



A Local Particle Filter and Its Gaussian Mixture Extension Implemented with Minor Modifications to the LETKF

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15 Abstract. A particle filter (PF) is an ensemble data assimilation method that does not assume Gaussian error distributions. Recent studies proposed local PFs (LPFs), which use localization as in the ensemble Kalman filter, to apply the PF for highdimensional dynamics efficiently. Among others, Penny and Miyoshi developed an LPF in the form of the ensemble transform matrix of the Local Ensemble Transform Kalman Filter (LETKF). The LETKF has been widely accepted for various geophysical systems including numerical weather prediction (NWP) models. Therefore, implementing consistently with an

20 existing LETKF code is useful.

This study developed a software platform for the LPF and its Gaussian mixture extension (LPFGM) by making slight modifications to the LETKF code with a simplified global climate model known as Simplified Parameterizations, Primitive Equation Dynamics (SPEEDY). A series of idealized twin experiments were accomplished under the ideal model assumption. With large inflation by the relaxation to prior spread, the LPF showed stable filter performance with dense observations but

- 25 became unstable with sparse observations. The LPFGM showed more accurate and stable performances than the LPF with both dense and sparse observations. In addition to the relaxation parameter, regulating the resampling frequency and the amplitude of Gaussian kernels was important for the LPFGM. With a spatially inhomogeneous observing network, the LPFGM was superior to the LETKF in sparsely observed regions where the background ensemble spread and non-Gaussianity are larger. The SPEEDY-based LETKF, LPF, and LPFGM systems were available as open-source software on Github
- 30 (https://github.com/skotsuki/speedy-lpf) and can be adapted to various models relatively easily like the LETKF.

Short Summary. Data assimilation takes an important part in numerical weather prediction (NWP) to combine forecasted states and millions of observations. While data assimilation methods in NWP usually assume the Gaussian error distribution,







some variables in the atmosphere are known to have non-Gaussian error statistics such as precipitation. This study extended a 35 widely used ensemble data assimilation algorithm for enabling to assimilate more non-Gaussian observations.

1 Introduction

Ensemble data assimilation (DA) has been broadly applied in geoscience fields such as weather and ocean predictions. The ensemble Kalman filter (EnKF) has been intensely investigated for the past two decades, such as for the perturbed observation method (Evensen, 1994; Burgers et al., 1998; Houtekamer and Mitchel, 1998) and ensemble square root filters

- 40 (e.g., Anderson, 2001; Bishop, 2001; Whitaker and Hamill, 2002; Hunt et al., 2007). The EnKF has advantages in flowdependent error estimates represented by an ensemble and in its relative ease of implementation to nonlinear dynamical systems such as numerical weather prediction (NWP) models. The degrees of freedom of dynamical models (e.g., $> O(10^8)$ for NWP models) are much larger than the typically affordable ensemble size ($< O(10^3)$). On the other hand, atmospheric and oceanic models shows local low dimensionality (Patil et al., 2001; Oczkowski et al. 2005), and practical EnKF with these systems uses
- 45 a localization technique that limits the impact of distant observations within a local area and reduces the effective degrees of freedom. Among various kinds of EnKFs, the local ensemble transform Kalman filter (LETKF; Hunt et al., 2007) is widely utilized in operational NWP centers in the same manner with the Deutscher Wetterdienst (DWD) and the Japan Meteorological Agency (JMA). Analysis updates of the LETKF are performed by multiplying the ensemble transform matrix by the prior ensemble perturbation matrix, following the ensemble transform Kalman filter (ETKF, Bishop et al. 2001).
- 50 The particle filter (PF) is another ensemble DA method broadly applicable to nonlinear and non-Gaussian problems (cf. van Leeuwen 2009 and van Leeuwen et al. 2019 for reviews on geoscience applications). The PF potentially solves some issues in EnKF, such as the nonlinear observation operator and non-Gaussian likelihood functions (Penny and Miyoshi, 2016). For example, assimilating precipitation observations with a standard EnKF is difficult partly because of their non-Gaussian errors (Lien et al., 2013, 2016; Kotsuki et al., 2017a). The PF can treat such variables with non-Gaussian errors properly.
- 55 Several PF methods have been explored for low-dimensional problems in early studies (Gordon et al. 1993; van Leeuwen et al. 2009). However, applying the PF to high-dimensional dynamical systems is generally difficult because the number of particles or the ensemble size need to be increased exponentially with the system size to avoid a weight collapse in which very few particles occupy most of the weights (Snyder et al., 2008, 2015). If a weight collapse occurs, the PF loses the diversity of the particles after resampling. Therefore, we need to assure that the weights are similarly distributed among particles. Previous
- 60 studies developed the equivalent-weights particle filter (ETPF; van Leeuwen et al. 2010; Ades and van Leeuwen 2013, 2015; Zhu et al. 2016) to avoid a weight collapse by using the proposal density to drive the particles toward the high-probability region of the posterior.

Alternatively, the local particle filter (LPF) uses localization to avoid a weight collapse by limiting the impact of observations within a local domain. Localization is a well-adopted method in EnKF to treat sampling errors due to a limited

65 ensemble size. Several LPFs have been proposed to apply the PF efficiently to high-dimensional systems (e.g., Bengston et





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al., 2003; van Leeuwen, 2009; Poterjoy, 2016; Penny and Miyoshi, 2016; Poterjoy and Anderson, 2016; Farchi and Bocquet, 2018; van Leeuwen et al. 2019). Among them, Penny and Miyoshi (2016) developed an LPF by means of the ensemble transform matrix of the LETKF. The LETKF has been commonly used for diverse geophysical systems, and consistent implementation with an available LETKF code would be useful. The DWD implemented the LPF in an operational global model based on the operational LETKF code and described stable performance in the operational setting (Potthast et al., 2019).

Walter and Potthast (2022; hereafter WP22) extended the LPF to the Gaussian mixture for further improvements.

The goal of this study is to develop and provide a software platform to accelerate research on LPF and its Gaussian mixture extension (hereafter, LPFGM). Although many studies on LPF have used simple idealized chaotic models, such as the 40-variable Lorenz model (hereafter, "L96"; Lorenz, 1996; Lorenz and Emanuel, 1998), the present study uses a simplified

- 75 atmospheric general circulation model defined as the Simplified Parameterizations, Primitive Equation Dynamics (SPEEDY) model (Molteni, 2003). Miyoshi (2005) coupled the LETKF with the SPEEDY model for the first time, and the source code is accessible at https://github.com/takemasa-miyoshi/letkf. This study extends the SPEEDY-LETKF code and implements the LPF and LPFGM. As demonstrated below, the LPF and LPFGM can be implemented easily with simple modifications to the existing LETKF code.
- 80 The remainder of this paper is organized as follows. Section 2 explains the mathematical formulation of the LETKF, LPF, and LPFGM, followed by the description of specific modifications made to the existing LETKF code. Section 3 presents the experimental settings. Section 4 outlines the results and discussions. Lastly, section 5 provides a summary.

