1	Combining Ensemble Kalman Filter and Reservoir Computing to
2	predict spatio-temporal chaotic systems from imperfect observations
3	and models
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11	Abstract
12	Prediction of spatio-temporal chaotic systems is important in various fields, such as Numerical
13	Weather Prediction (NWP). While data assimilation methods have been applied in NWP, machine
14	learning techniques, such as Reservoir Computing (RC), are recently recognized as promising tools to
15	predict spatio-temporal chaotic systems. However, the sensitivity of the skill of the machine learning
16	based prediction to the imperfectness of observations is unclear. In this study, we evaluate the skill of
17	RC with noisy and sparsely distributed observations. We intensively compare the performances of RC
18	and Local Ensemble Transform Kalman Filter (LETKF) by applying them to the prediction of the

19	Lorenz 96 system. In order to increase the scalability to larger systems, we applied parallelized RC
20	framework. Although RC can successfully predict the Lorenz 96 system if the system is perfectly
21	observed, we find that RC is vulnerable to observation sparsity compared with LETKF. To overcome
22	this limitation of RC, we propose to combine LETKF and RC. In our proposed method, the system is
23	predicted by RC that learned the analysis time series estimated by LETKF. Our proposed method can
24	successfully predict the Lorenz 96 system using noisy and sparsely distributed observations. Most
25	importantly, our method can predict better than LETKF when the process-based model is imperfect.
26	
27	1. Introduction
28	In Numerical Weather Prediction (NWP), it is required to obtain the optimal estimation of atmospheric
29	state variables by observations and process-based models which are both imperfect. Observations of
30	atmospheric states are sparse and noisy, and numerical models inevitably include biases. In addition,
31	models used in NWP are known to be chaotic, which makes the prediction substantially difficult. To
32	accurately predict the future atmospheric state, it is important to develop methods to predict spatio-
33	tempral chaotic dynamical systems from imperfect observations and models.
34	
35	Traditionally, data assimilation methods have been widely used in geosciences and NWP systems.
36	Data assimilation is a generic term of approaches to estimate the state from observations and model

37	outputs based on their errors. The state estimated by data assimilation is used as the initial value, and
38	the future state is predicted by models alone. Data assimilation is currently adopted in operational
39	NWP systems. Many data assimilation frameworks have been proposed, e.g. 4D variational methods
40	(4D-VAR; Bannister, 2017), Ensemble Kalman Filter (EnKF; Houtekamer & Zhang, 2016), or their
41	derivatives, and they have been applied to many kinds of weather prediction tasks, such as the
42	prediction of short-term rainfall events (e.g. Sawada et al., 2019; Yokota et al., 2018), and severe
43	storms (e.g. Zhang et al., 2016). Although data assimilation can efficiently estimate the unobservable
44	state variables from noisy observations, the prediction skill is degraded if the model has large biases.
45	
46	On the other hand, model-free prediction methods based on machine learning have received much
47	attention recently. In the context of dynamical system theory, previous works have developed the
48	methods to reproduce the dynamics by inferring it purely from observation data (Rajendra and
49	Brahmajirao, 2020), or by combining a data-driven approach and physical knowledge on the systems
50	(Karniadakis et al., 2021). In the NWP context, many previous studies have successfully applied
51	machine learning to predict chaotic dynamics. Vlachas et al. (2018) successfully applied Long-Short
52	Term Memory (LSTM; Hochreiter & Schmidhuber, 1997) to predict the dynamics of the Lorenz96
53	model, Kuramoto-Sivashinski Equation, and the barotropic climate model which is a simple
54	atmospheric circulation model. Asanjan et al. (2018) showed that LSTM can accurately predict the

future precipitation by learning satellite observation data. Nguyen & Bae (2020) successfully applied

LSTM to generate area-averaged precipitation prediction for hydrological forecasting.

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58 In addition to LSTM, Reservoir Computing (RC), which was first introduced by Jaeger & Haas (2004), 59 has been found to be suitable to predict spatio-temporal chaotic systems. Pathak et al. (2017) 60 successfully applied RC to predict the dynamics of Lorenz equation and Kuramoto-Sivashinski 61 Equation. Lu et al. (2017) showed that RC can be used to estimate state variables from sparse 62 observations if the whole system was perfectly observed as training data. (Pathak et al., 2018b) 63 succeeded in using a parallelized RC to predict each segment of the state space locally, which enhanced 64 the scalability of RC to much higher dimensional systems. Chattopadhyay et al. (2020) revealed that 65 RC can predict the dynamics of the Lorenz 96 model more accurately than LSTM and Artificial Neural 66 Network (ANN). In addition to the accuracy, RC also has an advantage in computational costs. RC 67 can learn the dynamics only by training a single matrix as a linear minimization problem just once, 68 while other neural networks have to train numerous parameters and need many iterations (Lu et al., 69 2017). Thanks to this feature, the computational costs needed to train RC is cheaper than LSTM and 70 ANN.

72	However, Vlachas et al. (2020) revealed that the prediction accuracy of RC is degraded when all of
73	the state variables cannot be observed. It can be a serious problem since the observation sparsity is
74	often the case in geosciences and the NWP systems. Brajard et al. (2020) pointed out this issue and
75	successfully trained the Convolutional Neural Network with sparse observations, by combining with
76	EnKF. However, their method needs to iterate the data assimilation and training until the prediction
77	accuracy of the trained model converges. Although one can stop the iteration in a few times, it can be
78	longer, and the training can be computationally expensive if one should wait until the convergence.
79	Bocquet et al. (2020) proposed a method to combine EnKF and machine learning methods to obtain
80	both the state estimation and the surrogate model online. They showed successful results without using
81	the process-based model at all. Dueben & Bauer (2018) mentioned that the spatio-temporal
82	heterogeneity of observation data made it difficult to train machine learning models, and they
83	suggested to use the model or reanalysis as training data. Weyn et al. (2019) successfully trained
84	machine learning models using the atmospheric reanalysis data.
85	
86	We aim to propose the novel methodology to predict spatio-temporal chaotic systems from imperfect
87	observations and models. First, we reveal the limitation of the stand-alone use of RC under realistic
88	situations (i.e., imperfect observations and models). Then, we propose a new method to maximize the
89	potential of RC to predict chaotic systems from imperfect models and observations, which is even

