap-
 178 ture non-Gaussian statistics of high-dimensional systems even with sparse and infre-
 179 quent observations. In the formulation of CPF, we assume that the observations are
 180 so sparse that each observation at different locations is uncorrelated with each other.

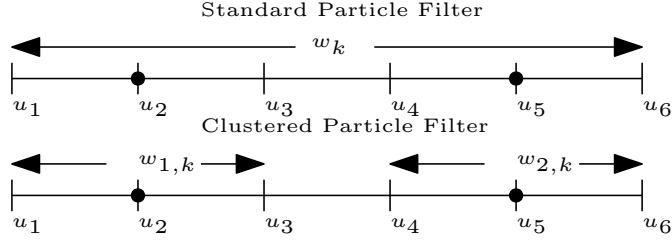


Figure 1: Schematics of particle weight for the k -th particle. Total dimension is 6 and there are two observations at u_2 and u_5 , which yields two clusters in CPF. The standard particle filter uses the same particle weight at different locations whereas the clustered particle filter uses different weights in different clusters but the weights are the same in the same cluster.

181 Thus, if there are N_o observation points, CPF partitions the state vectors into N_o non-
 182 overlapping clustered $\{C_l, l = 1, 2, \dots, N_o\}$ according to the observation location. Each
 183 cluster, C_l , is centered at the observation point and the cluster boundary is chosen as
 184 the middle point of the two adjacent observation locations, which can be applied to
 185 irregularly spaced observation networks. For the subspace state vector of each cluster,
 186 $\mathbf{u}_{C_l} = \{u_i | u_i \in C_l\}$ after clustering of the state variable, each cluster uses its own clus-
 187 ter particle weights $\{w_{l,k}\}$ to represent the marginalized probability distribution of each
 188 cluster (see Figure 1 which compares the schematics of the particle weights of the stan-
 189 dard and the clustered particle filters for a 6 dimensional system with two observa-
 190 tion points).

191 To use the particle adjustment step explained later in this section, CPF considers
 192 only the marginalized probability distribution of each cluster

$$p(\mathbf{u}_{C_l}) = \sum_k^K w_{l,k} \delta(\mathbf{u}_{C_l} - \mathbf{u}_{X_{C_l}}). \quad (4)$$

193 When we sequentially assimilate each observation v_j (which is possible as each obser-
 194 vation error is spatially uncorrelated), the observation v_j affects the marginalized PDF
 195 of the corresponding cluster C_j while the other clusters remain unaffected. From the
 196 forecast particle weights $\{w_{l,k}^f\}$ for the cluster C_j , the posterior particle weights $\{w_{j,k}^a\}$
 197 are given by

$$\omega_{l,k}^a = \begin{cases} \frac{\omega_{l,k}^f p(v_j | \mathbf{u}_k)}{\sum_m^K \omega_{l,m}^f p(v_j | \mathbf{u}_m)} & l = j, \\ \omega_{l,k}^f & l \neq j. \end{cases} \quad (5)$$

198 Therefore the clustering of the state variables plays the role of coarse-grained localiza-
 199 tion.

200 *Particle adjustment*

201 Another important key ingredient of the clustered particle filter is the particle ad-
 202 justment step, which translates and shrink the forecast particles instead of reweighing

203 when a special criterion related to the forecast statistics is satisfied. An important ob-
 204 servation for the standard particle filter is that the posterior statistics by combining the
 205 forecast statistics and observations is given by reweighing the forecast samples, which
 206 is a convex combination of the forecast samples. This fact implies that if the posterior
 207 mean cannot be represented by a convex combination of the forecast samples, it is not
 208 possible to represent the accurate posterior statistics using only the reweighing of the
 209 forecast samples. This situation can happen when the observation is of high-quality,
 210 i.e., the observation error variance is small and thus the observation is close to the true
 211 value. In that case, it is straightforward to check whether the observation can be rep-
 212 resented by a convex combination of the forecast samples. Otherwise, another method
 213 to represent the accurate posterior statistics is necessary.

214 The particle adjustment step of the hard threshold version clustered particle filter
 215 checks whether each observation v_j is in the convex hull of the forecast samples in the
 216 corresponding cluster C_j

$$v_j \in \left\{ \sum_k^K q_k \mathbf{H}(\mathbf{u}_{C_j,k}^f) \mid \forall q_k \geq 0 \text{ such that } \sum_k q_k = 1 \right\}. \quad (6)$$

217 If (6) is not satisfied, we trigger the particle adjustment step, which updates the forecast
 218 samples $\{\mathbf{u}_{C_l,k}^f\}$ through an adjustment matrix A (see the supporting information of [29]
 219 for a way to find the adjustment matrix A)

$$\mathbf{u}_{C_j,k}^a = \mathbf{u}_{C_j}^a + A(\mathbf{u}_{C_j,k}^f - \mathbf{u}_{C_j}^f). \quad (7)$$

220 to match the Kalman analysis mean $\mathbf{x}_{C_j}^a$ and covariance $R_{C_j}^a$ which are given as

$$\mathbf{u}_{C_j}^a = \mathbf{u}_{C_j}^f + G(y_j - H\mathbf{u}_{C_j}^f) \quad (8)$$

221 and

$$R_{C_j}^a = (I - GH)R_{C_j}^f \quad (9)$$

222 respectively, where $G = R^f H^T (H R^f H^T + r_o I)^{-1}$ is the Kalman gain matrix, $\mathbf{u}_{C_j}^f =$
 223 $\sum_k^K \omega_{j,k} \mathbf{u}_{C_j,k}^f$ is the forecast mean and $R_{C_j}^f = \sum_k^K \omega_{j,k} (\mathbf{u}_{C_j,k}^f - \mathbf{u}_{C_j}^f)(\mathbf{u}_{C_j,k}^f - \mathbf{u}_{C_j}^f)^T$ is
 224 the forecast covariance. In the particle adjustment step, the particle weights remain
 225 unchanged. There are other criteria to trigger particle adjustment than (6) (such as the
 226 soft threshold criterion in [29]). In our study, we use only the hard threshold criterion (6)
 227 as it shows robust results in our tests. Now we summarize the hard threshold clustered
 228 particle filter

229 **Hard Threshold Clustered Particle Filter Algorithm - one step assimila-**
 230 **tion.**

231 **Given :**

- 232 1) N_o observations $\{v_1, v_2, \dots, v_{N_o}\}$
 233 2) prior K particles $\{\mathbf{u}_{C_j,k}^f, k = 1, 2, \dots, K\}$ and weight vectors $\{\omega_{l,k}^f, k = 1, 2, \dots, K\}$ for
 234 each cluster $C_l, l = 1, 2, \dots, N_{obs}$

235 **For** v_j from $j = 1$ to N_o
 236 **If** The hard threshold criterion (6) is satisfied
 237 Update the prior particles using (7) to match the Kalman update (8) and (9)
 238 **Else** Use particle filtering
 239 Update $\{\omega_{j,k}^f\}$ using (5)
 240 **If** $K_{eff} = \frac{1}{\sum_k (\omega_{l,k}^a)^2} < \frac{K}{2}$
 241 Do resampling
 242 Add additional noise to the resampled particles

$$\mathbf{u}_{C_l, Resample(k)} \leftarrow \mathbf{u}_{C_l, Resample(k)} + \epsilon \quad (10)$$

243 where ϵ is IID Gaussian noise with zero mean and variance r_{noise}

244 **End If**
 245 **End If**
 246 **End For**

247 Note that there is a potential issue, dynamic imbalance of CPF through the coarse-
 248 grained localization [35, 36]. We emphasize that we consider sparse observations where
 249 each observation point is uncorrelated with each other (which is typical in geophysical
 250 systems due to the vast area of the system). Thus the effect of dynamic imbalance
 251 is marginal. In our tests in section 4, we do not find any issues related to dynamic
 252 imbalance.

253 *2.2. Multiscale clustered particle filter*

254 The basic idea of the multiscale clustered particle filter is to use the same coarse-
 255 grained localization and particle adjustment as in CPF. The only difference is that the
 256 particle weights in each cluster are updated using the multiscale particle filter method
 257 [22] in each cluster.

258 For the subspace state vector \mathbf{u}_{C_l} corresponding to the cluster C_l , we assume that
 259 there is a decomposition of the full state vector into resolved large-scale component \mathbf{x}_{C_l}
 260 and unresolved small-scale component \mathbf{y}_{C_l} . Using this decomposition into the resolved
 261 and unresolved scales, the marginalized PDF of \mathbf{u}_{C_l} is represented by the following
 262 conditional Gaussian mixture distribution (compare (11) with (4))

$$p(\mathbf{u}_{C_l}) = \sum_k^K w_{l,k} \delta(\mathbf{x} - \mathbf{x}_l) \mathcal{N}(\mathbf{y}_l(\mathbf{x}_{l,k}), \mathbf{R}'(\mathbf{x}_{l,k})). \quad (11)$$

263 where each summand is a Gaussian distribution conditional to the resolved scale $\mathbf{x}_{C_l,k}$.
 264 Note that the interactions between the resolved and unresolved scales through the de-
 265 pendence of the unresolved scale PDFs on the resolved scale can make non-trivial be-
 266 havior including non-Gaussian distributions.