2 Methodology

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2.1 Local ensemble transform Kalman filter

B5 Hunt et al. (2007) introduced the LETKF as a computationally efficient EnKF by combining the local ensemble Kalman filter (Ott et al., 2004) and ETKF (Bishop et al., 2001). Let \mathbf{X}_t be a matrix composed of *m* ensemble state vectors. The ensemble mean vector and perturbation matrix of \mathbf{X}_t are given by $\bar{\mathbf{x}}_t$ ($\in \mathbb{R}^n$) and $\mathbf{Z}_t \equiv \left\{ \mathbf{x}_t^{(1)} - \bar{\mathbf{x}}_t, \dots, \mathbf{x}_t^{(m)} - \bar{\mathbf{x}}_t \right\}$ ($\in \mathbb{R}^{n \times m}$), respectively, where *n* is the system size. The subscript *t* indicates the time, and the superscript (*i*) denotes the *i*th ensemble member. The analysis equations of the LETKF are specified by:

$$\mathbf{X}^{a}_{t,LETKF} = \bar{\mathbf{x}}^{b}_{t} \cdot \mathbf{1} + \mathbf{Z}^{b}_{t} \mathbf{T}_{t,LETKF},\tag{1}$$

$$\mathbf{\Gamma}_{t,LETKF} = \widetilde{\mathbf{P}}_{t}^{a} (\mathbf{Y}_{t}^{b})^{\mathrm{T}} \mathbf{R}_{t}^{-1} \left(\mathbf{y}_{t}^{o} - \overline{H_{t}(\mathbf{X}_{t}^{b})} \right) \cdot \mathbf{1} + \left[(m-1) \widetilde{\mathbf{P}}_{t}^{a} \right]^{1/2}, \tag{2}$$

where 1 is a row vector whose all elements are 1 ($\in \mathbb{R}^m$), **T** is the ensemble transform matrix ($\in \mathbb{R}^{m \times m}$), $\widetilde{\mathbf{P}}$ is the error covariance matrix in the ensemble space ($\in \mathbb{R}^{m \times m}$), $\mathbf{Y} \equiv \mathbf{HZ}$ is the ensemble perturbation matrix in the observation space ($\in \mathbb{R}^{p \times m}$), **R** is the observation error covariance matrix ($\in \mathbb{R}^{p \times p}$), **y** is the observation vector ($\in \mathbb{R}^p$), **H** is the linear observation

95 operator matrix ($\in \mathbb{R}^{p \times n}$), and *H* is the observation operator that may be nonlinear. Here, *p* is the number of observations. The





superscripts *o*, *b*, and *a* denote the observation, background (prior), and analysis (posterior), respectively. Transform matrix \mathbf{T}_{LETKF} denotes the ensemble transform matrix of the LETKF. The first and second terms of the right-hand side of Eq. (2) correspond to the updates of ensemble mean and perturbation, respectively. The ETKF computes the analysis error covariance matrix in the ensemble space $\mathbf{\tilde{P}}_{t}^{a}$ by:

$$\widetilde{\mathbf{P}}_{t}^{a} = [(m-1)\mathbf{I}/\beta + (\mathbf{Y}_{t}^{b})^{\mathrm{T}}\mathbf{R}_{t}^{-1}\mathbf{Y}_{t}^{b}]^{-1},$$
(3)

where β is a multiplicative inflation factor. Equations (1) and (2) are derived from the Kalman filter equations given by:

$$\bar{\mathbf{x}}_t^a = \bar{\mathbf{x}}_t^b + \mathbf{K}_t \left(\mathbf{y}_t^o - H_t(\mathbf{X}_t^b) \right),\tag{4}$$

$$\mathbf{K}_t = \mathbf{P}_t^b \mathbf{H}_t^{\mathsf{T}} (\mathbf{H}_t \mathbf{P}_t^b \mathbf{H}_t^{\mathsf{T}} + \mathbf{R}_t)^{-1} = \mathbf{P}_t^a \mathbf{H}_t^{\mathsf{T}} \mathbf{R}_t^{-1},$$
(5)

$$\mathbf{P}_t^a = (\mathbf{I} - \mathbf{K}_t \mathbf{H}_t) \mathbf{P}_t^b, \tag{6}$$

105 where **K** is the Kalman gain $(\in \mathbb{R}^{n \times p})$ and **P** is the error covariance matrix in the model space $(\in \mathbb{R}^{n \times n})$. The EnKF approximates the error covariance matrix by $\mathbf{P} \approx \frac{1}{m-1} \mathbf{Z}(\mathbf{Z})^{\mathrm{T}}$. Hunt et al. (2007) provides more details on deriving Eqs. (1) and (2) from the Kalman filter equations. For nonlinear observation operators, the following approximation is used:

$$\mathbf{Y} \equiv \mathbf{H}\mathbf{Z} \approx H(\mathbf{X}) - \overline{H(\mathbf{X})} \cdot \mathbf{1}.$$
 (7)

The LETKF provides $\widetilde{\mathbf{P}}_{t}^{a}$ and $(\widetilde{\mathbf{P}}_{t}^{a})^{1/2}$ of Eq. (2) by solving the eigenvalue decomposition of $(\widetilde{\mathbf{P}}_{t}^{a})^{-1} = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^{\mathsf{T}}$, where 110 U is a square matrix ($\in \mathbb{R}^{m \times m}$) composed of eigenvectors, and $\mathbf{\Lambda}$ is a diagonal matrix ($\in \mathbb{R}^{m \times m}$) composed of the corresponding eigenvalues. The eigenvalue decomposition leads to $\widetilde{\mathbf{P}}_{t}^{a} = \mathbf{U}\mathbf{\Lambda}^{-1}\mathbf{U}^{\mathsf{T}}$ and $(\widetilde{\mathbf{P}}_{t}^{a})^{1/2} = \mathbf{U}\mathbf{\Lambda}^{-1/2}\mathbf{U}^{\mathsf{T}}$.

The localization is practically important for mitigating sampling errors in the ensemble-based error covariance with a limited ensemble size (Houtekamer and Zhang, 2016). With localization, the LETKF computes the transform matrix T_{LETKF} at every model grid point independently by assimilating a subset of observations within the localization cut-off radius. The LETKF employs localization by inflating the observation error variance so that observations distant from the analysis model

grid point have fewer impacts (Hunt et al., 2007; Miyoshi and Yamane, 2007).

For local analysis schemes, a spatially smooth transition of the transform matrix \mathbf{T}_{LETKF} is essential to prevent abrupt changes in the analyses of neighboring grid points. The LETKF realizes a smooth transition of the transform matrix by using the symmetric square root of $\mathbf{\tilde{P}}_{t}^{a}$ (Hunt et al., 2007).

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The EnKF generally underestimates the error variance mainly because of model errors, nonlinear dynamics, and limited ensemble size. Therefore, a covariance inflation technique is used to inflate the underestimated error variance (Houtekamer and Mitchell, 1998). Among several kinds of covariance inflations methods, the present study considers multiplicative inflation (Anderson and Anderson, 1999) and relaxation to prior (Zhang et al., 2004). In multiplicative inflation, the ensemble-based covariance is multiplied by a factor $\beta (\mathbf{P}^b \rightarrow \beta \mathbf{P}^b)$. This multiplicative inflation is employed in Eq. (3) in



- Geoscientific Model Development Discussions
- 125 the LETKF. In this study, the LETKF experiments use the approach of Miyoshi (2011) which adaptively estimates a spatially varying inflation factor on the basis of the innovation statistics of Desroziers et al. (2005). In realistic problems, covariance relaxation methods are often used to inflate the posterior perturbation (e.g., Terasaki et al. 2019; Kotsuki et al., 2019b). This study utilizes the relaxation to prior spread (RTPS; Whitaker and Hamill, 2012) given by:

$$\mathbf{Z}_{t(k)}^{a} \leftarrow \left((1-\alpha) + \alpha \frac{\sigma_{t(k)}^{b}}{\sigma_{t(k)}^{a}} \right) \mathbf{Z}_{t(k)}^{a}, \tag{8}$$

130 where α is the RTPS parameter, and σ is the ensemble spread. The subscript (*k*) denotes the *k*th model variable or the *k*th component of state vector. Although this study uses only multiplicative inflation for the LETKF experiments, the posterior error perturbation is inflated by RTPS for LPF and LPFGM.