90	computationally feasible. As Dueben & Bauer (2018) proposed, we make RC learn the analysis data
91	series generated by a data assimilation method. Our new method can accurately predict from imperfect
92	observations. Most importantly, we found that our proposed method is more robust to model biases
93	than the stand-alone use of data assimilation methods.
94	
95	
96	2. Methods
97	2.1 Lorenz 96 model and OSSE
98	We used a low dimensional spatio-temporal chaotic model, the Lorenz 96 model (L96), to perform
99	experiments with various parameter settings. L96 is a model introduced by Lorenz & Emanuel (1998)
100	and has been commonly used in data assimilation studies (e.g. Kotsuki et al., 2017; Miyoshi, 2005;
101	Penny, 2014; Raboudi et al., 2018). L96 is recognized as a good testbed for the operational NWP
102	problems (Penny, 2014).
103	
104	In this model, we consider a ring structured and m dimensional discrete state space $x_1, x_2,, x_m$
105	(that is, x_m is adjacent to x_1), and define the system dynamics as follows:

106
$$\frac{dx_i}{dt} = (x_{i+1} - x_{i-2}) x_{i-1} - x_i + F$$
(1)

107 where *F* stands for the force parameter, and we define $x_{-1} = x_{m-1}$, $x_0 = x_m$, and $x_{m+1} = x_1$. 108 Each term of this equation corresponds to advection, damping and forcing respectively. It is known 109 that the model with m = 40 and F = 8 shows chaotic dynamics with 13 positive Lyapunov 110 exponents (Lorenz and Emanuel, 1998), and this setting is commonly used in the previous studies (e.g. 111 Kotsuki et al., 2017; Miyoshi, 2005; Penny, 2014; Raboudi et al., 2018). The time width $\Delta t = 0.2$ 112 corresponds to one day in real atmospheric motion from the view of dissipative decay time (Lorenz 113 and Emanuel, 1998).

114

115 As we use this conceptual model, we cannot obtain any observational data or "true" phenomena that 116 correspond to the model. Instead, we adopted Observing System Simulation Experiment (OSSE). We 117 first prepared a time series by integrating equation (1) and regarded it as the "true" dynamics (called 118 Nature Run). Observation data can be calculated from this time series adding some perturbation: $y^0 = Hx + \epsilon$ 119 (2) where $\mathbf{v}^{\mathbf{0}} \in \mathbb{R}^{h}$ is the observation value, **H** is the $m \times h$ observation matrix, $\boldsymbol{\epsilon} \in \mathbb{R}^{h}$ is the 120 121 observational error whose each element is independent and identically distributed from a Gaussian 122 distribution N(0, e) for observation error e. 123

124 In each experiment, the form of L96 used to generate Nature Run is unknown, and the model used to

125 make prediction can be different from that for Nature Run. The difference between the model used for

126 Nature Run and that used for prediction corresponds to the model's bias in the context of NWP.

127

- 128 **2.2 Local Ensemble Transform Kalman Filter**
- 129 We used the Local Ensemble Transform Kalman Filter (LETKF, Hunt et al., 2007) as the data
- 130 assimilation method in this study. LETKF is one of the ensemble-based data assimilation methods,
- 131 which is considered to be applicable to the NWP problems in many previous studies (Sawada et al.,
- 132 2019; Yokota et al., 2018). LETKF is also used for the operational NWP in some countries (e.g.
- 133 Germany; Schraff et al., 2016).
- 134
- 135 LETKF and the family of ensemble Kalman filters have two steps; forecast and analysis. The analysis

136 step makes the state estimation based on the forecast variables and observations. The forecast step

- 137 makes the prediction from the current analysis variables to the time for the next analysis using the
- 138 model. The interval for each analysis is called "assimilation window".
- 139 Considering the stochastic error in the model, system dynamics can be represented as follows 140 (hereafter the subscript k stands for the variable at time k, and the time width between k and k +
- 141 1 corresponds to the assimilation window):
- 142 $\boldsymbol{x}_{\boldsymbol{k}}^{f} = \boldsymbol{\mathcal{M}}(\boldsymbol{x}_{\boldsymbol{k}-1}^{a}) + \boldsymbol{\eta}_{\boldsymbol{k}}, \qquad \boldsymbol{\eta}_{\boldsymbol{k}} \sim N(\boldsymbol{0}, \boldsymbol{Q})$ (3)

where $x_k^f \in \mathbb{R}^m$ is the forecast variables, $x_{k-1}^a \in \mathbb{R}^m$ is the analysis variables, $\mathcal{M}: \mathbb{R}^m \to \mathbb{R}^m$ is 143 144 the model dynamics operator, $\eta \in \mathbb{R}^m$ is the stochastic error and $N(\mathbf{0}, \mathbf{Q})$ means the multivariate 145 Gaussian distribution with mean 0 and $n \times n$ covariance matrix Q. Since the error in the model is assumed to follow the Gaussian distribution, forecasted state x^{f} can also be considered as a random 146 147 variable from the Gaussian distribution. When the assimilation window is short, the Gaussian nature 148 of the forecast variables is preserved even if the model dynamics is nonlinear. In this situation, the probability distribution of x^{f} (and also x^{a}) can be parametrized by mean $\overline{x^{f}}(\overline{x_{k}^{a}})$ and covariance 149 matrix $P^f(P^a_k)$. 150

151 Using the computed state vector x_k^f , observation variables can be estimated as follows:

152
$$\mathbf{y}_{k}^{f} = \mathcal{H}\left(\mathbf{x}_{k}^{f}\right) + \boldsymbol{\epsilon}_{k}, \quad \boldsymbol{\epsilon}_{k} \sim N(\mathbf{0}, \mathbf{R})$$
 (4)

153 where $y^{f} \in \mathbb{R}^{h}$ is the estimated observation value, $\mathcal{H}: \mathbb{R}^{m} \to \mathbb{R}^{h}$ is the observation operator and 154 $\epsilon \in \mathbb{R}^{h}$ is the observation error sampled from $N(\mathbf{0}, \mathbf{R})$. Although \mathcal{H} can be either linear or 155 nonlinear, we assume it to be linear in this study and expressed as a $h \times m$ matrix H (the treatment 156 of the nonlinear case is discussed in Hunt et al., 2007).