267 When the observation \mathbf{v} has the following form (which can be regarded as a Taylor
 268 expansion of general nonlinear observation operators around the resolved scale)

$$\mathbf{v} = \mathbf{H}(\mathbf{x}, \mathbf{y}) + \xi = \bar{\mathbf{H}}\mathbf{x} + \mathbf{H}'(\mathbf{x})\mathbf{y} + \xi, \quad (12)$$

269 where \mathbf{H}' has rank N_o , the posterior marginalized distribution of \mathbf{u}_{C_l} taking into account
 270 the observation v_j is in the same form as the forecast PDF (see Proposition 3.1 of [22])
 271 and its analysis weight is given by

$$w_{l,k}^a = \begin{cases} \frac{w_{l,k}^f I_k}{\sum_k w_{l,k}^f I_k} & l = j, \\ w_{l,k}^f & l \neq j \end{cases} \quad (13)$$

272 where $I_k = \int p(v_j | \mathbf{x}_{C_l,k}, \mathbf{y}_{C_l}) p(\mathbf{y}_{C_l} | \mathbf{x}_k) d\mathbf{y}_{C_l}$.

273 To trigger particle adjustment for the multiscale clustered particle filter, we use the
 274 hard threshold version in the observation space

$$v_j \in \left\{ \sum_k^K q_k \mathbf{H}(\mathbf{x}_{C_j,k}^f, \mathbf{y}_{C_j,k}^f) \mid \forall q_k \geq 0 \text{ such that } \sum_k q_k = 1 \right\}, \quad (14)$$

275 that is, we check whether each observation is in the convex combination of the full state
 276 vector as the observation does not separate the resolved and unresolved scales. When
 277 this criterion (14) is satisfied, we trigger particle adjustment, which is the standard
 278 particle adjustment step (7) except that the posterior mean and covariance is given by
 279 (8) and (9) with an increased observation error [24, 22]

$$G = R^f H^T (H R^f H^T + r_o I + R')^{-1} \quad (15)$$

280 accounting for the contribution from the unresolved small-scales, i.e., the representation
 281 error.

282 **Hard Threshold Multiscale Clustered Particle Filter Algorithm - one step**
 283 **assimilation.**

284 **Given :**

- 285 1) N_o observations $\{v_1, v_2, \dots, v_{N_o}\}$
 286 2) prior K particles $\{(\mathbf{x}_{C_j,k}^f, \mathbf{y}_{C_j,k}^f), k = 1, 2, \dots, K\}$ and weight vectors $\{\omega_{l,k}^f, k = 1, 2, \dots, K\}$
 287 for each cluster $C_l, l = 1, 2, \dots, N_{obs}$

288 **For** v_j from $j = 1$ to N_o

289 **If** The hard threshold criterion (14) is satisfied

290 Update the prior particles using (7) to match the Kalman update (8) and (9)
 291 with the Kalman gain G is given by (15)

292 **Else** Use particle filtering

293 Update $\{\omega_{j,k}^f\}$ using (13)

294 **If** $K_{eff} = \frac{1}{\sum_k (\omega_{l,k}^a)^2} < \frac{K}{2}$

295 Do resampling

296 Add additional noise to the resampled particles

$$\mathbf{u}_{C_l, Resample(k)} \leftarrow \mathbf{u}_{C_l, Resample(k)} + \epsilon \quad (16)$$

297 where ϵ is IID Gaussian noise with zero mean and variance r_{noise}

298 **End If**
 299 **End If**
 300 **End For**
 301

302 *2.3. Multiscale ensemble filter*

303 As a benchmark method, we use the multiscale ensemble method [22, 24], which
 304 uses a Gaussian assumption for the multiscale forecast PDF. Under this assumption,
 305 the multiscale ensemble filter becomes the standard ensemble filter except that the
 306 update formula uses an increased observation variance, i.e., the representation error,
 307 coming from the contribution of the unresolved scales. As we believe that the qualitative
 308 behavior of the multiscale ensemble filter is not strongly dependent on the particular
 309 choice of ensemble filters, we choose the ensemble adjustment Kalman filter [37] for the
 310 multiscale ensemble filter (we call it Multiscale EAKF (MsEAKF) hereafter).

311 **3. Multiscale Dynamical Systems with Non-Gaussianity and Extreme Events**
 312 **: A Paradigm Model**

313 A preliminary result of the multiscale clustered particle filter is reported in [29] with
 314 a successful application of the multiscale CPF for an one-dimensional wave turbulence
 315 model with breaking solitons and shallow energy spectrum but with a Gaussian dis-
 316 tribution. Here we propose a multiscale turbulence model with interesting features of
 317 geophysical turbulence flows such as non-Gaussian statistics and extreme events to test
 318 the multiscale data assimilation method.

319 Our test model, which we call advective two-layer Lorenz-96 model, is given by the
 320 following two-layer coupled Lorenz-96 system

$$\begin{aligned} \frac{dx_i}{dt} &= x_{i-1}(x_{i+1} - x_{i-2}) + \lambda_1 \sum_{j=1}^J y_{i,j} - d_1 x_i + F, \quad i = 1, 2, \dots, I \\ \frac{dy_{i,j}}{dt} &= \frac{a_L x_i + a_S y_{i,j+1}}{\epsilon} (y_{i,j-1} - y_{i,j+2}) - \lambda_2 x_i - d_2 y_{i,j}, \quad j = 1, 2, \dots, J \end{aligned} \tag{17}$$

321 where x_i is periodic in i and $y_{i,j}$ is periodic in both i and j . This model is characterized
 322 by two sets of variables, slow-climate variable $\mathbf{x} = \{x_i\}$ of size I and fast-weather
 323 variable $\mathbf{y} = \{y_{i,j}\}$ of size IJ . Here $\epsilon > 0$ is an explicit time-scale separation parameter,
 324 F is an external slow forcing (which is constant in our study), λ_1 and λ_2 (which are
 325 not necessarily equal) are coupling parameters, and $d_1 > 0$ and $d_2 > 0$ are damping
 326 coefficients to stabilize the system. For the fast variable \mathbf{y} , there are large- and small-
 327 scale advection corresponding to the terms a_L and a_S respectively, which yields the
 328 slow-fast system when $a_L = 0$.

329 In our study, we fix $I = 40$ and $J = 10$ so that there are 440 variables in total
 330 (40 x_i 's and 400 $y_{i,j}$'s). Note that when $\lambda_1 = 0$, the equation of x_i is the standard
 331 Lorenz-96 model designed to mimic baroclinic turbulence in the midlatitude atmosphere

332 with energy-conserving nonlinear advection and dissipation [38, 3]. As the coupling
 333 parameters are set to nonzero values ($\lambda_1 \neq 0, \lambda_2 \neq 0$), this model problem is a good test
 334 model for filtering slow variables influenced by fast variables, which is crucial for the
 335 problems of medium-range weather prediction that is given by both the slow advective
 336 wave and the slowly varying envelope of the fast gravity waves. Note that without
 337 damping ($d_1 = d_2 = 0$) and no large-scale advection to the small-scale ($a_L = 0$) along
 338 with the same coupling parameters $\lambda_1 = \lambda_2$, this equation becomes the inviscid full
 339 Lorenz-96 model designed to study high skill prediction using FDT in [39].

340 3.1. Linear stability

341 To find interesting test regimes with extreme events and intermittency, which are
 342 represented by non-Gaussian fat-tails, we use the linear stability analysis of the model.
 343 First we consider the equation for the stationary homogeneous solution, $x_i = \bar{x}$ and
 344 $y_{ij} = \bar{y}$. As this solution has no spatial dependence, the equation of the homogeneous
 345 solution becomes

$$\frac{d\bar{x}}{dt} = \lambda_1 J \bar{y} - d_1 \bar{x} + F = 0 \quad (18)$$

$$\frac{d\bar{y}}{dt} = -\lambda_2 \bar{x} - d_2 \bar{y} = 0, \quad (19)$$

346 which yields

$$\bar{x} = \frac{F}{d_1 - \lambda_1 \lambda_2 J / d_2}, \quad \bar{y} = \frac{\lambda_2}{d_2} \bar{x}. \quad (20)$$

If we denote the perturbations of x_i and y_{ij} around the steady state by x'_i and y'_{ij} respectively so that

$$x_i = \bar{x} + x'_i \quad \text{and} \quad y_{ij} = \bar{y} + y'_{ij},$$

347 the equations of x'_i and y'_{ij} are given by

$$\frac{dx'_i}{dt} = (\bar{x} + x'_i)(x'_{i+1} - x'_{i-2}) + \lambda_1 \sum_j y'_{ij} - d_1 x'_i \quad (21)$$

$$\frac{dy'_{ij}}{dt} = (a_L(\bar{x} + x'_i) + a_S(\bar{y} + y'_{ij}))(y'_{ij-1} - y'_{ij+2}) - \lambda_2 x'_i - d_2 y'_{ij} \quad (22)$$

348 To check the linear stability, we linearize (21) and (22) and obtain

$$\frac{dx'_i}{dt} = \bar{x}(x'_{i+1} - x'_{i-2}) + \lambda_1 \sum_j y'_{ij} - d_1 x'_i \quad (23)$$

$$\frac{dy'_{ij}}{dt} = (a_L \bar{x} + a_S \bar{y})(y'_{ij-1} - y'_{ij+2}) - \lambda_2 x'_i - d_2 y'_{ij}$$