2.2 Local particle filter with ensemble transform matrix

Here, we describe the LPF in the form of the ensemble transform matrix of the LETKF (Reich, 2013; Penny and Miyoshi, 2016; Potthast et al. 2019). The PF is a direct Monte Carlo realization of Bayes' theorem given by:

$$\pi(\mathbf{x}_{t}|\mathbf{y}_{1:t}^{o}) = \frac{\pi(\mathbf{y}_{t}^{o}|\mathbf{x}_{t})\pi(\mathbf{x}_{t}|\mathbf{y}_{1:t-1}^{o})}{\pi(\mathbf{y}_{t}^{o}|\mathbf{y}_{1:t-1}^{o})},\tag{9}$$

where $\pi(\mathbf{x}_t | \mathbf{y}_{1:t}^o)$ is the probability of state \mathbf{x} given all observations \mathbf{y}^o up to time *t*. The PF approximates the prior probability density function (PDF), which appears in the numerator of Eq. (9), using an ensemble forecast:

$$\pi_{LPF}(\mathbf{x}_t | \mathbf{y}_{1:t-1}^o) \approx \sum_{i=1}^m w_t^{b(i)} \delta(\mathbf{x}_t - \mathbf{x}_t^{b(i)}),$$
(10)

140 where δ is the Dirac's delta function and $w^{b(i)}$ is the prior weight of the *i*th particle (i.e., ensemble member) at the previous analysis time. If particles are resampled at the previous analysis time, all particles have the same weight $w^{b(i)} = 1/m$ (i = 1, ..., m). The sum of the weights $\sum_{i=1}^{m} w_t^{a,b(i)}$ is always 1. The denominator of the right-hand side of Eq. (9) can be estimated by:

$$\pi(\mathbf{y}_{t}^{o}|\mathbf{y}_{1:t-1}^{o}) = \int \pi(\mathbf{y}_{t}^{o}|\mathbf{x}_{t})\pi(\mathbf{x}_{t}|\mathbf{y}_{1:t-1}^{o})d\mathbf{x}_{t} \approx \sum_{i=1}^{m} w_{t}^{b(i)}\pi(\mathbf{y}_{t}^{o}|\mathbf{x}_{t}^{b(i)}).$$
(11)

145 This study assumes a Gaussian likelihood function given by:

$$\pi(\mathbf{y}_t^o|\mathbf{x}_t) \propto \exp\left[-\frac{1}{2}(H_t(\mathbf{x}_t) - \mathbf{y}_t^o)^{\mathsf{T}} \mathbf{R}_t^{-1}(H_t(\mathbf{x}_t) - \mathbf{y}_t^o)\right].$$
(12)

Then, the posterior can be expressed by:

$$\pi_{LPF}(\mathbf{x}_t|\mathbf{y}_{1:t}^o) \approx \sum_{i=1}^m w_t^{a(i)} \delta(\mathbf{x}_t - \mathbf{x}_t^{b(i)}),\tag{13}$$

$$w_t^{a(i)} = w_t^{b(i)} \pi_{LPF} (\mathbf{y}_{1:t}^o | \mathbf{x}_t^{b(i)}) / \sum_{j=1}^m w_t^{b(i)} \pi_{LPF} (\mathbf{y}_{1:t}^o | \mathbf{x}_t^{b(j)}) = w_t^{b(i)} q_t^{(i)} / \sum_{k=1}^m w_t^{b(k)} q_t^{(k)},$$
(14)



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$$q_t^{(l)} = \exp\left[-\frac{1}{2} \left(H_t(\mathbf{x}_t^{b(l)}) - \mathbf{y}_t^o\right)^{\mathsf{T}} \mathbf{R}_t^{-1} \left(H_t(\mathbf{x}_t^{b(l)}) - \mathbf{y}_t^o\right)\right],\tag{15}$$

where q is the likelihood. Equation (14) results in posterior weights that satisfy $\sum_{i=1}^{m} w_t^{a(i)} = 1$.

To mitigate weight collapse, the local PF (LPF) solves the PF equations by assimilating local observations surrounding the analysis grid point. This study uses Penny and Miyoshi (2016)'s approach that computes the analysis at every model grid point independently with the observation error covariance R being inflated by the inverse of a localization function

155 as in the LETKF (Penny and Miyoshi, 2016).

Sampling importance resampling (SIR) is a technique for applying the PF for high-dimensional dynamics with a limited amount of particles. The resampling process rearranges the particles to effectively represent the densest areas of the posterior PDF. After resampling, each particle has equal weights and the posterior PDF is given by:

$$\pi_{LPF}(\mathbf{x}_t | \mathbf{y}_{1:t}^o) \approx \frac{1}{m} \sum_{i=1}^m \delta(\mathbf{x}_t - \mathbf{x}_t^{a(i)}).$$
(16)

160 The resampling process can be expressed equally valid to the ensemble transform matrix of the ETKF (Reich, 2013; Penny and Miyoshi, 2016) given by:

$$\mathbf{X}_{t,LPF}^{a} = \mathbf{X}_{t}^{b} \mathbf{T}_{t,LPF} = (\bar{\mathbf{x}}_{t}^{b} \cdot \mathbf{1} + \mathbf{Z}_{t}^{b}) \mathbf{T}_{t,LPF} = \bar{\mathbf{x}}_{t}^{b} \cdot \mathbf{1} + \mathbf{Z}_{t}^{b} \mathbf{T}_{t,LPF}.$$
(17)

where \mathbf{T}_{LPF} denotes the ensemble transform matrix of the LPF. Here, we applied $(\bar{\mathbf{x}}_t^b \cdot \mathbf{1})\mathbf{T}_{t,LPF} = \bar{\mathbf{x}}_t^b \cdot \mathbf{1}$ based on the following necessary condition of the ensemble transform matrix for the LPF:

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$$\sum_{i=1}^{m} \mathbf{T}_{t,LPF}^{(i,j)} = 1, \qquad j = 1,...,m$$
 (18)

In addition to Eq. (18), the ideal resampling matrix satisfies the following two conditions:

•
$$\sum_{j=1}^{m} \mathbf{T}_{t,LPF}^{(i,j)} = m \cdot w_t^{a(i)}, \qquad i = 1, \dots, m$$
$$\Leftrightarrow \bar{\mathbf{x}}_t^b = \sum_{i=1}^{m} \mathbf{x}_t^{b(i)} \cdot w_t^{a(i)} \qquad , \tag{19}$$

spatially smooth transition of $\mathbf{T}_{t.LPF}$.

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The resampling matrix significantly affects the filter performance (Farchi and Bocquet, 2018). The present study constructs resampling matrices based on the Monte-Carlo approach. This resampling method uses m random numbers $\mathbf{r}^{(i)}$ (i = 1, ..., m) drawn from uniform distribution U([0,1]) and accumulated weights $w_{t,acc}$:

$$w_{t,acc}^{(0)} = 0, \qquad w_{t,acc}^{(i)} = w_{t,acc}^{(i-1)} + w_t^{a(i)}, \qquad i = 1, \dots, m.$$
 (20)

By definition, $w_{t,acc}^{(m)}$ is 1. After sorting **r** to be the ascending order **r**_{sorted}, we generate the resampling matrix using **Algorithm** 1.75 1. This procedure is similar to the resampling of Potthast et al. (2019), but it employs an additional treatment so that the resampling matrix is close to the identity matrix (line 10 of Algorithm 1; Fig. 1 b and c).



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Classical resampling can produce the same particles resulting in the loss of diversity of posterior particles. Therefore, additional treatments are required to generate slightly different posterior particles. Potthast et al. (2019) proposed adding Gaussian random noise to $\mathbf{T}_{t,LPF}$ to prevent the generation of the same particles. As an alternative, the present study uses the

- 180 Monte-Carlo approach that repeats Algorithm 1 many times with different random numbers and takes the average of the generated resampling matrices (Fig. 1). Using different random numbers r, the resampling matrices differ (Fig. 1 b, c) even if the same weight is used (Fig. 1 a). By averaging the resampling matrices generated by using different random numbers, we get matrices that have higher weights in the diagonal components and lower weights in the off-diagonal components (Fig. 1 d, e). The Monte-Carlo approach makes the resampling matrix closer to the identity matrix, which is beneficial for a smooth
- 185 transition in space. In addition, this stochastic approach approximates Eq. (19) using the Monte-Carlo approach. The generated transform matrix with 200 samples (Fig. 1 c) is close to that with 10,000 samples (Fig. 1 d) in the case of 40 particles. Therefore, the transformation matrices are generated by averaging 200 sampled matrices in subsequent LPF experiments. Hereafter, we call this resampling method "MC resampling" which is used in the following experiments.