157

158 LETKF uses an ensemble of state variables to estimate the evolution of $\overline{x_k^f}$ and P_k^f . The time 159 evolution of each ensemble members is as follows:

160
$$x_{k}^{f,(i)} = \mathcal{M}\left(x_{k-1}^{a,(i)}\right)$$
(5)

161 where $\mathbf{x}_{k}^{f,(i)}$ is the *i*th ensemble member of forecast value at time *k*. Then the mean and covariance

162 of state variables can be expressed as follows:

163
$$\overline{\boldsymbol{x}_{k}^{f}} \approx \frac{1}{N_{e}} \sum_{i=1}^{N_{e}} \boldsymbol{x}_{k}^{f,(i)}, \qquad \boldsymbol{P}_{k}^{f} = \frac{1}{N_{e} - 1} \boldsymbol{X}_{k}^{f} \left(\boldsymbol{X}_{k}^{f}\right)^{T}$$
(6)

164 where N_e is the number of ensemble members and X_k^f is the matrix whose *i*th column is the 165 deviation of the *i*th ensemble member from the ensemble mean.

166

assimilated observations are different at different grid points and the analysis variables of each grid

- 169 points are computed separately.
- 170 For each grid points, observations to be assimilated are chosen. The rows or elements of y^o , H, and
- 171 **R** corresponding to non-assimilated observations should be removed as the localization procedure.
- 172 "Smooth localization" can also be performed by multiplying some factors to each row of \mathbf{R} based on
- the distance between target grid point and observation points (Hunt et al., 2007).

174 From the forecast ensemble, the mean and the covariance of the analysis ensemble can be calculated

175 in the ensemble subspace as follows:

176
$$\overline{w_{k}^{a}} = \widetilde{P}_{k}^{a} \left(HX_{k}^{f}\right)^{T} R^{-1} \left(y^{o} - H\overline{x_{k}^{f}}\right)$$
$$\widetilde{P}_{f}^{a} = \left[(k-1)I + \left(HX_{k}^{f}\right)^{T} R^{-1}HX_{k}^{f}\right]^{-1}$$
(7)

177 where $w_{k}^{a}, \tilde{P}_{f}^{a}$ stands for the mean and covariance of the analysis ensemble calculated in the ensemble

178 subspace. They can be transformed into model space as follows:

179
$$\overline{x_k^a} = \overline{x_k^f} + X_k^f \overline{w_k^a}$$

180
$$\boldsymbol{P}_{k}^{a} = \boldsymbol{X}_{k}^{f} \widetilde{\boldsymbol{P}}_{k}^{a} \left(\boldsymbol{X}_{k}^{f}\right)^{T}$$
(8)

181 On the other hand, as equation (6), we can consider the analysis covariance as the product of the

182 analysis ensemble matrix:

183
$$\boldsymbol{P}_{k}^{a} = \frac{1}{N_{e} - 1} \boldsymbol{X}_{k}^{a} (\boldsymbol{X}_{k}^{a})^{T}$$
(9)

184 where X_k^a is the matrix whose *i*th column is the variation of the *i*th ensemble member from the 185 mean for the analysis ensemble. Therefore, decomposing \tilde{P}_k^a of equation (7) into square root, we can 186 get each analysis ensemble member at time *k* without explicitly computing the covariance matrix in 187 the state space:

188
$$W_k^a (W_k^a)^T = \widetilde{P}_k^a, \qquad x_k^a = \overline{x_k^f} + \sqrt{N_e - 1} X_k^f w_k^a$$
(10)

189 where w_k^a is the *i*th column of W_k^a in the first equation. A covariance inflation parameter is 190 multiplied to take measures for the tendency of data assimilation to underestimate the uncertainty of 191 state estimate by empirically accounting for model noise (see equation (3)). See Hunt et al. (2007) for 192 more detailed derivation. Now, we can return to the equation (5) and iterate forecast and analysis step. 193

194 As in the real application, we consider the situation that the observations are not available in the

195 prediction period. Predictions are made by the model alone, using the latest analysis state variables as

the initial condition:

197
$$\boldsymbol{x}_{K+1}^{f} = \widetilde{\boldsymbol{\mathcal{M}}}(\overline{\boldsymbol{x}_{K}^{a}}), \ \boldsymbol{x}_{K+2}^{f} = \widetilde{\boldsymbol{\mathcal{M}}}(\boldsymbol{x}_{K+1}^{f}), \ \dots$$
(11)

198 where \mathbf{x}_{k}^{f} is the prediction variables at time k, $\widetilde{\mathbf{M}}$ is the prediction model (an imperfect L96 model), 199 and $\overline{\mathbf{x}_{K}^{a}}$ is the mean of the analysis ensemble at the initial time of the prediction. This way of making 200 prediction is called "Extended Forecast", and we call this prediction "LETKF-Ext" in this study, to 201 distinguish it from the forecast-analysis iteration of LETKF.

202

203 2.3 Reservoir Computing

204 2.3.1 Description of Reservoir Computing Architecture

205 We use Reservoir Computing (RC) as the machine learning framework. RC is a type of Recurrent

206 Neural Network, which has a single hidden layer called reservoir. Figure 1 shows its architecture. As

207 mentioned in Section 1, previous works have shown that RC can predict the dynamics of spatio-

208 temporal chaotic systems.