Now we define Y_j as the average of y'_{ij} over j

$$Y_i := \frac{1}{J} \sum_j y'_{ij}.$$

349 By summing the second equation of (23) over j and divide it by J , we obtain the
 350 following system

$$\begin{aligned}\frac{dx'_i}{dt} &= \bar{x}(x'_{i+1} - x'_{i-2}) + \lambda_1 \sum_j y'_{ij} - d_1 x'_i \\ \frac{dY_i}{dt} &= -\lambda_2 x'_i - d_2 Y_i\end{aligned}\tag{24}$$

351 Using Fourier series expansions of $x'_i = \sum_k \hat{x}'_k \exp(\frac{2\pi i k i}{I})$ and $Y_i = \sum_k \hat{Y}_k \exp(\frac{2\pi i k i}{I})$,
 352 plug them in (24), which yields the following equations for the Fourier coefficients

$$\frac{d}{dt} \begin{pmatrix} \hat{x}'_k \\ \hat{Y}_k \end{pmatrix} = A \begin{pmatrix} \hat{x}'_k \\ \hat{Y}_k \end{pmatrix} = \begin{pmatrix} \bar{x}(\exp(\frac{2\pi i k}{I}) - \exp(-\frac{4\pi i k}{I})) - d_1 & \lambda_1 J \\ -\lambda_2 & -d_2 \end{pmatrix} \begin{pmatrix} \hat{x}'_k \\ \hat{Y}_k \end{pmatrix}\tag{25}$$

353 The real and imaginary parts of the matrix A are given by

$$\Re(A) = \begin{pmatrix} \bar{x}(\cos(\frac{2\pi k}{I}) - \cos(\frac{4\pi k}{I})) - d_1 & \lambda_1 J \\ -\lambda_2 & -d_2 \end{pmatrix},\tag{26}$$

354 and

$$\Im(A) = \begin{pmatrix} \bar{x}(\sin(\frac{2\pi k}{I}) + \sin(\frac{4\pi k}{I})) - d_1 & 0 \\ 0 & 0 \end{pmatrix}\tag{27}$$

355 respectively. Note that the real and imaginary parts commute and thus the linear
 356 stability is related to the eigenvalues of the real part matrix (26). For simplicity, we use
 357 the following notations for the components of the real part matrix

$$\begin{aligned}a_{11} &= \bar{x}(\cos(\frac{2\pi k}{I}) - \cos(\frac{4\pi k}{I})) - d_1, \\ a_{12} &= \lambda_1 J, \\ a_{21} &= -\lambda_2, \\ a_{22} &= -d_2.\end{aligned}\tag{28}$$

358 If the discriminant of the characteristic function of the real part matrix

$$D := (a_{11} + a_{22})^2 - 4(a_{11}a_{22} + a_{12}a_{21})\tag{29}$$

is positive there are two real eigenvalues. In this case, the condition for one positive
 and one negative eigenvalues is

$$a_{11}a_{22} - a_{12}a_{21} < 0$$

359 that is,

$$\frac{\lambda_1 \lambda_2 J}{d_2} < \bar{x}(\cos(\frac{2\pi k}{I}) - \cos(\frac{4\pi k}{I})) - d_1.\tag{30}$$

On the other hand, the condition for two positive eigenvalues for linear instability is

$$a_{11} + a_{22} > 0 \quad \text{and} \quad a_{11}a_{22} - a_{12}a_{21} > 0$$

360 that is,

$$\frac{\lambda_1 \lambda_2 J}{d_2} > \bar{x} \left(\cos\left(\frac{2\pi k}{I}\right) - \cos\left(\frac{4\pi k}{I}\right) \right) - d_1 > d_2 \quad (31)$$

361 If D is negative (or zero), the eigenvalues are complex (or repeated real) and thus
 362 the condition for a positive real part of the eigenvalues (or positive repeated real), which
 363 guarantee linear instability, becomes

$$a_{11} + a_{22} > 0. \quad (32)$$

364 In addition to the linear stability analysis of x_i and the local average of y_{ij} , Y_i , we
 365 check the linear stability analysis of y_{ij} conditional to x_i . If we assume that there is
 366 time scale separation between x'_i and y'_{ij} , that is, x'_i can be assumed to be constant
 367 compared with y'_{ij} , we can check the linear stability of y'_{ij} directly from the second
 368 equation of (23). For fixed x'_i (and i), we use the Fourier series expansion of $y'_{ij} =$
 369 $\frac{-\lambda_2 x'_i}{d_2} + \sum_m \hat{y}'_m \exp\left(\frac{2\pi i m j}{J}\right)$ (where the first term $\frac{-\lambda_2 x'_i}{d_2}$ is the steady state solution to
 370 the second equation of (23)) and plug it into the second equation of (23), which yields

$$\frac{d}{dt} \hat{y}'_m = \left((a_L \bar{x} + a_S \bar{y}) \left(\exp\left(-\frac{2\pi i m}{J}\right) - \exp\left(\frac{4\pi i m}{J}\right) \right) - d_2 \right) \hat{y}'_m. \quad (33)$$

371 Thus \hat{y}'_m is linearly unstable when

$$\begin{aligned} & \Re \left((a_L \bar{x} + a_S \bar{y}) \left(\exp\left(-\frac{2\pi i m}{J}\right) - \exp\left(\frac{4\pi i m}{J}\right) \right) - d_2 \right) \\ & = \left((a_L \bar{x} + a_S \bar{y}) \left(\cos\left(\frac{2\pi m}{J}\right) - \cos\left(\frac{4\pi m}{J}\right) \right) - d_2 \right) > 0 \end{aligned} \quad (34)$$

372 3.2. Three parameter regimes

373 Depending on the presence of the large-scale and small-scale advection to the small-
 374 scale variable, we consider three parameter regimes. For each combination of advection,
 375 the other parameters are chosen to make instability in the system of x_i and y_{ij} (23) or the
 376 system of x_i and Y_i (24) (see Table 1 for the parameters of each regime). For the slow-fast
 377 system case, where ($a_L = 0, a_S = 1$), λ_1 and λ_2 are equal and thus the interaction terms
 378 conserve the energy. This regime is a slow-fast system, which is typical in geophysical
 379 systems, for example, in atmosphere where a slow advective vortical Rossby wave is
 380 coupled with fast inertia-gravity waves [30, 31]. It is straightforward to check that the
 381 discriminant (29) is negative and thus the real part matrix has two complex eigenvalues.
 382 Further analysis shows that the real part of these complex numbers are negative and
 383 thus the linearized x_i and Y_i system is stable. However, if we assume that there is
 384 time-scale separation between x_i and y_{ij} , which is true for this system (see Table 2 for

	Slow-fast system	Strongly chaotic	Weakly chaotic
a_L	0	1	1
a_S	1	1	0
F	1	5	5
λ_1	-3	1/4	1/4
λ_2	-3	-1	-1
d_1	0.01	1	1.5
d_2	0.1	2	2.5
ϵ	0.1	1	1

Table 1: Three parameter regimes of the test model (17). I and J are fixed at 10 and 40 respectively.

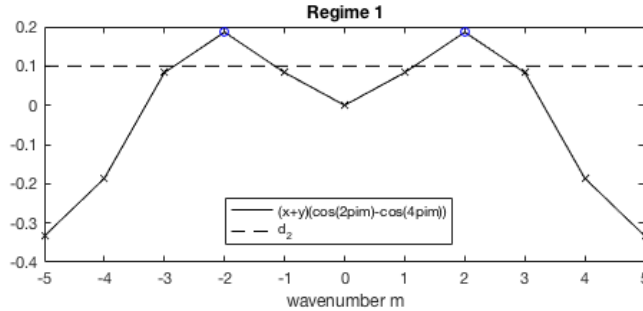


Figure 2: Slow-fast system. Linear stability of y_{ij} by assuming scale-separation between x_i and y_{ij} (34). Wavenumber 2 is linearly unstable. Solid line : $\bar{y}(\cos(\frac{2\pi m}{J}) - \cos(\frac{4\pi m}{J}))$. Dash line : d_2 .

385 the decorrelation times of x_i and y_{ij}), the linear stability analysis of y_{ij} (34) shows that
386 y_{ij} is unstable (Figure 2 shows linearly unstable modes of y_{ij} for fixed i). Note that
387 in this regime, only a small number of fast waves corresponding to wavenumber 2 are
388 unstable.

389 When $\lambda_1 > 0$ and $\lambda_2 < 0$ (strongly chaotic and weakly chaotic cases), the discrim-
390 inant (29) is positive and thus the system is unstable when (30) or (31) are satisfied.
391 Figure 3 shows linearly unstable modes of the x_i and Y_i system (marked with blue
392 circles) of the strongly chaotic and weakly chaotic cases. In the weakly chaotic regime,
393 for low wavenumber k , the system of x_i and Y_i is unstable with one positive eigenvalue
394 for the real part matrix of the linearized equation. In the strongly chaotic regime, low
395 wavenumbers except 7-10 are unstable. Note that the eigenvector of (24) is a linear
396 combination of x_i and Y_i . If we assume that there is time-scale separation between x_i
397 and y_{ij} , the linear stability of y_{ij} (34) implies y_{ij} is linearly stable.