The effective particle size N_{eff} (Kong et al., 1994) is useful to measure the diversity of particles in LPF:

$$N_{t,eff} = 1/\sum_{i=1}^{m} {\binom{u^{a(i)}}{t}}^2 \in [1,m].$$
⁽²¹⁾

If N_{eff} is sufficiently large ($N_{eff} \approx m$), no resampling is needed. This study considers a tunable parameter N_0 as a criterion for resampling:

$$\mathbf{T}_{t,LPF} \leftarrow \begin{cases} \mathbf{I} & if \quad N_{t,eff} > N_0 \\ \mathbf{T}_{t,LPF} & else \end{cases}.$$
(22)

Without resampling $(N_{t,eff} > N_0)$, the posterior weight is succeeded for the subsequent forecast as follows:

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$$\mathbf{w}_{t+1}^b \leftarrow (1-\tau) \cdot \mathbf{w}_t^a + \tau/m, \tag{23}$$

where τ is the tunable forgetting factor $\tau \in [0: 1]$. This weight succession (Eq. 23) can be interpreted as a temporal localization that reduces the impact of observations distant from the assimilation time. Here, the weight succession in *local* PF is not trivial because the weight (or likelihood of particles) would move with the dynamical flow. Similar discussions can be found for the advection of localization functions (e.g., Ota et al., 2013; Kotsuki et al. 2019a). This study assumes no flow motion of the weights and simply use Eq. (23) at each grid point independently.

200 weights and simply

Although the LETKF applies inflation to the prior error covariance (i.e., $\mathbf{P}^b \rightarrow \beta \mathbf{P}^b$), this inflation is suboptimal to the LPF partly because the weight collapse occurs more easily if multiplicative inflation is applied to the prior perturbation (cf. Eq. 15). Therefore, the LPF usually applies inflation to the posterior particles (e.g., Farchi and Bocquet 2018). The present study uses the RTPS to inflate posterior perturbations for the LPF. We do not use the RTPS for the LETKF experiments since

205 the Miyoshi (2011)'s adaptive multiplicative inflation is known to outperform the manually-tuned RTPS for idealized twin experiments with SPEEDY based on authors' preliminary experiments and personal communication (Ota et al. 2021).







Preliminary experiments showed that the RTPS outperformed the relaxation to prior perturbation (RTPP; Zhang et al., 2004) for the LPF. Having some noise in the transform matrix is important, so that the LPF can maintain the diversity of posterior particles. The RTPP makes the transform matrix closer to the identity matrix, resulting in less diverged posterior particles. Therefore, the RTPS would be a more suitable relaxation method than the RTPP for LPF.

2.3 LPF with Gaussian mixture extension

Assimilating too many independent observations in the local area is not desirable for the LPF to avoid weight collapse (van Leuuwen et al., 2019). To solve this problem, hybrid algorithms of EnKF and PF have been explored to efficiently assimilate massive observation data. The Gaussian mixture extension of the LPF is a kind of such hybrid algorithms (Hoteit et

215 al. 2008; Stordal et al., 2011; WP22). In the Gaussian mixture extension, the previous PDF is approximated by a combination of Gaussian distributions centered at the values of the particles, given by:

$$\pi_{LPFGM}(\mathbf{x}_t|\mathbf{y}_{i:t-1}^o) \approx \sum_{t=1}^m w_t^{b(t)} N(\mathbf{x}_t^{b(t)}, \widehat{\mathbf{P}}_t^b), \tag{24}$$

where $N(\mathbf{x}_t^{b(i)}, \hat{\mathbf{P}}_t^b)$ is the Gaussian kernel with mean $\mathbf{x}_t^{b(i)}$ and covariance $\hat{\mathbf{P}}_t^b$. Here, hut indicates matrices for the Gaussian kernels (e.g., prior error covariance $\hat{\mathbf{P}}^b$, observation error covariance $\hat{\mathbf{R}}$ and Kalman gain $\hat{\mathbf{K}}$). The covariance of the Gaussian kernel were the covariance and the transformation of the formula of

220 kernel uses the sampled covariance matrix \mathbf{P}_t^b such that:

$$\widehat{\mathbf{P}}_{t}^{b} = \gamma \mathbf{P}_{t}^{b} \approx \frac{\gamma}{m-1} \mathbf{Z}_{t}^{b} (\mathbf{Z}_{t}^{b})^{\mathsf{T}}, \tag{25}$$

where γ (>0) is a tunable parameter that regulates the amplitude and width of the Gaussian kernel (i.e., uncertainty of particles). For example, larger γ reduces amplitude and increases width of the Gaussian kernel.

The Gaussian mixture performs a two-step update to obtain the posterior particles. The first update moves the center of the Gaussian kernel with observations. Since kernels are Gaussian, we can use the Kalman filter for the first update:

$$\mathbf{x}_{t}^{a(i)} = \mathbf{x}_{t}^{b(i)} + \widehat{\mathbf{K}}_{t} \left(\mathbf{y}_{t}^{o} - H(\mathbf{x}_{t}^{b(i)}) \right), \qquad (i = 1, \dots, m)$$

$$\Leftrightarrow \mathbf{X}_{t,GM}^{a} = \mathbf{X}_{t}^{b} + \widehat{\mathbf{K}}_{t} \left(\mathbf{y}_{t}^{o} \cdot \mathbf{1} - H_{t}(\mathbf{X}_{t}^{b}) \right), \qquad (26)$$

where $\hat{\mathbf{K}} = \hat{\mathbf{P}}^{a} \mathbf{H}^{T} \mathbf{R}^{-1}$ as in Eq. (5). In the LETKF, the Kalman gain **K** is computed by $\mathbf{K} = \mathbf{P}^{a} \mathbf{H}^{T} \mathbf{R}^{-1} \approx \frac{1}{m-1} \mathbf{Z}^{b} \tilde{\mathbf{P}}^{a} (\mathbf{Z}^{b})^{T} \mathbf{H}^{T} \mathbf{R}^{-1}$. Since the Gaussian kernel uses the ensemble-based error covariance (Eq. 25), we can apply the exact algorithms of the LETKF by replacing β of Eq. (3) with γ . Consequently, Eq. (26) is equivalent to:

$$\mathbf{X}_{t,GM}^{a} = \bar{\mathbf{x}}_{t}^{b} \cdot \mathbf{1} + \mathbf{Z}_{t}^{b} \mathbf{T}_{t,GM},\tag{27}$$

where

$$\mathbf{S}_{t} = \widetilde{\mathbf{P}}_{t}^{a} (\mathbf{Y}_{t}^{b})^{\mathsf{T}} \mathbf{R}_{t}^{-1} \left(\mathbf{y}_{t}^{o} \cdot \mathbf{1} - H_{t} (\mathbf{X}_{t}^{b}) \right), \text{ and}$$

$$\tag{28}$$





$$\mathbf{T}_{t,GM} = \mathbf{S}_t + \mathbf{I}.$$
(29)

235 Here, \mathbf{T}_{GM} denotes the ensemble transform matrix of the Gaussian mixture.

The second update resamples the particles based on the likelihood of the posterior kernel given by:

$$q_t^{(i)} = \exp\left[-\frac{1}{2}\left(H_t(\mathbf{x}_t^{b(i)}) - \mathbf{y}_t^o\right)^{\mathrm{T}} \widehat{\mathbf{R}}_t^{-1}\left(H_t(\mathbf{x}_t^{b(i)}) - \mathbf{y}_t^o\right)\right],\tag{30}$$

where

$$\mathbf{R}_t = \mathbf{R}_t + \mathbf{H}_t \mathbf{P}_t^{D} \mathbf{H}_t^{T}. \tag{31}$$