209

210 The state of the reservoir layer at timestep k is represented as a vector $\mathbf{r}_k \in \mathbb{R}^{D_r}$, which evolves

211 given the input vector $\boldsymbol{u}_k \in \mathbb{R}^m$ as follows:

212
$$\boldsymbol{r}_{k+1} = \tanh[\boldsymbol{A}\boldsymbol{r}_k + \boldsymbol{W}_{in}\boldsymbol{u}_k] \tag{12}$$

where W_{in} is the $D_r \times m$ input matrix which maps the input vector to the reservoir space, and Ais the $D_r \times D_r$ adjacency matrix of the reservoir which determines the reservoir dynamics. W_{in} should be determined to have only one nonzero component in each row, and each nonzero component is sampled from uniform distribution of [-a, a] for some parameter a. A has a proportion of dnonzero components with random values from uniform distribution, and it is normalized to have the maximum eigenvalue ρ . The reservoir size D_r should be determined based on the size of the state space. From the reservoir state, we can compute the output vector \boldsymbol{v} as follows:

$$v_k = W_{out} f(r_k) \tag{13}$$

where W_{out} is the $M \times D_r$ output matrix which maps the reservoir state to the state space, and $f: \mathbb{R}^{D_r} \to \mathbb{R}^{D_r}$ is an operator of nonlinear transformation. The nonlinear transformation is essential for the accurate prediction (Chattopadhyay et al., 2020). It is important that A and W_{in} are fixed and only W_{out} will be trained by just solving a linear problem. Therefore, the computational cost required to train RC is small and it is an outstanding advantage of RC compared to the other neural network frameworks.

227

In the training phase, we set the switch in the Figure 1 to the training configuration. Given a training data series $\{u_0, u_1, ..., u_K\}$, we can generate the reservoir state series $\{r_1, r_2, ..., r_{K+1}\}$ by equation (12). By using the training data and reservoir state series, we can determine the W_{out} matrix by ridge regression. We minimize the following square error function with respect to W_{out} :

232
$$\sum_{i=1}^{n} \|\boldsymbol{u}_{k} - \boldsymbol{W}_{out}\boldsymbol{f}(\boldsymbol{r}_{k})\|^{2} + \beta \cdot trace(\boldsymbol{W}_{out}\boldsymbol{W}_{out}^{T})$$
(14)

where $||\mathbf{x}|| = x^T x$ and β is the ridge regression parameter (normally a small positive number). Since the objective function (14) is quadratic, it is differentiable. The optimal value can be obtained by just solving a linear equation as follows:

236 $W_{out} = UR^T (RR^T + \beta I)^{-1}$ (15)

237 where I is the $D_r \times D_r$ identity matrix and R, U are the matrices whose kth column is the vector

238 $f(r_k)$, u_k , respectively.

239

240Then, we can shift to the predicting phase. Before we predict with the network, we first need to "spin 241 up" the reservoir state. The spin up process was done by giving the time series before the initial value 242 $\{u_{-k}, u_{-k+1}, \dots, u_{-1}\}$ to the network and calculate the reservoir state right before the beginning of the 243 prediction via equation (12). After that, the output layer is connected to the input layer, and the network 244becomes recursive. In this configuration, the output value v_k of equation (13) is used as the next 245 input value u_k of equation (12). Once we give the initial value u_0 , the network will iterate equation 246 (12) and (13) spontaneously, and the prediction will be yielded. At this point, RC can now be used as 247the surrogate model that mimics the state dynamics:

248
$$\boldsymbol{x}_{k+1}^{f} = \widetilde{\mathcal{M}}_{RC} \left(\boldsymbol{x}_{k}^{f}, \left\{ \boldsymbol{x}_{k}^{train} \right\}_{1 \le k \le K} \right)$$
(16)

where \mathbf{x}_{k}^{f} is the prediction variables at time k, $\widetilde{\mathcal{M}}_{RC}$ is the dynamics of RC (equations (12) and (13)) and $\{\mathbf{x}_{k}^{train}\}_{1 \le k \le K} = \{\mathbf{x}_{1}^{train}, \mathbf{x}_{2}^{train}, \dots, \mathbf{x}_{K}^{train}\}$ is the time series of training data.

- 251
- 252 Considering the real application, it is natural to assume that the observation data can only be used as
 253 the training data and the initial value for the RC prediction. In this paper we call this type of prediction
- 254 "RC-Obs". Prediction time series here can be expressed using equation (16) as follows:

255
$$\boldsymbol{x}_{K+1}^{f} = \widetilde{\mathcal{M}}_{RC} \left(\boldsymbol{y}_{K}^{O} \{ \boldsymbol{y}_{k}^{O} \}_{1 \le k \le K} \right), \quad \boldsymbol{x}_{K+2}^{f} = \widetilde{\mathcal{M}}_{RC} \left(\boldsymbol{x}_{K+1}^{f}, \{ \boldsymbol{y}_{k}^{O} \}_{1 \le k \le K} \right), \dots$$
(17)

where $\{y_k^o\}_{1 \le k \le K} = \{y_1^o, y_2^o, ...\}$ is the observation time series and y_k^o is the observation at the initial time of the prediction. As in equation (14), input and output of RC must be in the same space. Therefore, in this case, prediction variables x_k^f has the same dimensionality as y_k^o , and the nonobservable grid points are not predicted by this prediction scheme.

260

261 2.3.2 Parallelized Reservoir Computing

262 In general, the required reservoir size D_r for accurate prediction increases as the dimension of the

- state space m increases. Since the RC framework needs to keep adjacency matrix A on the memory,
- and to perform inverse matrix calculation of $D_r \times D_r$ matrix (equation (15)), too large reservoir size
- leads to unfeasible computational cost. (Pathak et al., 2018b) proposed a solution to this issue, which
- is called the parallelized reservoir approach.