398 Table 2 shows the climatological properties of the three regimes. For the slow-fast
399 and the strongly chaotic regimes, there are strongly non-Gaussian features (non-zero
400 skewness and kurtosis away from 3). In the weakly chaotic regime, the decorrelation
401 times of x_i and y_{ij} are inverted (y_{ij} has a longer decorrelation time than that of x_i)
402 while the slow-fast and the strongly chaotic regimes have correct orders for decorrelation
403 times; the presence of the small-scale advection makes the signal decorrelate rapidly in

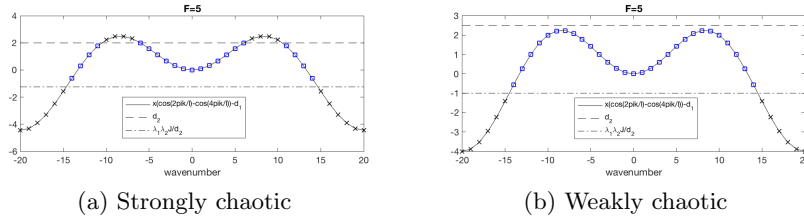


Figure 3: Strongly chaotic and weakly chaotic cases. Linear stability of x_i and $Y_i = \frac{1}{J} \sum_j y_{ij}$. Unstable wavenumbers are marked with squares while stable wavenumbers are marked with crosses. Solid line : $\bar{x}(\cos(\frac{2\pi k}{T}) - \cos(\frac{4\pi k}{T})) - d_1$. Dash-dot line : d_2 . Dash line : $\lambda_1 \lambda_2 J / d_2$

	Slow-fast system		Strongly chaotic		Weakly chaotic	
	x_i	y_{ij}	x_i	y_{ij}	x_i	y_{ij}
mean	0.022	0.033	1.69	-0.04	2.01	0.80
variance	0.009	0.021	5.71	6.80	8.51	0.75
skewness	0.261	-0.139	-0.02	-0.89	0.18	0.38
kurtosis	7.421	3.914	2.57	6.93	2.40	2.68
corr length	≤ 1	≤ 1	≤ 1	≤ 1	≤ 1	≤ 1
corr time	1.91	0.88	0.92	0.22	2.93	3.52

Table 2: Climatological properties of the system (17).

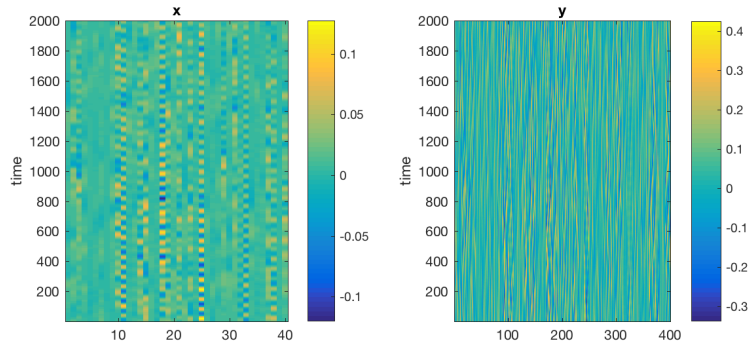
404 time.

405 Space-time diagrams of x_i and y_{ij} for all regimes are shown in Figure 4. In the
 406 slow-fast system case, there are random standing waves for \mathbf{x} with intermittent local
 407 bursts and \mathbf{y} is strongly mixing with no significant spatial structure. In the strongly
 408 chaotic case, \mathbf{x} has westward moving waves and \mathbf{y} has local bursts following the pattern
 409 of the moving waves of \mathbf{x} . In the weakly chaotic case, there are breaking waves while
 410 \mathbf{y} has local bursts corresponding to the pattern of \mathbf{x} . Thus all three regimes have
 411 characteristics of turbulent flows, from strongly turbulent to weakly turbulent along
 412 with extreme events.

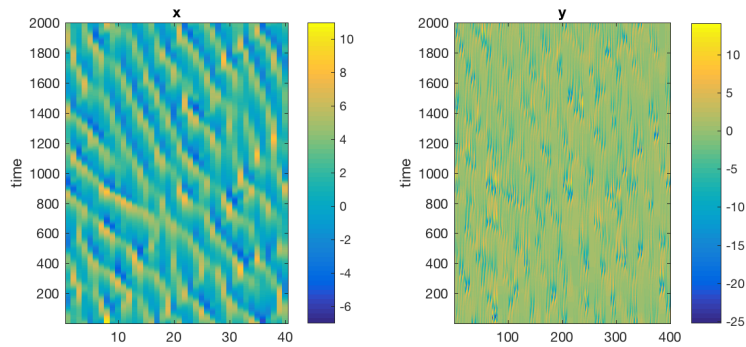
413 As a qualitative measure of non-Gaussian statistics, the stationary state PDFs of
 414 $x_i + y_{ij}$, x_i and y_{ij} of all regimes are shown in Figure 5 along with the Gaussian fits to
 415 the true. The top row of each figure shows the PDFs in log-scale (note that the log-
 416 scale of a Gaussian distribution is a parabola) while the bottom row of the figure shows
 417 the PDF without scaling. In all regimes, we can check that the system has strongly
 418 non-Gaussian statistics with fat-tails, which imply local extreme events.

419 Figure 6 shows the time series of x_i and y_{ij} at a grid point, $i = 2$ and $j = 5$. In
 420 the slow-fast system case, x_2 shows strong intermittency and $y_{2,5}$ has intermittent fast
 421 oscillation when there is intermittency in x_2 . In the strongly and weakly chaotic cases,
 422 $y_{2,5}$ shows intermittent local bursts explaining the fat-tails of y_{ij} .

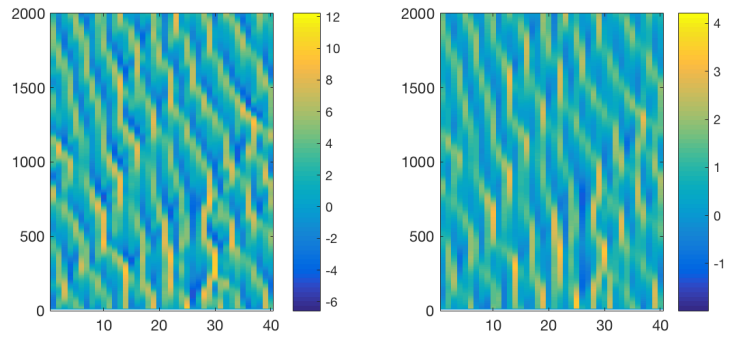
423 Another important statistical property of the turbulent system for data assimilation
 424 is decorrelation times and spatial correlation lengths. In Figure 7, the autocorrelation



(a) Slow-fast system



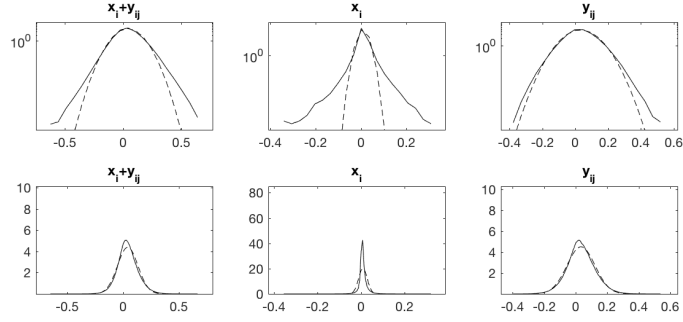
(b) Strongly chaotic



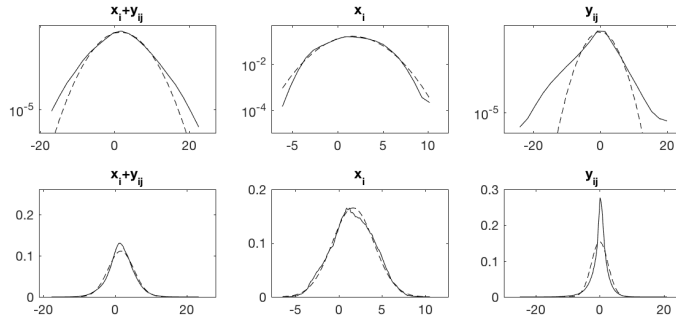
(c) Weakly chaotic

Figure 4: Space-time diagrams of \mathbf{x} and \mathbf{y} of the advective two-layer Lorenz-96 model (17) for all regimes.