Hoteit et al. (2008) and Stordal et al. (2011) used Equation (30) for computing the likelihood of posterior kernels. Alternatively, WP22 suggested that using Eq. (15) instead of Eq. (30) is a reasonable approximation in the case of a smaller variance of $\hat{\mathbf{P}}_t^b$ compared to the observation departure $H_t(\mathbf{x}_t^{b(i)}) - \mathbf{y}_t^o$. This study follows the WP22's approximation because computing inverse of Eq. (31) is computationally much more expensive than computing inverse of diagonal **R**. Using WP22's approximation, the solution of the LPFGM is given by:

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$$\mathbf{X}_{t,LPFGM}^{a} = \mathbf{X}_{t,GM}^{a} \mathbf{T}_{t,LPF} = \left(\bar{\mathbf{x}}_{t}^{b} \cdot \mathbf{1} + \mathbf{Z}_{t}^{b} \mathbf{T}_{t,GM} \right) \mathbf{T}_{t,LPF} = \bar{\mathbf{x}}_{t}^{b} \cdot \mathbf{1} + \mathbf{Z}_{t}^{b} \mathbf{T}_{t,GM} \mathbf{T}_{t,LPF}.$$
(32)

Here, we used $(\bar{\mathbf{x}}_{t}^{b} \cdot \mathbf{1})\mathbf{T}_{t,LPF} = \bar{\mathbf{x}}_{t}^{b} \cdot \mathbf{1}$ (cf. Eq. (18)). Consequently, the transform matrix of the LPFGM (\mathbf{T}_{LPFGM}) is given by:

$$\mathbf{T}_{t,LPFGM} = \mathbf{T}_{t,GM} \mathbf{T}_{t,LPF}.$$
(33)

Namely, the LPFGM can be described as the ensemble transform matrix form.

- The two-step update of the LPFGM may appear using the same observations twice, but this is not true. To understand the principles, here we consider a simple scalar example with H=1.0 with illustrations of Fig. 2. Let $\pi(y_t^o)$ be an observation PDF (Fig. 2 top row), and the prior and posterior PDFs of the LPF are given by $\pi_{LPF}(x_t) \approx \frac{1}{m} \sum_{i=1}^{m} \delta(x_t - x_t^{b(i)})$ and $\pi_{LPF}(x_t|y_t^o)$, respectively (Fig. 2a, 2nd and 3rd rows). The LPF employs resampling by approximating the posterior PDF as *a combination of prior particles* such that $\pi_{LPF}(x_t|y_t^o) \approx \sum_{i=1}^{m} w_t^{a(i)} \delta(x_t - x_t^{b(i)})$ (Fig. 2a, bottom row). Next, we focus on the 5th particle of the LPFGM (Fig. 2b). Prior and posterior PDFs of the 5th particle are given by $\pi(x_t^{(5)}) = N(x_t^{b(5)}, \hat{p}_t^b)$ and $\pi(x_t^{(5)}|y_t^o) = N(x_t^{b(5)}, \hat{p}_t^b) \cdot N(y_t^o, R_t)$, respectively (Fig. 2b, 2nd and 3rd rows). Since the Gaussian kernels are assumed for $f(x_t^{(5)}) = N(x_t^{b(5)}, \hat{p}_t^b) \cdot N(y_t^o, R_t)$, respectively (Fig. 2b, 2nd and 3rd rows). Since the Gaussian kernels are assumed for
- the prior particles, the center of the posterior kernel moves such that $\pi(x_t^{(5)}|y_t^o) \propto N(x_t^{a(5)}, \hat{P}_t^a)$, where $x_t^{a(5)}$ and \hat{P}_t^a can be computed by the Kalman filter (from the blue circle to the red circle in Fig. 2b). Since the LPFGM moves all particles, the posterior PDF of the LPFGM is given by $\pi_{LPFGM}(x_t|y_t^o) \approx \frac{1}{m} \sum_{i=1}^m \pi(x_t^{(i)}|y_t^o)$ (Fig. 2c, 3rd row). These movements correspond to the first update of the LPFGM. In contrast to the LPF, the posterior PDF of the LPFGM is approximated by *a* 260 *combination of the posterior Gaussian kernels* (red circles of Fig. 2c, 3rd row). The LPFGM employs the resampling based on
- the moved particles such that $\pi_{LPFGM}(x_t|y_t^o) \approx \sum_{i=1}^m w_t^{a(i)} N(x_t^{a(i)}, \hat{P}_t^a)$ (Fig. 2c, bottom row). This resampling corresponds





to the second update of the LPFGM. As seen in this example, the two-step update of the LPFGM does not use the same observations twice.

2.4 Implementation and computational complexity

265 We implemented the LPFGM based on the available LETKF code from Miyoshi (2005) and follow-on studies (Miyoshi and Yamane 2007, Kondo and Miyoshi 2019; Kotsuki et al. 2020; <u>https://github.com/takemasa-miyoshi/letkf</u>). Figure 3 compares the workflows of the LETKF, LPF, and LPFGM. All DA methods execute the same first four steps (steps A–D). After step D, the LETKF involves four additional steps (steps E–H) to compute **T**_{LETKF}. The LPF computes the weights of particles (step J), followed by the generation of the transform matrix **T**_{LPF} (step K). The LPFGM first executes steps E–G,

as in the LETKF, and then executes step I to compute \mathbf{T}_{GM} , followed by the LPF algorithms to compute \mathbf{T}_{LPF} (steps J and K). Finally, the LPFGM multiplies \mathbf{T}_{GM} and \mathbf{T}_{LPF} to compute \mathbf{T}_{LPFGM} (step L). At the end of the process, the transform matrix is applied to the prior perturbation matrix \mathbf{Z}^{b} to produce the analysis ensemble (step M), followed by the RTPS (step N).

If the LETKF code is available, the LPF in the transform matrix form can be developed by coding two steps J and K. The LPFGM can also be developed easily by coding two more steps I and L if the LETKF and LPF codes are available.

275

Here we compare the computational complexities of the LETKF, LPF and LPFGM algorithms (Table 1). The total cost (C_T) of a DA cycle is identical to the overhead of the assimilation system (C_H), plus *n* times the average local analysis cost (C_L), and *m* times the cost of one-member model forecast (C_M):

$$C_T(n, p, m) = C_H(n, p, m) + n \cdot C_L(p_L, m) + m \cdot C_M,$$
(34)

where p_L is the number of local observations within the localization cut-off radius. We assume that the overhead and model costs are equivalent among the three methods. In addition, the total computational cost of DA usually depends on the local analysis cost (C_L):

$$C_L^{LETKF} = O(m^3 + m^2 p_L), (35)$$

$$C_L^{LPF} = O(m^2 N_{MC}), \tag{36}$$

$$C_L^{LPFGM} = O(m^3 + m^2 p_L + m^2 N_{MC}), \tag{37}$$

where N_{MC} is the number of times the resampling matrices are generated by Algorithm 1. The number of local observations p_L is usually much greater than the ensemble size *m* and N_{MC} . In this case, $O(m^2 p_L)$ is dominant for the LETKF, and LPFGM.

The computational cost of LPF here is more expensive than that with a simpler resampling algorithm such as the stochastic uniform resampling (O(m); Penny and Miyoshi 2016, Farchi and Bocquet, 2018) due to the relatively complex **Algorithm 1** ($O(m^2 N_{MC})$). We could not use such simpler approaches in this study since they do not yield ideal resampling 290 matrices that satisfy the two conditions (Eq. 19 and spatially smooth transition of $\mathbf{T}_{t,LPF}$).