267 In this approach, the state space is divided into g groups, all of which contains q = m/g state 268 variables:

269
$$\boldsymbol{g}_{k}^{(i)} = \left(u_{k,(i-1)\times q+1}, u_{k,(i-1)\times q+2}, \dots, u_{k,i\times q}\right)^{T}, i = 1, 2, \dots, g$$
(18)

where $\boldsymbol{g}_{k}^{(i)}$ is the *i*th group at time *k*, $u_{k,j}$ is the *j*th state variable at time *k*. Each group is predicted by different reservoir placed in parallel. *i*th reservoir accepts the state variables of *i*th group as well as adjacent *l* grids, which can be expressed as follows:

273
$$\boldsymbol{h}_{k}^{(i)} = \left(u_{k,(i-1)\times q+1-l}, u_{k,(i-1)\times q+2-l}, \dots, u_{k,i\times q+l}\right)^{T}$$
(19)

274 where $\boldsymbol{h}_{k}^{(i)}$ is the input vector for *i*th reservoir at time *k*. The dynamics of each reservoir can be

275 expressed as follows according to equation (12):

276
$$\boldsymbol{r}_{k+1}^{(i)} = \tanh\left[\boldsymbol{A}^{(i)}\boldsymbol{r}_{k}^{(i)} + \boldsymbol{W}_{in}^{(i)}\boldsymbol{h}_{k}^{(i)}\right]$$
(20)

277 where $\mathbf{r}_{k}^{(i)}$, $\mathbf{A}^{(i)}$, $\mathbf{W}_{in}^{(i)}$ and $\mathbf{W}_{out}^{(i)}$ are the reservoir state vector, adjacency matrix input matrix, and

278 output matrix for *i*th reservoir. Each reservoir is trained independently using equation (13) so that:

279
$$\boldsymbol{g}_{k}^{(i)} = \boldsymbol{W}_{out}^{(i)} \boldsymbol{f}\left(\boldsymbol{r}_{k}^{(i)}\right)$$
(21)

where $W_{out}^{(i)}$ is the output matrix in the *i*th reservoir. The prediction scheme of parallelized RC is summarized in Figure 2. The strategy of parallelization is similar to the localization of data assimilation. As LETKF ignores correlations between distant grid points, parallelized reservoir computing assumes that the state variable of a grid point at the next time step depends only on the state variables of neighboring points. In contrast, ordinary RC assumes that the time evolution at one

grid point is affected by all points in the state space, which may be inefficient in many applications in

286 geoscience such as NWP.

287

288 2.4 Combination of RC and LETKF

289 As discussed so far and we will quantitatively discuss in the section 4, LETKF-Ext and RC-Obs have 290 contrasting advantages and disadvantages. LETKF-Ext can accurately predict even if the observation 291 is noisy and/or sparsely distributed, while RC-Obs is vulnerable to the imperfectness in observation. 292 On the other hand, LETKF-Ext can be strongly affected by the model biases since the prediction of 293 LETKF-Ext depends only on the model after obtaining the initial condition, while RC-Obs has no 294 dependence to the accuracy of the model as it only uses the observation data for training and prediction. 295 296 Therefore, the combination of LETKF and RC has a potential to push the limit of these two individual 297 prediction methods and realize accurate and robust prediction. The weakness of RC-Obs is that we 298 can only use the observational data directly, which is inevitably sparse in the real application, although 299 RC is vulnerable to this imperfectness. In our proposed method, we make RC learn the analysis time 300 series generated by LETKF instead of directly learning observation data. 301

302 Suppose we have sparse and noisy observations for the training data. If we take observations as inputs

303 and analysis variables as outputs, LETKF can be considered as an operator to estimate the full state

304 variables from the sparse observations:

305
$$\left\{\overline{\boldsymbol{x}_{k}^{a}}\right\}_{1 \le k \le K} = \left\{\mathcal{D}(\boldsymbol{y}_{k}^{O})\right\}_{1 \le k \le K}$$
(22)

where $\{\overline{x_k^a}\}_{1 \le k \le K} = \{x_1^a, x_2^a, ..., x_K^a\}$ is the full-state variables (time series of the LETKF analysis 306 ensemble mean), \mathbf{y}_k^0 is the observation, and $\mathcal{D}: \mathbb{R}^n \to \mathbb{R}^m$ represents the state estimation operator, 307 which is realized by LETKF in this study. Then, RC is trained by using $\{x_k^a\}_{1 \le k \le K}$ as the training 308 309 data set. In this way, RC can mimic the dynamics of analysis time series computed by forecast-analysis 310 cycle of LETKF. Prediction can be generated by using the analysis variables at current time step (\boldsymbol{x}_{K}^{a}) 311 as the initial value. Since RC is trained with LETKF analysis variables, we call this method "RC-Anl". 312 By using the notation of equation (16), the prediction of RC-Anl can be expressed as follows: $\boldsymbol{x}_{K+1}^f = \widetilde{\mathcal{M}}_{RC}(\boldsymbol{x}_K^a, \{\boldsymbol{x}_k^a\}_{1 \le k \le K}), \qquad \boldsymbol{x}_{K+2}^f = \widetilde{\mathcal{M}}_{RC}\big(\boldsymbol{x}_{K+1}^f, \{\boldsymbol{x}_k^a\}_{1 \le k \le K}\big), \dots$ 313 (23)where $\{x_k^a\}_{1 \le k \le K} = \{x_1^a, x_2^a, ..., x_k^a\}$ is the time series of the LETKF analysis variables. The 314 315 schematics of the LETKF-Ext, RC-Obs, and RC-Anl are shown in the figure 3. Initial values and

model dynamics used in each method are compared in Table 1.

317

316

318 Our proposed combination method is expected to predict more accurately than RC-Obs since the 319 training data always exist in all the grid points, even if the observation is sparse. Also, especially if the 320 model is substantially biased, the analysis time series generated by LETKF is more accurate than the 321 model output itself. It means that RC-Anl is expected to be able to predict more accurately than322 LETKF-Ext.

323

324 **3. Experiment Design**

325 To generate the Nature Run, L96 with m = 40, F = 8 was used, and it was numerically integrated

326 by 4th order Runge-Kutta method by time width $\Delta t = 0.005$. Before calculating the Nature Run, the

327 L96 equation was integrated for 1440000 timesteps for spin up. In the following experiment, the F

328 term in the model was changed to represent the model bias.