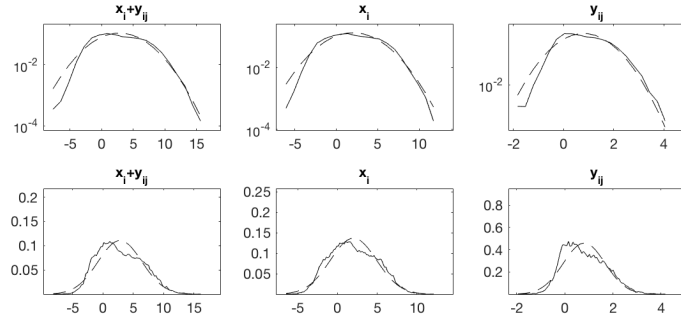
425 functions and spatial correlation functions are shown to analyze the decorrelation time
 426 and spatial correlation length. Except Regime 3, the decorrelation time of x_i is longer
 427 than that of y_{ij} , which are physical for slow-climate variable x_i and fast-weather variable



(a) Slow-fast system



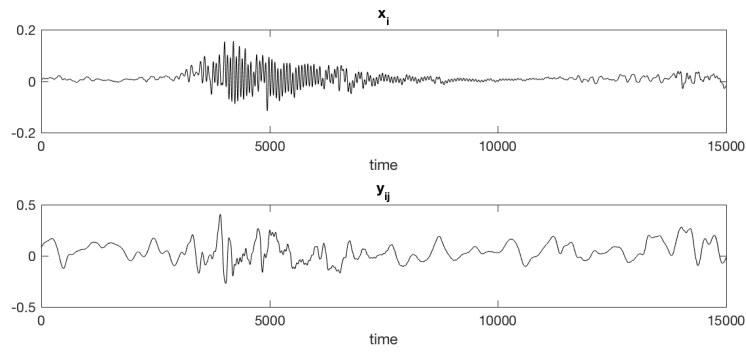
(b) Strongly chaotic



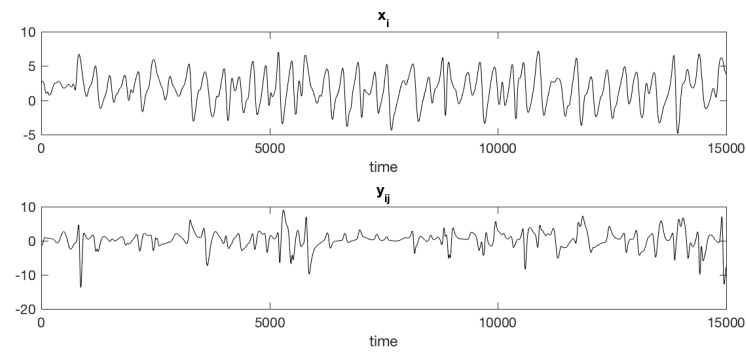
(c) Weakly chaotic

Figure 5: Stationary state PDFs of $x_i + y_{ij}$, x_i and y_{ij} . Log-scale (top) and without scaling (bottom). Dash lines are Gaussian fits. Note that the log-scale of a Gaussian distribution is a parabola.

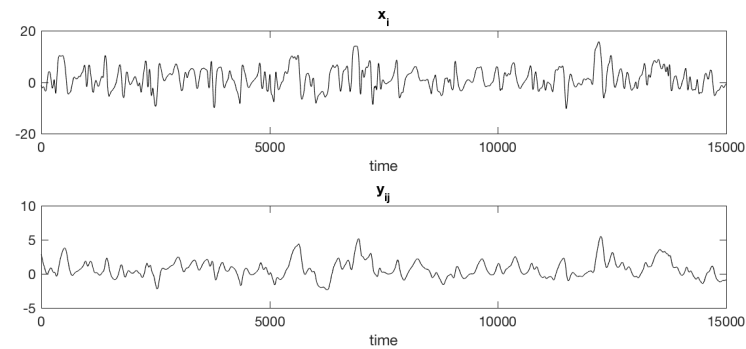
428 y_{ij} . Also, the spatial correlation length is less than 1 spatial grid point and thus all
 429 regimes are difficult test models for multiscale data assimilation.



(a) Slow-fast system



(b) Strongly chaotic

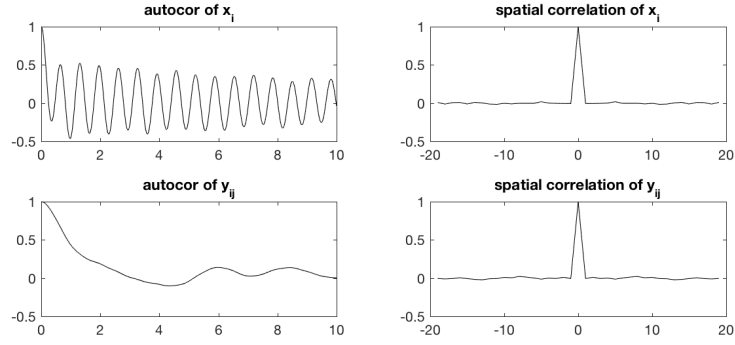


(c) Weakly chaotic

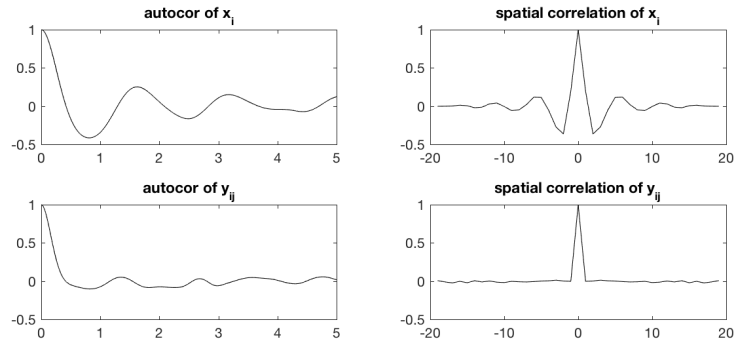
Figure 6: Time series at a grid point, x_2 and $y_{2,5}$

430 **4. Numerical Experiments for Data Assimilation and Prediction using the**
 431 **Multiscale Particle Filter**

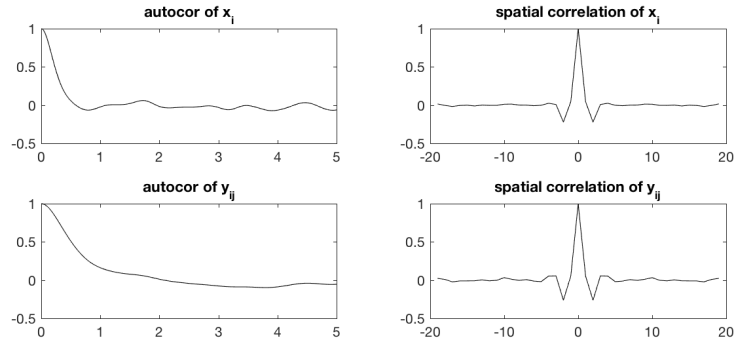
432 In this study, we are interested in the effect of the observation model error, i.e. the
 433 representation error, on the forecast skill for complex systems (see [11] for the study



(a) Slow-fast system



(b) Strongly chaotic



(c) Weakly chaotic

Figure 7: Autocorrelation (left) and spatial-correlation (right) functions of x_i (top) and y_{ij} (bottom)

434 of the effect of forecast model errors on the filter performance). To minimize the ef-
 435 fect from the forecast model error, we use the perfect model as the forecast model.
 436 In the multiscale data assimilation setup, it is important to estimate the small-scale
 437 variance $\mathbf{R}'(\mathbf{x}_{l,k})$ for each large-scale variable. In our experiments, we approximate the

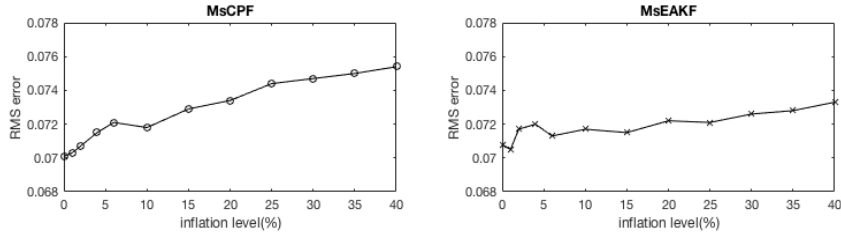


Figure 8: Slow-fast system. Time-averaged forecast RMS errors as functions of covariance inflation level. MsCPF (left) and MsEAKF (right). 20 observations.

438 small-scale covariance as a diagonal matrix whose diagonal components are given by
 439 the variance of $\{y_{ij}\}$ for each i . The original multiscale data assimilation framework
 440 provides a method to update the small-scale variables. However, this update is com-
 441 putationally expensive in real applications. Therefore, we update only the large-scale
 442 variables using the multiscale data assimilation method while the small-scale variables
 443 remain unchanged. This approximation is not optimal as it ignores information for the
 444 small-scale variables and thus there is an information barrier to get the optimal result.
 445 Although this is an interesting research topic, we do not investigate the barrier in the
 446 current study.

447 *4.1. Experiment setup*

448 We test the multiscale clustered particle filter (MsCPF) and the multiscale ensemble
 449 adjustment filter (MsEAKF) for the advective two-layer Lorenz 96 model. We first
 450 consider the experiments for the slow-fast and the strongly chaotic regimes. In each
 451 experiment, the true signal is given by one realization of the model. Both the true model
 452 and the forecast model use the same time integration method, the Euler-Maruyama
 453 method with a time step 10^{-3} . To mimic the incomplete partial observations in real
 454 applications, we test two scenarios, 40 full observations and 20 uniformly distributed
 455 observations that are available for each even i . Each observation component v_j directly
 456 observes the sum of x_j and $y_{j,5}$

$$v_j = x_j + y_{j,5} + \xi_i, \quad \xi_i : \text{iid random noise} \quad (35)$$

457 which has contributions from both the large-scale and the small-scale variables where
 458 the fifth component of y_{ij} contributes to the observation for each i . The observation
 459 interval varies from 0.1 to 0.8 for the slow-fast system case and from 0.05 to 0.1 for
 460 the strongly chaotic case, which are frequent compared with the decorrelation times
 461 of the large-scale variables in each regime. Observation error variance is only 1% of
 462 the total variance; however, the contribution from the unresolved small-scale variables,
 463 i.e., the representation error, is more than 50% of the total variance. Thus recovering
 464 accurate estimation and prediction skill for the resolved large-scale is difficult for both
 465 test regimes.