3 Experimental settings

3.1 SPEEDY model

This study used the intermediate global atmospheric general circulation model SPEEDY (Molteni, 2003) to compare the LETKF, LPF and LPFGM. The SPEEDY model is a computationally-inexpensive hydrostatic model with fundamental physical parameterization schemes such as surface flux, radiation, convection, cloud and condensation. The SPEEDY model has 96 × 48 grid points in the horizontal plane (T30 ~ 3.75° × 3.75°) and sigma-coordinate seven vertical layers. The SPEEDY consists of five prognostic variables: temperature (T), specific humidity (Q), zonal wind (U), and meridional wind (V) at seven layers, as well as surface pressure (Ps). Although running the SPEEDY model is, the model contains The SPEEDY model coupled with the LETKF (SPEEDY–LETKF) has been widely used in DA studies (Miyoshi 2005 and many follow-on studies, e.g., Miyoshi 2011; Kondo et al., 2013; Kondo and Miyoshi, 2016, 2019; Kotsuki and Bishop 2021). We implemented the

LPF and LPFGM based on the existing SPEEDY-LETKF code following the procedures described in section 2.4.

3.2 Experimental design

The experimental settings follow the previous SPEEDY–LETKF experiments (Miyoshi 2005 and follow-on studies, e.g., Kotsuki et al., 2020). A series of idealized twin experiments (also known as observing system simulation experiments) were conducted without model errors. We first performed a spin-up run for one year initialized by the standard atmosphere during rest, followed by the nature run started at 0000 UTC on January 1 of the second year. We assumed diagonal observation error covariance **R** (i.e., uncorrelated observation error). Gaussian noises were added to the nature run to produce observation data whose interval is 6 h. The standard deviations of the Gaussian noise are 1.0 K for T, 1.0 m s⁻¹ for U and V, 0.1 g kg⁻¹

for Q, and 1 hPa for surface pressure. This study considered two observing networks (Figs. 4 a and b): the regularly distributed network (hereafter REG2) and the radiosonde-like inhomogeneous network (hereafter RAOB). We observe T, U and V at every seven layers, whereas Q was observed at the 1st-4th layers. The ensemble size is 40 and their initial conditions were taken from an independent nature run.

Table 2 summarizes the settings of the LETKF, LPF, and LPFGM experiments. The observation error variance was inflated for the localization, by using the Gaussian-based function given by:

$$l = \begin{cases} \exp\left[-\frac{1}{2}\{(d_h/\rho_h)^2 + (d_v/\rho_v)^2\}\right] & \text{if } d_h < 2\sqrt{10/3}\rho_h \text{ and } d_v < 2\sqrt{10/3}\rho_v \\ 0 & \text{else} \end{cases}$$
(38)

where *l* is the localization function, and its inverse l^{-1} is multiplied and used to inflate **R**. d_h and d_v are horizontal and vertical distances (km and log(Pa)) between the observation and analysis grid point. ρ_h and ρ_v are tunable horizontal and vertical localization scales (km and log(Pa)). Subscripts *h* and *v* represent horizontal and vertical, respectively. This study set the vertical localization scale ρ_v be 0.1 log(Pa) following Greybush et al. (2011) and Kondo et al. (2013). The horizontal





320 localization scales of the LETKF were optimized manually before the experiments to minimize the first-guess root mean square error (RMSE) of the fourth layer temperature of the SPEEDY-LETKF.

The LETKF experiments used the adaptive multiplicative inflation method of Miyoshi (2011) in which the inflation factor β was estimated adaptively. On the basis of sensitivity experiments for γ , we chose $\gamma = 1.5$. Sensitivity to γ is discussed in section 4.3.3.

325 We first performed a one-year SPEEDY-LETKF experiment over the second year from January to December following the one-year spin-up. We then performed LETKF, LPF, and LPFGM experiments from January to April in the third year initialized by the first-guess ensemble of the LETKF at 0000 UTC on January 1 of the third year. The results from the last three months, i.e., February to April, were used for verification. We assessed the 6-h forecast or background RMSE for T at the fourth model level (~500 hPa) since this is among the most important variables for medium-range NWP. This study

330 mainly discusses the RMSE and ensemble spread for T, similar results are observed for other variables.

4 Results and discussion

4.1 Experiments with a regularly distributed observing network

We first compare the LETKF, LPF, and LPFGM with REG2 in which the manually-tuned horizontal localization scale for the LETKF is 600 km.

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First, sensitivities to the horizontal localization scale (ρ_h) and RTPS parameter (α) are investigated for the LPF. Figure 5 indicates the time-mean background RMSEs and ensemble spreads for LETKF and LPF. The LPF requires large inflation ($\alpha \ge 1.0$) to avoid filter divergence. With large inflation ($\alpha \ge 1.0$), the LPF experiment with $\rho_h = 600$ km resulted in the smallest RMSEs among the three LPF experiments. The optimal localization scale of LPF was found similar to that of the LETKF. The four LPF experiments exhibited larger RMSEs than the LETKF, as demonstrated by the previous studies with a low-

340 dimensional L96 model (Poterjoy, 2016; Penny and Miyoshi, 2016; Farichi and Bouquet, 2018). The LPF experiment with ρ_h = 700 km shows filter divergence when α = 1.0. The ensemble spreads of LPF are smaller than the RMSEs when α = 1.0. This under dispersive ensemble is a typical behavior of LPF (e.g., Poterjoy and Anderson 2016).

Second, we compare the time series of the background RMSEs, ensemble spreads, and effective particle sizes N_{eff} (Fig. 6). The RMSE and ensemble spread are consistent in the LETKF. However, the LPF shows generally smaller ensemble 345 spreads than the RMSEs. Since the beginning of the experiments on January 1, the three LPF experiments showed rapid increases in the ensemble spread (Fig. 6 a), and a rapid decrease in the effective particle size (Fig. 6 b) within two weeks. After the rapid changes, the ensemble spreads and effective particle sizes were stabilized. The three LPF experiments increased RMSEs until the beginning of March. The LPF with $\rho_h = 500$ km showed filter divergence in April. The LPF with $\rho_h = 400$ km and $\rho_h = 600$ km also showed increasing trends in RMSE until the end of April while their ensemble spreads and effective particle sizes were stable.





Next, sensitivities to the RTPS parameter (α), resampling frequency (N_0), and forgetting factor (τ) are investigated for the LPFGM. The optimal localization scale of LPF was identical to that of the LETKF (Fig. 5). Therefore, we choose the same 600-km localization scale for the LPFGM. Figure 7 compares the time-mean background RMSEs and ensemble spreads for LETKF and LPFGM. In the LPFGM experiments, we investigate two experimental settings: with weight successions (τ =

- 355 0.0, Figs. 7 a) and without weight successions ($\tau = 1.0$, Figs. 7 b). With weight successions (Fig. 7 a), the LPFGM shows RMSEs similar to those of LETKF with optimal parameters for α and N_0 . Regulating the resampling frequency (N_0) would be needed for LPFGM because the LPFGM shows filter divergence when resampling is employed at all assimilation steps excluding the case of $\alpha = 1.0$ (magenta line in Fig. 7 a). The LPFGM employs two ensemble updates: the Gaussian mixture and resampling. Owing to the first update by the Gaussian mixture, the LPFGM would not require resampling at all assimilation
- 360 steps. With weight succession, the optimal relaxation parameter α is approximately 0.6–0.9, excluding the case employing resampling at all assimilation steps.