329

330 Here, we assume that the source of the model bias is unknown. When the source of bias is only the 331 uncertainty in model parameters, and uncertain parameters which significantly induce the model bias 332 are completely identified, optimization methods can estimate the value of the uncertain parameters to 333 minimize the gaps between simulation and observation. This problem can also be solved by data 334 assimilation methods (e.g. Bocquet and Sakov, 2013). However, it is difficult to calibrate the model 335 when the source of uncertainty is unknown. Our proposed method does not need to identify the source 336 of model bias so that it may be useful especially when the source of model bias is unknown. This is 337 often the case in the large and complex model such as NWP systems. 338

The setting for LETKF was based on Miyoshi and Yamane (2007). As the localization process, the observation points within 10 indices are chosen to be assimilated for every grid point. The "smooth localization" is also performed on observation covariance \mathbf{R} . Since we assume that each observation error is independent and thus \mathbf{R} is diagonal, the localization procedure can be done just by dividing each diagonal elements of observation covariance \mathbf{R} by the value w calculated as follows:

349
$$w(r) = \exp\left(-\frac{r^2}{18}\right) \tag{24}$$

where r is the distance between each observation point and each analyzed point. For every grid point, the observation point with $w(r) \ge 0.0001$ are chosen to be assimilated. In equation (10), a "covariance inflation factor", which was set to 1.05 in our study, was multiplied to \tilde{P}_{k}^{a} in each iteration to maintain the sufficiently large background error covariance by empirically accounting for model noise (see equation (3)). Ensemble size N_{e} was set to 20.

350

The parameter values of parallelized RC used in this study is similar to Vlachas et al. (2020), but was slightly modified. Parameter settings used in the RC experiments are shown in Table 1. Jiang and Lai (2019) revealed that the performance of RC is sensitive to ρ and it needs to be tuned. We identified the proper value of ρ by sensitivity studies. Other parameters do not substantially affect the prediction accuracy, and we selected them based on the settings in previous works such as Vlachas et al. (2020). The nonlinear transformation function for the output layer in equation (13) is the same as 357 Chattopadhyay et al. (2020), which is represented as follows:

358
$$f(r_i) = \begin{cases} r_i & (i \text{ is odd})\\ r_{i-1} \times r_{i-2} & (i \text{ is even}) \end{cases}$$
(25)

where r_i is the *i*th element of r. Note that the form of the transformation function can be flexible; one can use a different form of the function to predict Lorenz 96 (Chattopadhyay et al., 2020), or the same function can be used to predict other systems (Pathak et al., 2017). In the prediction phase, we used the data for 100 timesteps before the prediction initial time for the reservoir spin up.

363

364 We implement numerical experiments to investigate the performance of RC-Obs, LETKF-Ext and RC-Anl to predict L96 dynamics. First, we evaluate the performance of RC-Obs under perfect 365 366 observations (all the grid points are observed with no error) and quantify the effect of the observation 367 imperfectness (i.e. observation error and spatio-temporal sparsity), to investigate the prediction skill 368 of the stand-alone use of RC and LETKF. Second, we evaluate the performance of RC-Anl. We 369 investigate the performance of RC-Anl and LETKF-Ext as the functions of the observation density 370 and model biases. 371 372 In each experiment, we prepare 200000 timesteps of Nature Run. The first 100000 timesteps are used 373 for the training of RC or for the spinning up of LETKF, and the rest of them are used for the evaluation

374 of each method. Every prediction is repeated 100 times to avoid the effect of the heterogeneity of data.

For the LETKF-Ext prediction, the analysis time series of all the evaluation data is firstly generated. Then, the analysis variables for one every 1000 timestep is taken as the initial conditions and total 100 prediction runs are performed. For the RC-Obs prediction, evaluation data are equally divided into 100 sets and the prediction is identically done for each set. For the RC-Anl prediction, the analysis time series of training data are used for training, and the prediction is performed using the same initial condition as LETKF-Ext. Each prediction set of LETKF-Ext, RC-Obs, and RC-Anl corresponds to the same time range.

382

383 The prediction accuracy of each method is evaluated by taking the average of RMSE of 100 sets for

ach timestep. We call this metric mean RMSE (*mRMSE*), and can be represented as follows:

385
$$mRMSE(t) = \frac{1}{100} \sum_{i=1}^{100} \sqrt{\frac{1}{m} \sum_{j=1}^{m} \left(u_j^{(i)}(t) - x_j^{(i)}(t) \right)^2}$$
(26)

where t is the number of the steps elapsed from the prediction initial time, $x_j^{(i)}(t)$ is the *j*th nodal value of the *i*th prediction set at time t and $u_j^{(i)}(t)$ is the corresponding value of Nature Run. Using this metric, we can see how the prediction accuracy is degraded as time elapses from initial time (so called "forecast lead time").

390

391 **4. Results**

392 Figure 4 shows the Hovmöller diagram of a prediction of RC-Obs and Nature Run. Figure 4 also

393	shows the difference between prediction and Nature Run, as well as the actual prediction results so
394	that we can see how long we can keep the prediction accurate. RC is trained with perfect observation
395	(e = 0 at all grid point). Figure 4 shows that RC-Obs predicts accurately within approximately 200
396	timesteps.

398	Figure 5 shows the time variation of the $mRMSE$ (see equation (26)) of RC-Obs with perfect
399	observation. It also shows that RC-Obs can predict with good accuracy for approximately 200
400	timesteps. It should be noted that LETKF (as well as other data assimilation methods) just replaces
401	the model's forecast with the initial conditions identical to Nature Run when all state variables can be
402	perfectly observed, and thus the prediction accuracy of LETKF-Ext will be perfect if we have no
403	model bias. LETKF-Ext is much superior to RC-Obs under this regime (not shown).
404	
405	Next, we evaluated the sensitivity of the prediction skill of both LETKF-Ext and RC-Obs to the
406	imperfectness of the observations. Figure 6a and 6b show the effect of the observation error on the
407	prediction skill. The value of observation error e is changed from 0.1 to 1.5 and the <i>mRMSE</i> time
408	series is drawn. We can see that LETKF-Ext is more sensitive to the increase of observation error than
409	RC-Obs, although the LETKF-Ext is superior in accuracy to RC-Obs within this range of observation
410	error.