466 In each test, we run 5000 cycles and use the last 3000 cycles to measure the filter
 467 performance. Both MsCPF and MsEAKF use 50 samples and EAKF uses covariance
 468 localization using the smooth localization function by Gaspari and Cohn [40]. As the
 469 large-scale variable has a short decorrelation length (see Figure 7 and Table 2), we
 470 use a localization radius 2 that affects only the adjacent state variables. Covariance
 471 inflation plays an important role in recovering filter skill in the presence of model and
 472 sampling error [18, 19, 11]. In our multiscale data assimilation test, the covariance
 473 inflation plays no significant role in improving the filter performance. For the slow-fast
 474 system case, we tested several inflation levels and compare the time-averaged forecast
 475 RMS errors (Figure 8 shows the time-averaged forecast RMS errors as functions of the
 476 inflation level for both methods). Except the MsEAKF using a small inflation level and
 477 marginal gain, covariance inflation degrades the filter performance for both MsCpF and
 478 MsEAKF. Thus, the covariance inflation is not utilized in our tests.

479 *4.2. Data Assimilation and Prediction*

480 *4.2.1. Slow-fast system regime*

481 The slow-fast system system is typical in geophysical systems such as the atmosphere
 482 system where a slow advective vortical Rossby wave is coupled with fast inertia-gravity
 483 waves [30, 31]. Also more than two thirds of the total variance is carried by the un-
 484 resolved small-scale variables, which is a difficult test problem for data assimilation as
 485 the unresolved small-scale variable plays an role of additional observation error in the
 486 estimation of x_i (i.e., the representation error).

487 As a quantitative path-wise measure, we check the RMS error of the forecast es-
 488 timates. Figure 9 shows the time series of forecast RMS errors with 20 observations
 489 and observation time 0.1 by MsCPF and MsEAKF along with two benchmark values.
 490 The dash line is the climatological error given by the standard deviation of the resolved
 491 scale x_i , which is the error when we use the steady state mean. The other line, dash-
 492 dot line, is the effective observation error, which is the square root of the unresolved
 493 small-scale variance in addition to the raw observation error variance, which accounts
 494 for the representation error from the unresolved scale variables. From the figure, both
 495 MsCPF and MsEAKF have RMS errors staying below the climatological error except
 496 intermittent times, which shows filter skill from the noisy observational data both from
 497 the raw instrumental observation error and the unresolved scale error. Table 3 shows the
 498 time-averaged RMS errors and pattern correlation in parenthesis for several observation
 499 times and 40 full and 20 partial observations. As the observation time increases and
 500 the observation number decreases, the RMS error increases. However both methods are
 501 comparable and the RMS errors are smaller than the climatological error, which show
 502 filter skill.

503 One of the important measures in filtering high-dimensional systems is the recovery
 504 of the true PDF, which assess the lack of information in the filtered estimation and
 505 prediction. The RMS error and pattern correlation, which are path-wise measures of
 506 filter performance and are related to the Shannon entropy and the mutual information
 507 in information theory [3], fail to assess the lack of information in the filter estimates

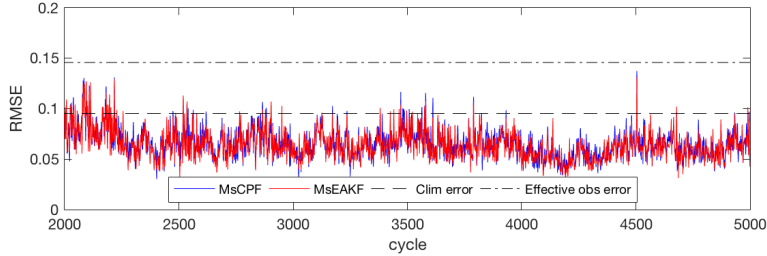


Figure 9: Slow-fast system. Time series of x -estimation RMS errors by MsCPF (blue) and MsEAKF (red). 20 observations and observation time 0.1. Dash line : climatological error. Dash-dot line : effective observation error.

	40 observations		20 observations	
obs time	MsCPF	MsEAKF	MsCPF	MsEAKF
0.1	0.061 (0.781)	0.061 (0.758)	0.079 (0.467)	0.078 (0.451)
0.3	0.062 (0.727)	0.060 (0.736)	0.080 (0.453)	0.078 (0.449)
0.5	0.072 (0.633)	0.069 (0.643)	0.085 (0.413)	0.085 (0.421)
0.8	0.075 (0.600)	0.071 (0.606)	0.087 (0.397)	0.085 (0.406)

Table 3: Slow-fast system. Time averaged RMS errors and pattern correlation in parenthesis. Climatological error is 0.095. Effective observation error is 0.145.

508 and the predicted states [41, 42]. It is shown in [42] that two filtered trajectories with
 509 disparate amplitudes can have the same RMS error and pattern correlation. Especially
 510 in complex high-dimensional systems, which show extreme events and non-Gaussian
 511 statistics, it is important to quantify the ability of filters in capturing extreme events
 512 and non-Gaussian statistics. Figure 10 shows the climatological PDFs ((a) in log-scale
 513 and (b) without scaling) of the forecast estimates of x_i . The true PDF of x_i shows
 514 a strongly non-Gaussian PDF with fat-tails (see Figure 10 (a)). Both MsCPF and
 515 MsEAKF have fat-tails but MsCPF has a better fit to the true PDF than MsEAKF.
 516 From the PDFs without scaling (Figure 10 (b)), we can check more significant difference
 517 between MsCPF and MsEAKF; MsCPF has a comparable PDF with the true PDF with
 518 marginal misfit but MsEAKF has a very sharp peak and shallow tails with significant
 519 misfit from the true PDF.

520 The relative entropy, which is also called Kullback-Leibler divergence in probability
 521 theory and information theory, is defined as follows

$$\mathcal{P}(\pi, \pi^{filter}) = \int \pi(\mathbf{x}) \ln \frac{\pi(\mathbf{x})}{\pi^{filter}(\mathbf{x})} d\mathbf{x} \quad (36)$$

522 where $\pi(\mathbf{x})$ and $\pi^{filter}(\mathbf{x})$ are the true and filtered forecast PDFs of \mathbf{x} respectively. The
 523 relative entropy measures the lack of information in estimating the true PDF π using
 524 the filtered forecast PDF π^{filter} and this has been successfully applied in quantifying
 525 the filter performance in several contexts [5, 43]. Note that if we have $\pi^{filter} = \pi$ the

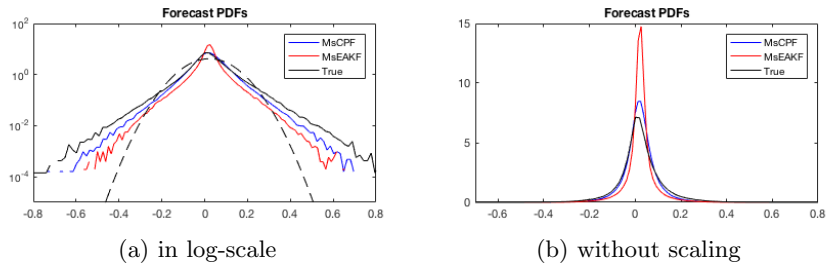


Figure 10: Slow-fast system. Forecast PDFs of \mathbf{x} by MsCPF (blue) and MsEAKF (red) along with the true value (black). Dash-line is the Gaussian fit to the true PDF. 20 observations

526 relative entropy is 0 and a large value means much lack of information of the filtered
 527 PDF. The forecast relative entropy using the forecast PDFs by MsCPF and MsEAKF
 528 are shown in Table 4 for 40 and 20 observations and observation times from 0.1 to 0.8.
 529 As we use the forecast PDFs for the relative entropy, a smaller relative entropy means
 530 better prediction and forecast skill than a larger relative entropy. As expected from
 531 the recovery of the true PDF, the forecast relative entropy of MsCPF is smaller than
 532 one of MsEAKF, the relative entropy of MsEAKF is about four times larger than that
 533 of MsCPF. As the number of observations and the observation interval increase, the
 534 lack of information in the forecast filter estimate increases, that is, the relative entropy
 increases. However, the ratio between MsCPF and MsEAKF does not change.

	40 observations		20 observations	
obs time	MsCPF	MsEAKF	MsCPF	MsEAKF
0.1	0.0365	0.1647	0.0398	0.1701
0.3	0.0383	0.1783	0.0403	0.1795
0.5	0.0410	0.1812	0.0421	0.1819
0.8	0.0437	0.1841	0.0438	0.1881

Table 4: Slow-fast system. Forecast relative entropy using the forecast estimate PDFs by MsCPF and MsEAKF.

535
 536 The filter performance between MsCPF and MsEAKF in capturing the non-Gaussian
 537 statistics also can be investigated from the time series of the forecast estimate of x_{10}
 538 shown in Figure 11. The true value of x_{10} stays bounded but it shows amplified fast
 539 oscillations extreme events beginning from time 2100. Both methods capture the be-
 540 ginning of fast oscillations; however the amplitude of MsEAKF is less than half of the
 541 true amplitude at time around 2700 while MsCPF has a comparable amplitude of the
 542 true value, which explains the narrower tail bounds of MsEAKF and the sharp peak in
 543 the forecast PDF of x_i (Figure 10).