Without weight succession, the RMSEs of the LPFGM are less sensitive to the resampling parameter N_0 and RTPS parameter α (Fig. 7 b), implying that the LPFGM is more stable without weight succession. Owing to the first update by the Gaussian mixture, succeeding weights may be unnecessary for the LPFGM. In addition, the method of succeeding weights in

- 365 the *local* PF is not trivial because the weights would move with the dynamical flow. While this study considers only two weight succession patterns for the LPFGM (i.e., τ = 0.0 or 1.0), the optimal parameter may exist in the definition range of the forgetting factor (τ ∈ [0:1]). Such additional investigations on the weight succession are important research directions for our future studies. Because the results of the LPFGM experiments without weight succession were superior to those with weight succession, the remainder of this paper focuses on the LPFGM experiments without weight succession.
- 370 The time series of background RMSEs, and effective particle sizes for LPFGM experiments show that the LPFGM with every-time resampling ($N_0 = 40$) exhibits large RMSEs and the smallest effective particle sizes (Fig. 8, magenta). In contrast, the LPFGM experiments with infrequent resampling ($N_0 = 10$, 5, and 2) show small RMSEs similar to that of the LETKF and maintain larger effective particle sizes than the LPF (Fig. 8, red, blue and green lines).
- Finally, we compare the spatial patterns of the RMSEs at a fourth model level for the LETKF, LPF, and LPFGM with 375 optimal parameter settings (Fig. 9). The LETKF and LPFGM show larger RMSEs in the tropics and polar regions (Figs. 9 a and c), possibly because of uncertainties from convective dynamics in the tropics and sparser observations in the polar regions. The LPF shows a larger RMSE than the LETKF globally (Fig. 9 b, d). By contrast, slight improvements were observed globally in the LPFGM relative to the LETKF as indicated by generally warm colors in Fig. 9 (e), especially around the North Pole.

4.2 Experiments with a realistic observing network

380 Here we compare the LETKF, LPF, and LPFGM with the realistic observing network RAOB. With this spatially inhomogeneous observing network, all LPF experiments showed filter divergence, even with a broad range of the localization and RTPS parameters. In addition, the LPFGM was unstable with weight succession. Therefore, this section focuses on the comparison of the LETKF and LPFGM without weight succession ($\tau = 1.0$) only.







First, sensitivities to the RTPS parameter (α) and resampling frequency (N_0) are investigated for the LPFGM. Figure 10 compares the time-mean background RMSEs and ensemble spreads for the LETKF and LPFGM. The optimal horizontal localization scale for the LETKF is 1100 km, and the same localization scale is used for the LPFGM. The LPFGM with everytime resampling ($N_0 = 40$) shows the largest RMSEs (Fig. 10 a, magenta). By contrast, some LPFGM experiments show smaller RMSEs than the LETKF (Fig. 10 b). In this experimental setting, the resampling parameter of $N_0 = 2.0$ shows the most stable performance. With $N_0 = 2.0$, the LPFGM outperforms the LETKF slightly for α =0.5–0.7 (green line of Fig. 10 b).

The time series of the background RMSEs and effective particle sizes show that the LPFGM with every-time resampling ($N_0 = 40$; Fig. 11 a, magenta), and relatively-frequent resampling ($N_0 = 10$; Fig. 11 a, red) caused filter divergences. The times when the filters diverged seem to correspond to the times when the effective particle sizes decreased (Fig. 11 b, magenta and red). This reduction in effective particle size is a typical sign of filter divergence for PF (Snyder et al., 2008). In contrast, the LPFGM experiments with infrequent resampling ($N_0 = 5$ and 2) show stable RMSEs and maintain a larger effective particle size. These stable LPFGM experiments maintain the amplitude of the ensemble spreads similar to that of the

We further explore regions where the LPFGM outperforms the LETKF. Figure 12 compares the space-based patterns of the background RMSEs for T (K) at the fourth model level for LETKF and LPFGM. Errors in sparsely recognized regions, such as the South Pacific Ocean, Indian Ocean, and polar regions, tend to be larger (Figs. 12 a and b). The LPFGM outperforms

400 the LETKF in such sparsely observed regions (Fig. 12 c). The regions showing improvements correspond to the regions where the ensemble spreads and first-guess non-Gaussianity are larger (Fig. 13). Here, we measure the non-Gaussianity by Kullback– Leibler divergence (Kullback and Leibler, 1951).

The first update of the LPFGM (the Gaussian mixture) is similar to the LETKF update as discussed. Therefore, the improvements of the LPFGM with respect to the LETKF would be owing to the resampling step. Previous studies demonstrated

405 that the LPF outperformed the LETKF for non-Gaussian DA with non-Gaussian observation and prior PDFs (Poterjoy et al. 2016a, 2016b, Penny and Miyoshi 2016). Therefore, the improvements of the LPFGM would come from the consideration of non-Gaussian prior PDF in sparsely observed regions.

4.3 Factors requiring further investigation

Finally, we discuss other issues for potential further improvement of the LPF and LPFGM in future studies.

410 4.3.1 Inflation

RMSEs.

This study used the RTPS to inflate the posterior perturbation for the LPF and LPFGM. As shown in Figs. 5, 7 and 10, the RMSEs of the LPF and LPFGM are sensitive to the RTPS parameter. There is a need to investigate methods that estimate the RTPS parameter adaptively, as in the EnKF (Ying and Zhang, 2015; Kotsuki et al., 2017b). However, the adaptive relaxation methods used in the EnKF cannot be applied directly to the LPF because they use the innovation statistics





415 (Desroziers et al., 2005) that assume analysis updates by the Kalman filter. Therefore, substantially different adaptive relaxation methods should be investigated for the LPF and LPFGM.

An alternative method of inflation is adding random noise to the transform matrix (Potthast et al., 2019). However, regulating the amplitude of the random noise was not trivial in the authors' preliminary experiments with L96 (not shown). Too small random noise results in loss of diversity of posterior particles, whereas excessively large random noise results in an

420 overly dispersive ensemble. Therefore, a method to determine the optimum amplitude of random noise should be investigated as well. Moreover, additive inflation methods, as used in the EnKF, can be beneficial for producing diverse prior particles (Mitchell and Houtekamer, 2000; Corazza et al., 2003).

4.3.2 Transform matrix for LPF

The transform matrix significantly affects the filter performance. Farchi and Bocquet (2018) demonstrated that the optimal transport method of Reich (2013) resulted in lower RMSE than the commonly used stochastic uniform resampling approach with the L96 model. However, it is not clear if optimal transport is beneficial for high-dimensional systems such as the SPEEDY model.

In this study, all-time resampling was detrimental for the LPFGM experiments (Figs. 7 and 10). This may be due to the MC resampling that satisfies Eq. (19) $(\bar{\mathbf{x}}_t^b = \sum_{i=1}^m \mathbf{x}_t^{b(i)} \cdot w_t^{a(i)})$ not exactly, but approximately. With a small effective

430 particle size, the MC resampling almost satisfies Eq. (19) since the resampling is not affected by the sampling noise in the selection of particles. In contrast, satisfying Eq. (19) is more difficult when the effective particle size is larger due to the sampling noise. A possible solution to this problem is to use the optimal transport method (Reich 2013) that satisfies Eq. (19) exactly. However, the optimal-transport-based resampling was inferior to the MC resampling with SPEEDY in the authors' preliminary experiments (not shown). It is necessary to investigate better methods for generating resampling matrices.

435 4.3.3 Tunable parameters of LPF and LPFGM

The tunable parameters of the LPF and LPFGM should be investigated further. For example, parameter N_0 , which controls the resampling frequency, significantly affected the filter accuracy and stability. Adaptive determination of this parameter can prevent time-consuming parameter tuning.

- The sensitivity to parameter γ should also be investigated for the LPFGM. WP22 proposed using $\gamma = 2.5$. Since γ 440 controls the amplitude and width of Gaussian kernels, the filter accuracy and stability of the LPFGM would be sensitive to this parameter. We briefly examined the sensitivity to this parameter with REG2 and RAOB (Fig. 14; $\gamma = 2.5$, 1.5, and 0.5 for red, blue, and green lines). The results indicate that the filter accuracy of the LPFGM is sensitive to this parameter, especially for spatially-inhomogeneous RAOB observing network. For our experimental settings, the optimal γ was 1.5 for both REG2 and RAOB. However, the optimal parameter would differ for different models, ensemble sizes, observing networks, and observing
- 445 frequency. Therefore, adaptive determination of this parameter is helpful.