412	However, RC-Obs showed a greater sensitivity to the density of observation points than LETKF-Ext.
413	Figures 7a and 7b show the sensitivity of the prediction accuracy of LETKF-Ext and RC-Obs,
414	respectively, to the number of observed grid points. Observation is reduced as uniformly as possible.
415	The observation network in each experiment is shown in Table 2. Even though we can observe a small
416	part of the system, the accuracy of LETKF-Ext changed only slightly. On the other hand, the accuracy
417	of RC-Obs gets worse when we remove a few observations. As assumed in the section 2.4, we verified
418	that RC-Obs is more sensitive to the observation sparsity than LETKF-Ext.
419	
420	We tested the prediction skill of our newly proposed method, RC-Anl, under perfect models and sparse
421	observations. Here, we used the observation error $e = 1.0$. Figure 8 shows the change of the <i>mRMSE</i>
422	time series of RC-Anl with the different number of observed grid points. It indicates that the
423	vulnerability of the prediction accuracy to the change of the number of observed grid points, which is
424	found in RC-Obs, no longer exists in RC-Anl. Although the prediction accuracy is lower than LETKF-
425	Ext (Figure 7a), our new method indicates a robustness to the observation sparsity and overcomes the
426	limitation of the stand-alone RC.
427	

428 Moreover, when the model used in LETKF is biased, RC-Anl outperforms LETKF-Ext. Figures 9a

and 9b show the change of the *mRMSE* time series when changing the model biases. The number of the observed points was set to 20. The *F* term in equation (1) was changed from the true value 8 (the *F* value of the model for Nature Run) to values in [5.0, 11.0] as the model bias, and the accuracy of LETKF-Ext and RC-Anl is plotted. The accuracy of LETKF-Ext was slightly better than that of RC-Anl when the model was not biased (F = 8; green line). However, when the bias is large (e.g. F =10; gray line), RC-Anl showed the better prediction accuracy.

435

436 We confirmed this result by comparing the *mRMSE* value of RC-Anl and LETKF-Ext at the specific 437 forecast lead-time. Figure 10 shows the value of mRMSE(80) (see equation (26)) as the function of 438 the value of the F term. Both two lines that show the skill of RC-Anl (blue) and LETKF-Ext (red) 439 are convex downward and have a minimum at F = 8, meaning that the accuracy of both prediction methods are the best when the model is not biased. In addition, as long as F value is in the interval 440 441 [7.5, 8.5], LETKF-Ext has the better accuracy than RC-Anl. However, if the model bias become larger 442 than that, RC-Anl becomes more accurate than LETKF-Ext. As the bias increases, the difference 443 between the mRMSE(80) of two methods becomes larger, and the superiority of RC-Anl becomes 444 more obvious. We found that RC-Anl can predict more accurately than LETKF-Ext when the model 445 is biased.

447	We also checked the robustness for the training data size. Figure 11 shows the change of the accuracy
448	of RC-Anl by changing the size of training data from 100000 to 10000 timesteps. We confirmed that
449	the prediction accuracy did not change until the size was reduced to 25000 timesteps. Although we
450	have used a large size of training data (100000 timesteps; 68 model years) so far, the results are robust
451	to the reduction of the size of the training data.
452	
453	5. Discussion
454	By comparing the prediction skill of RC-Obs and LETKF-Ext, we confirmed that RC-Obs can predict
455	with accuracy comparable to LETKF-Ext, if we have perfect observations. This result is consistent
456	with Chattopadhyay et al. (2020), Pathak et al. (2017), and Vlachas et al. (2020), and we can expect
457	that RC has a potential to predict various kinds of spatio-temporal chaotic systems.
458	
459	However, Vlachas et al. (2020) revealed that the prediction accuracy of RC is substantially degraded
460	when the observed grid points are reduced, compared to other machine learning techniques such as
461	LSTM. Our result is consistent with their study. In contrast, Chattopadhyay et al. (2020) showed that
462	RC can predict the multi-scale chaotic system correctly even though only the largest scale dynamics
463	is observed. Comparing these results, we can suggest that the states in the scale of dominant dynamics
464	should be observed almost perfectly to accurately predict the future state by RC.

466	Therefore, when we use RC to predict spatio-temporal chaotic systems with sparse observation data,
467	we need to interpolate them to generate the appropriate training data. However, the interpolated data
468	inevitably includes errors even if the observation data itself has no error, so it should be verified that
469	RC can predict accurately by training data with some errors. Previous works such as Chattopadhyay
470	et al. (2020), Pathak et al. (2017), or Vlachas et al. (2020) have not considered the impact of error in
471	the training data. We found that the prediction accuracy of RC degrades as the error in training data
472	grows, but the degradation rate is not so large (if all the training data of all the grid points are obtained).
473	We can expect from this result that RC trained with the interpolated observation data can predict
474	accurately to some extent, but the interpolated data should be as accurate as possible.
475	
476	In this study, LETKF was used to prepare the training data for RC, since LETKF can interpolate the
477	observations and reduce their error at the same time. We showed that our proposed approach correctly
478	works. Brajard et al. (2020) also made Convolutional Neural Network (CNN) learn the dynamics from
479	sparse observation data and successfully predict the dynamics of the L96 model. However, as
480	mentioned in the introduction section, Brajard et al. (2020) iterated the learning and data assimilation
481	until they converge, because it replaced the model used in data assimilation with CNN. Although their
482	model-free method has an advantage that it was not affected by the process-based model's

483	reproducibility of the phenomena, it can be computationally expensive since the number of iterates
484	can be relatively large. By contrast, we need to train RC just one time, because we use the process-
485	based model (i.e. data assimilation method) to prepare the training data. We overcome the problem of
486	computational feasibility.
487	
488	Note also that the computational cost to train RC is much cheaper than the other neural networks.
489	Since the framework of our method does not depend on a specific machine learning framework, we
490	believe that we can flexibly choose other machine learning methods such as RNN, LSTM, ANN, etc.
491	Previous studies such as Chattopadhyay et al. (2020) or Vlachas et al. (2020) revealed that these
492	methods show competitive performances compared to RC in predicting spatio-temporal chaos. Using
493	them instead of RC in our method would probably give similar results. However, the advantage of RC
494	is its cheap training procedure. RC does not need to perform an expensive back-propagation method
495	for training, unlike other neural networks (Chattopadhyay et al., 2020; Lu et al., 2017). Therefore, RC
496	is considered as a promising tool for predicting spatio-temporal chaos. Although our method has
497	flexibility in the choice of machine learning methods, we consider that the good performance with RC
498	is important in this research context.
499	

500 The good performance of our proposed method supports the suggestion of Dueben & Bauer (2018),

501 in which machine learning should be applied to the analysis data generated by data assimilation

- 502 methods as the first step of the application of machine learning to weather prediction. As Weyn et al.
- 503 (2019) did, we successfully trained the machine learning model with the analysis data.