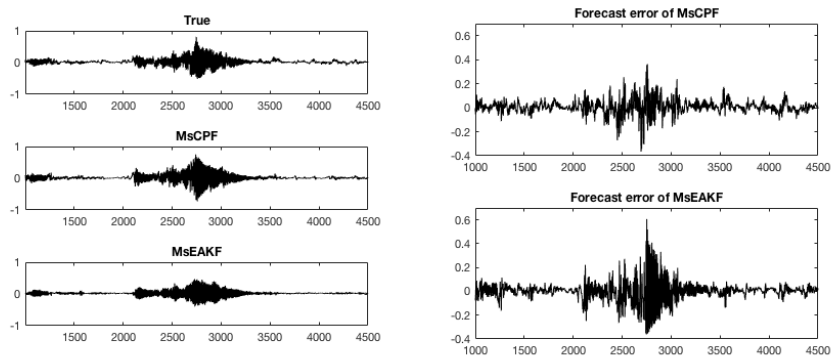


Figure 11: Slow-fast system. Time series of x_{10} forecast estimates (left) and forecast error (right) by MsCPF and MsEAKF. 20 observations

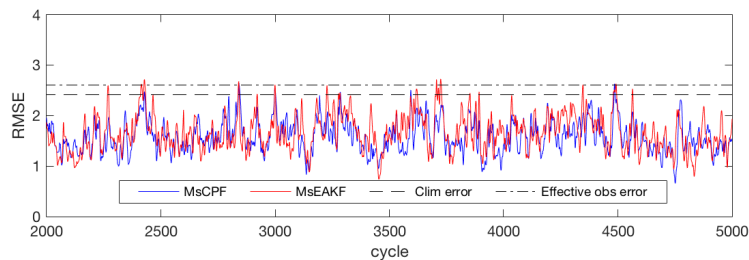


Figure 12: Strongly chaotic case. Time series of x -estimation RMS errors by MsCPF (blue) and MsEAKF (red). Dash line : climatological error. Dash-dot line : effective observation error.

544 *4.2.2. Strongly chaotic regime*

545 We now investigate the filter performance of MsCPF and MsEAKF applied for the
 546 second test regime, which has both the large- and small-scale advection to the small-
 547 scale dynamics ($a_L \neq 0, a_S \neq 0$). The westward moving waves seen in x_i is typical in
 548 the midlatitude atmosphere, i.e., the Rossby waves and x_i has non-Gaussian statistics,
 549 which is of our interest to recover using the multiscale data assimilation method.

550 As in Slow-fast system, we compare the filter performance using the path-wise mea-
 551 sures, RMS error and pattern correlation. Figure 12 shows the forecast estimate RMS
 552 errors of x_i as a function of time (the blue line is MsCPF and the red line is MsEAKF
 553 along with the climatological error (dash line) and the effective observation error (dash-
 554 dot line)). Both methods have filter skill and have comparable RMS errors that are
 555 smaller than both the climatological and the effective observation errors. Table 5 shows
 556 the time averaged forecast RMS errors and pattern correlations in parenthesis for fre-
 557 quent observation times 0.05 and 0.1 and 40 full and 20 sparse observations. Sparse
 558 observation and long observation time degrade the filter performance but both methods
 559 show skillful filter performance with RMS errors smaller than the climatological error
 560 along with pattern correlations larger than 88% and 73% for 40 and 20 observations

respectively.

	40 observations		20 observations	
obs time	MsCPF	MsEAKF	MsCPF	MsEAKF
0.05	1.12 (0.885)	1.17 (0.896)	1.66 (0.747)	1.67 (0.747)
0.10	1.17 (0.879)	1.21 (0.890)	1.76 (0.732)	1.79 (0.731)

Table 5: Strongly chaotic case. Time averaged RMS errors and pattern correlation in parenthesis. Climatological error is 2.39. Effective observation error is 2.620.

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In the slow-fast system, the filter performance between MsCPF and MsEAKF is observed in quantifying the lack of information in the filter estimates and the predicted states, that is, the recovery of the true PDF. The climatological PDFs of the forecast estimates of x_i by both methods along with the true PDF are shown in Figure 13. In the log-scale plot (Figure 13 (a)), we can check that the forecast PDF of MsCPF is on top of the true PDF, which has sub-Gaussian tails. On the other hand, the PDF of the ensemble-based method, MsEAKF, is a Gaussian fit to the true PDF. Without scaling, we can check more significant performance difference between MsCPF and MsEAKF. In Figure 13 (b), the PDF of MsCPF is on top of the true PDF capturing the non-symmetric peak of the true PDF. However, the PDF of MsEAKF fails to capture the non-symmetric peak of the true PDF.

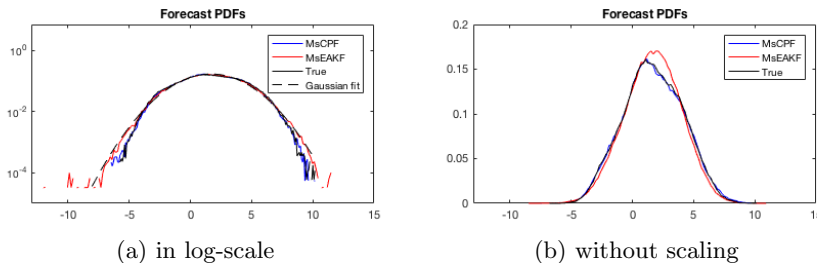


Figure 13: Strongly chaotic case. Forecast PDFs of \mathbf{x} by MsCPF (blue) and MsEAKF (red) along with the true value (black). Dash-line is the Gaussian fit to the true PDF.

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As in the slow-fast system, the forecast relative entropy using the forecast estimate PDFs by MsCPF and MsEAKF are shown in Table 6, which measure the prediction skill and the lack of information in the forecast. The lack of information in the forecast prediction is much larger for MsEAKF; the forecast relative entropy of MsCPF is about four times smaller than the relative entropy of MsEAKF. This result implies that the filter prediction can have significant performance difference in quantifying the uncertainty although they have comparable performance measured by path-wise measures such as the RMS error and pattern correlation [17, 43].

The space-time diagrams of the forecast estimates of x_i along with the true x_i are shown in Figure 14. Both methods have wave patterns comparable to the true state however the wave of MsEAKF has artificial local intermittency (for example, check the

	40 observations		20 observations	
obs time	MsCPF	MsEAKF	MsCPF	MsEAKF
0.05	0.0016	0.0069	0.0018	0.0078
0.10	0.0018	0.0072	0.0019	0.0089

Table 6: Strongly chaotic case. Forecast relative entropy using the forecast estimate PDFs by MsCPF and MsEAKF.

584 time around 350). This comparison also shows that there is no significant evidence of
 585 dynamic imbalance in MsCPF although MsCPF uses the coarse-grained localization.
 As another qualitative measure of filter performance, Figure 15 shows the time series

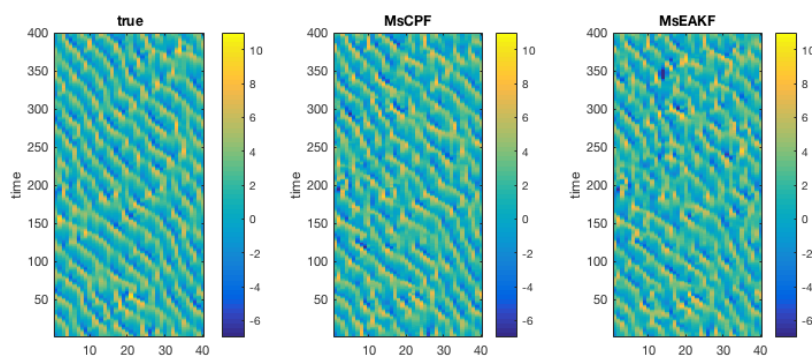


Figure 14: Snapshots of the forecast estimates of \mathbf{x} by MsCPF (middle) and MsEAKF (right) along with the true value (left)

586 of x_{10} . At the 3320th and 3430th cycles, MsCPF captures the correct local peaks but
 587 the ensemble-based multiscale filter fails to capture the comparable peaks.

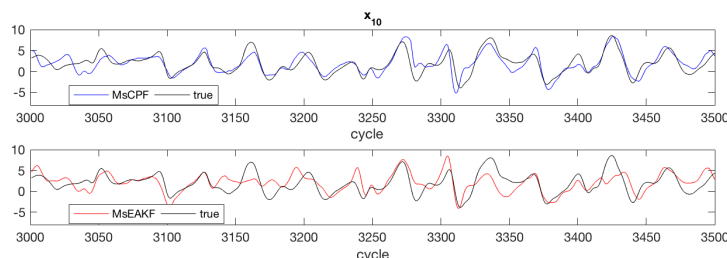


Figure 15: Strongly chaotic case. Time series of x_{10} forecast estimates by MsCPF (top) and MsEAKF (bottom) along with the true value.