504

505	Most importantly, we also found that the prediction by RC-Anl is more robust to the model biases than
506	the extended forecast by LETKF (i.e. LETKF-Ext). This result suggests that our method can be
507	beneficial in various real problems, as the model in real applications inevitably contains some biases.
508	Pathak et al. (2018a) developed the hybrid prediction system of RC and a biased model. Although
509	Pathak et al. (2018a) successfully predicted the spatio-temporal chaotic systems using the biased
510	models, they needed perfect observations to train their RC. The advantage of our proposed method
511	compared to these RC studies is that we allow both models and observation networks to be imperfect.
512	As in the review by Karniadakis et al. (2021), methodologies to train the dynamics from noisy
513	observational data by integrating data and physical knowledge are attracting attentions. In the NWP
514	context, some studies proposed methods to combine data assimilation and machine learning to emulate
515	the system dynamics from imperfect model and observations (e.g. Bocquet et al., 2019, 2020; Brajard
516	et al., 2020; Dueben and Bauer, 2018), and these approaches are getting popular. Our study
517	significantly contributes to this emerging research field.
518	

519	Although we tested our method only on 40-dimensional Lorenz 96 system, (Pathak et al., 2018b)
520	indicated that parallelized RC can be extended to predict the dynamics of substantially high
521	dimensional chaos such as 200-dimensional Kuramoto-Sivashinski equation with small computational
522	costs. Moreover, the applicability to the realistic NWP problems has also been discussed by their
523	sequel study (Wikner et al., 2020). These studies imply It implies that the findings of this study can
524	also be applied to higher dimensional systems.
525	
526	In NWP problems, it is often the case that homogenous observation data of high resolution are not
527	available over a wide range of time and space, which can be an obstacle to applying machine learning
528	to NWP tasks (Dueben & Bauer, 2018). We revealed that RC is robust for the temporal sparsity of
529	observations, and RC can be trained with relatively small training data sets.
530	
531	However, since the Lorenz 96 model (and other conceptual models such as Kuramoto-Sivashinski
532	equation) is ergodic, it is unclear that our method can be applied to real NWP problems directly, which
533	are possibly non-ergodic. Although our proposed method has a potential to extend to larger and more
534	complex problems, further studies are needed.
535	

537 **6.** Conclusion

538	The prediction skills of the extended forecast with LETKF (LETKF-Ext), RC that learned the
539	observation data (RC-Obs), and RC that learned the LETKF analysis data (RC-Anl) were evaluated
540	under imperfect models and observations, using the Lorenz 96 model. We found that the prediction by
541	RC-Obs is substantially vulnerable to the sparsity of the observation network. Our proposed method,
542	RC-Anl, can overcome this vulnerability. In addition, RC-Anl could predict more accurately than
543	LETKF-Ext when the process-based model is biased. Our new method is robust to the imperfectness
544	of both models and observations and we might obtain similar results higher dimensional and more
545	complexed systems. Further studies on more complicated models or operational atmospheric models
546	are expected.
547	
548	Code Availability
549	The source code for RC and Lorenz96 model is available at:

- 550 https://doi.org/10.5281/zenodo.3907291, and for LETKF at:
- 551 https://github.com/takemasa-miyoshi/letkf

552

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557

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- 649
- 650

Table 1. Parameter values of RC used in each experiment

Parameter	Description	Value
D_r	reservoir size	2000
а	Input matrix scale	0.5
d	adjacency matrix density	0.005
ρ	adjacency matrix spectral radius	1.0
β	ridge regression parameter	0.0001
g	number of reservoir groups	20
l	reservoir input overlaps	4

_

Table 2. Summary of three prediction frameworks

Name	Initial Value	Model for prediction
LETKF-Ext	LETKF analysis	the model used in LETKF
RC-Obs	observation	RC trained with observation
RC-Anl	LETKF analysis	RC trained with LETKF analysis

 Table 3. The indices of observed grid points.





657 Figure 1. The conceptual diagram of reservoir computing architecture. The network consists of an

658 input layer, a hidden layer called reservoir, and an output layer.



Figure 2. The conceptual diagram of parallelized reservoir computing architecture. The state space is





665 Figure 3. The algorithm flow of LETKF-Ext, RC-Anl, and RC-Obs. Solid and dotted lines show the

flow of variables and models (either process-based or data-driven surrogate), respectively.



667 **Figure 4.** The Hovmöller diagram of (a) Nature Run, (b) A prediction of RC-Obs, (c) difference of (a)

and (b). Horizontal axis shows the timesteps and vertical axis shows the nodal number. Value at each

timestep and node is represented by the color.

670



671 **Figure 5**. The *mRMSE* time series of the predictions of RC-Obs with perfect observation. Horizontal

672 axis shows the timestep and vertical shows the value of *mRMSE*.

673

674



675 Figure 6. The *mRMSE* time series of the predictions of (a)LETKF-Ext and (b)RC-Obs with noisy

676 observation. Each color corresponds to the observation error indicated by the legend.



Figure 7. The *mRMSE* time series of the predictions of (a)LETKF-Ext and (b)RC-Obs with spatially

680 sparse observation. Each color corresponds to the number of the observation points.



Figure 8. The same as figure4, for the RC-Anl prediction.



685 Figure 9. The *mRMSE* time series of the predictions of (a)LETKF-Ext and (b)RC-Anl with biased

686 model. Each color corresponds to each value of *F* term.

687



688 Figure 10. The *mRMSE(80)* of the predictions of LETKF-Ext(red) and RC-Anl(blue) for each model

bias. Horizontal axis shows the value of the force parameter of equation (1) (8 is the true value) and

690 vertical axis shows the value of *mRMSE*.



691 **Figure 11**. The *mRMSE* time series of the predictions of RC-Anl with various length of training data,

692 with perfect observation and perfect model. Each color corresponds to the value of the size of training

693 data.