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589 4.3. Weakly chaotic regime : prediction of the large-scale of y_{ij}

590 In the previous two test regimes, we were interested in the estimation and prediction
 591 of the slow resolved variable x_i , which has a longer decorrelation time than the one of

592 y_{ij} . In the weakly chaotic regime, the decorrelation times of x_i and y_{ij} are reversed
 593 and thus it is a non-physical and uninteresting test to predict x_i instead of y_{ij} as the
 594 unresolved y_{ij} is easier to predict than x_i and thus this setup is not a typical situation of
 595 data assimilation in real applications. In this section, we change the role of x_i and y_{ij} ,
 596 that is, we compare the multiscale filtering methods in the estimation and prediction of
 597 y_{ij} instead of x_i .

598 More precisely, we use the following observation $\mathbf{v} = \{v_1, v_2, \dots, v_j\}$

$$v_j = x_j + Y_j + \xi_i, \quad \xi_i : \text{iid random noise} \quad (37)$$

599 where Y_j is the local average of y_{ij}

$$Y_j = \frac{1}{J} \sum_j y_{ij} \quad (38)$$

600 so that there are equal number of variables for x_i and Y_i . This setup is not artificial
 601 but practical in that in real applications, many observations have collective information
 602 of different locations or variables such as radiation information from satellites [44].
 603 This coupled observation test and its mathematical analysis has already been studied
 604 in Chapter 7 of [1]. Our experiment setup is comparable to the setup in [1] but our
 605 test in this study is different from them as we test computationally efficient and cheap
 606 multiscale data assimilation methods instead of single-scale standard data assimilation
 607 methods.

608 Except the new observation operator (37), the other setup parameters are the same
 609 as in the previous two tests. We test 40 and 20 full and sparse observations with frequent
 610 observation intervals 0.05 and 0.10. Observation error variance is only 1% of the total
 611 variance and thus most of the observation error comes from the unresolved scale, i.e.,
 612 the representation error. Both MsCPF and MsEAKF use 50 samples and run 5000
 613 assimilation cycles and use the last 3000 cycles to measure the filter performance.

614 4.3.1. Data assimilation and prediction in the weakly chaotic regime

615 The time series of the forecast RMS errors by MsCPF (blue) and MsEAKF (red)
 616 with 20 observations and an observation interval 0.05 are shown in Figure 16 along with
 617 the climatological (dash) and effective observation (dash-dot) errors. In contrast to the
 618 previous two test regimes, there is significant performance difference in the RMS error,
 619 a path-wise filter measure; the RMS error of MsCPF stays below the climatological
 620 error, which shows significant filter skill but the RMS error of MsEAKF is larger than
 621 the climatological error without any filter skill. For other test scenarios (40 observations
 622 and an observation interval 0.10), the time averaged RMS errors and pattern correlations
 623 are shown in Table 7. For all possible observation scenarios, the RMS errors of MsCPF
 624 is at least 30% less than the climatological error while MsEAKF has errors larger than
 625 the climatological error. Regarding the forecast pattern correlations, which explains
 626 how much of the spatial variation is explained by the forecast, the pattern correlations

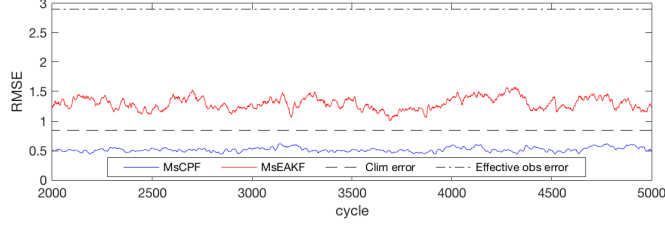


Figure 16: Weakly chaotic case. Time series of forecast Y -estimation RMS errors by MsCPF (blue) and MsEAKF (red). Dash line : climatological error. Dash-dot line : effective observation error.

	40 observations		20 observations	
obs time	MsCPF	MsEAKF	MsCPF	MsEAKF
0.05	0.52 (0.90)	1.30 (0.64)	0.55 (0.83)	1.46 (0.52)
0.10	0.54 (0.87)	1.32 (0.63)	0.61 (0.81)	1.53 (0.50)

Table 7: Weakly chaotic case. Time averaged RMS errors and pattern correlation in parenthesis. Climatological error is 0.844. Effective observation error is 2.900.

627 of MsCPF is at least 80% but the forecast pattern correlation of MsEAKF is less than
 628 65% for all scenarios and is marginally above 50% for the toughest test scenario.

629 Next we consider the recovery of the true PDF using the forecast estimates and the
 630 relative entropy to assess the lack of information in the forecast estimates and predic-
 631 tions. The forecast PDFs of Y_i (blue : MsCPF, red : MsEAKF) using 20 observations
 632 and an observation time 0.05 along with the true PDF of Y_i (black) are shown in Fig-
 633 ure 17. The PDF of MsCPF captures the comparable variance and shape of the true
 634 PDF although it is not on the top of the true PDF compared to the previous two test
 635 regimes. In contrary, the PDF of MsEAKF has a too large variance compared to the
 636 true PDF. This result shows that forecast using MsEAKF is inadequate as it provides
 637 incorrect weights on large deviated values while MsCPF has comparable weights to the
 true PDF. As a quantitative measure of the lack of information, the relative entropy for

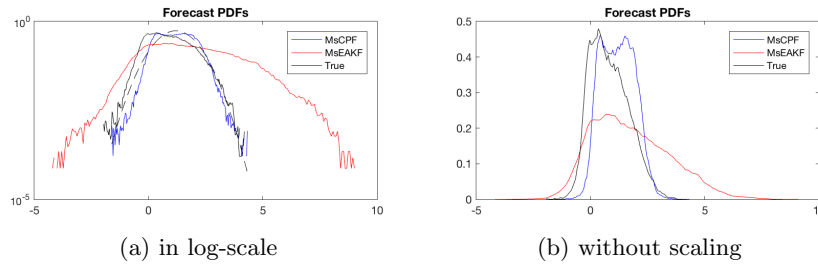


Figure 17: Weakly chaotic case. Forecast PDFs of x by MsCPF (blue) and MsEAKF (red) along with the true value (black). Dash-line is the Gaussian fit to the true PDF.

638 several scenarios are shown in Table 8. As discussed before, a smaller relative entropy
 639

	40 observations		20 observations	
obs time	MsCPF	MsEAKF	MsCPF	MsEAKF
0.05	0.1631	0.3024	0.1787	0.4328
0.10	0.1791	0.3234	0.1891	0.4523

Table 8: Weakly chaotic case. Forecast relative entropy using the forecast estimate PDFs by MsCPF and MsEAKF.

640 implies a better prediction or less lack of information. In comparison between MsCPF
641 and MsEAKF, it is obvious that MsCPF has a superior prediction skill with relative
642 entropies half of those of MsEAKF. As the number of observation decreases or the ob-
643 servation interval increases, the relative entropy decreases, which implies performance
644 degradation. However, the relative entropies of MsEAKF never becomes smaller than
645 those of MsCPF.

646 5. Conclusions

647 In the data assimilation of high-dimensional complex systems such as turbulent
648 geophysical systems, it is indispensable to use coarse-resolution forecast models as it
649 is computationally prohibitive to resolve all active spatiotemporal scales. To mitigate
650 the problem related to the incorporation of coarse-resolution forecast models, i.e., mixed
651 contributions from both the resolved and unresolved scales, we have proposed and tested
652 the multiscale clustered particle filter (MsCPF). MsCPF follows the single-scale clus-
653 tered particle filter [29] that use coarse-grained localization and particle adjustment
654 while the update in each cluster follows the general multiscale particle filter [22] instead
655 of the standard particle filter update.

656 To test the multiscale algorithm under effect of the observation model error, we
657 proposed and developed an advective two-layer Lorenz-96 system. Using several com-
658 bination of large- and small-scale advection on the small-scale equation, the model can
659 mimic several different test regimes including the standard slow-fast system that is typ-
660 ical in atmosphere where a slow advective vortical Rossby wave is coupled with fast
661 inertia-gravity waves. All different regimes we considered in this study have impor-
662 tant features of turbulent systems such as non-Gaussian statistics including fat-tails
663 and intermittent extreme events. The multiscale clustered particle filter shows robust
664 skill in recovering the true non-Gaussian PDF using a relatively few particles while
665 an ensemble-based method fails to capture the non-Gaussian feature. In the weakly
666 chaotic test regime with collective observation of the slow variables, which mimics one
667 of the difficult test scenario in real-applications such as radiation observation from satel-
668 lites, MsCPF shows superior performance to the ensemble based multiscale methods,
669 MsEAKF, in both the path-wise measure, RMS errors and pattern correlations and the
670 information theoretic measure, recovery of true PDF and relative entropy.

671 In this study, we focused on the investigation of the effect of the observation model
672 error, which is indispensable in the multiscale data assimilation as the forecast model

673 provides only the resolved large-scale components. For this purpose, only the perfect
674 forecast model has been tested in our study to minimize the error from the forecast
675 model error, which is another important factor for filter performance. Thus it is natural
676 to extend the current study to the investigation of the forecast model error, especially
677 from the coarse-resolution model error. Also we believe that the information barrier
678 related to the ignored small-scale update in our study could hinder further performance
679 improvement of the multiscale clustered particle filter. In the near future, we plan to
680 investigate the effects of the information barrier and the forecast model error on the
681 multiscale filter performance.

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