This study considered two experimental settings with and without weight succession, i.e., $\tau = 0.0$ and 1.0, respectively. The LPFGM without weight succession ($\tau = 1.0$) resulted in lower RMSE than that with weight succession ($\tau = 0.0$). However, the optimal parameter τ would be somewhere between 0.0 and 1.0. In addition, the weight succession at each model grid point would be suboptimal. Hence, the method for weight succession should also be explored further.

450 5 Summary

This study aims to develop a software platform for the LETKF, LPF, and LPFGM with the intermediate global atmospheric model SPEEDY. The main results of this investigation are briefly listed as follows:

- The LPF and LPFGM were developed by only minor modifications to the existing LETKF system with the SPEEDY model.
- 455 2) With dense observations (REG2), the LPF showed stable filter performance with large inflation by the RTPS. The optimal localization scale of the LPF was identical to that of the LETKF. The LPF forecast was less accurate than the LETKF forecast. With sparse observations (RAOB), the LPF did not work.
 - 3) The LPFGM showed more stability and lower forecast RMSEs than the LPF. In addition to the RTPS parameter, regulating the resampling frequency and the amplitude of Gaussian kernels was important for the LPFGM. The LPFGM
- 460 without weight succession resulted in more stability and lower RMSEs than that with weight succession. With RAOB, the LPFGM forecast was more accurate than the LETKF forecast in a sparsely observed regions where the background ensemble spread and non-Gaussianity are larger.

As discussed in section 4.3, there is much room for improvement in the LPF and LPFGM. While the LPFGM potentially provides a more accurate forecast than the LETKF, the LPFGM has more tunable parameters than the LETKF.

465 Manually tuning these parameters by trying numerous experiments is computationally expensive. Therefore, adaptive methods for determining such tuneable parameters need to be explored. Also, it is important to investigate computationally more efficient methods to generate resampling matrices for the LPF and LPFGM.

The SPEEDY-based LETKF, LPF, and LPFGM used in this study are available as open-source software on Github (<u>https://github.com/skotsuki/speedy-lpf</u>). This can act as a useful platform to investigate the LPF and LPFGM further in 470 comparison with the well-known LETKF.

Author contributions

SK developed the data assimilation system, conducted the experiments, analyzed the results and wrote this manuscript. TM is the PI and directed the research with substantial contribution to the development of this paper. KK developed the data assimilation system with SK. RP contributed substantially to the introduction of the LPFGM to the standard local particle filter.





475 Data and code availability

Developed data assimilation system is available at (https://github.com/skotsuki/speedy-lpf), which is based on the exiting SPEEDY-LETKF system (https://github.com/takemasa-miyoshi/letkf). The data assimilation system used in this manuscript is archived on Zonodo (https://zenodo.org/record/6586309; doi: 10.5281/zenodo.6586309). Due to the large volume of data (> 6 TB) and limited disk space, processed data and scripts for visualization are also shared on Zenodo at the same link.

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Algorithms

Algorithm 1: Generation of the resampling matrix T

Requirement: \mathbf{r}_{sorted} and $\mathbf{w}_{t,acc}$

1.	All components of T and z are initialized to be 0						
1:	#z: an indicator of resampled particles						
2:	do <i>j</i> =1 to <i>m</i>	# index of posterior particle					
3:	do <i>i</i> =1 to <i>m</i>	# index of prior particle					
4:	if $\{w_{t,acc}^{(i-1)} < r_{sored}^{(j)} \le w_{t,acc}^{(i)}\} z^{(j)} =$	= i # resampled particle					
5:	end do						
6:	end do						
7:	do <i>j</i> =1 to <i>m</i>						
8:	$i = z^{(j)}$						
9:	if $\{T^{(i,i)} = 0\}$ then						
10:	$\mathbf{T}^{(i,i)} = 1$	# diagonal components					
11:	$z^{(j)} = 0$						
12:	end if						
13:	end do						
14:	do <i>i</i> =1 to <i>m</i>	# (loop for rows of T)					
15:	if $\{z^{(j)} \neq 0\}$ then						
16:	do <i>j</i> =1 to <i>m</i>	# (loop for columns of T)					
17:	if $\{sum(\mathbf{T}^{(:,j)}) = 0\} \mathbf{T}^{(i,j)} = 1$	# off-diagonal components					
18:	end do						
19:	end if						
20:	end do						

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625 Tables

Table 1: Computational complexities of LETKF, LPF, and LPFGM. Each step corresponds to the steps in Fig. 1. Cross-marks

 represent the steps used for LETKF, LPF and LPFGM.

	Step	Computational complexity	LETKF	LPF	LPFGM
	А	<i>m</i> applications of <i>H</i>	Х	Х	Х
C_{H}	В	2 <i>mp</i>	Х	Х	Х
	С	2 <i>nm</i>	Х	Х	Х
	D	※ 1	Х	Х	Х
	Е	mp_L (≈ 2)	Х		Х
	F	$\leq 2m^2p_L$	Х		Х
	G	$O(m^3)$	Х		Х
$C_{\rm L}$	Н	$O(m(m+p_L))$	Х		
	Ι	$O(m(m+p_L))$			Х
	J	$O(mp_L)$ (≈ 2)		Х	Х
	К	$O(m^2 \cdot N_{MC})$		Х	Х
	L	$\leq 2m^3$			Х
-	М	$\leq 2nm^2$	Х	Х	X
\mathcal{L}_{H}	Ν	O(nm)	Х	Х	Х

%1: This computation depends on the localization scale

630 %2: These computations assume the diagonal **R** (i.e., uncorrelated observation error)

n: system size

m: ensemble size

p: the number of observations

 p_L : the number of local observations

635 N_{MC} : the number of times resampling matrices to be generated by Algorithm 1





Obs	DA	Purpose	$\rho_h(\mathrm{km})$	α	γ	N ₀	τ	Figures
	LETKF	control experiment	600	※ 1	/	/	/	
	LPF	sensitivity to ρ_h and α	400/500/ 600/700	0.0-1.0	/	/	/	Figs. 5, 6, 9
REG2	LPFGM	sensitivity to α , N_0 , and τ	600	0.0-1.0	1.5	2/4/ 10/40	0.0/1. 0	Figs. 7, 8, 9
	LPFGM	sensitivity to α and γ	600	0.0-1.0	0.5/1.5/2. 5	2	1.0	Figs. 14 (a)
	LETKF	control experiment	1,100	₩1				
	LPF	sensitivity to ρ_h and α	1,100	0.0-1.0	/	/	/	not shown
RAOB	LPFGM	sensitivity to α and N_0	1,100	0.0-1.0	1.5	2/4/ 10/40	1.0	Figs. 10, 11, 12, 13
	LPFGM	sensitivity to α and γ	1,100	0.0-1.0	0.5/1.5/2. 5	2	1.0	Figs. 14 (b)

 Table 2:
 List of experiments

 ρ_h : horizontal localization scale (Eq. 38)

645 α: relaxation parameter of RTPS (Eq. 8)

y: amplitude of Gaussian kernel of the LPFGM (Eq. 25)

 N_0 : parameter controls resampling frequency (Eq. 22)

 τ : forgetting factor of weight (Eq. 23)

%1: Instead of RTPS, the LETKF uses Miyoshi (2011)'s adaptive multiplicative inflation

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Figures



660 Figure 1: Examples of the resampling matrix in the case of 40 particles with a given weight generated by uniform random numbers. (a) Weight for 40 particles. (b, c) Examples of sampled resampling matrices by Algorithm 1 using different random numbers r. (d, e) Resampling matrices using the Monte Carlo stochastic approach with 200 and 10,000 sampled matrices, respectively.







665 **Figure 2:** A simple scalar example of observation, prior and posterior PDFs for (a) LPF, (b) 5th particle of LPFGM and (c) LPFGM. Green, blue, red, purple dashed circles represent an observation and prior particles, moved particles, posterior particles, and replaced particles respectively.







Figure 3: Workflows of LETKF, LPFGM, and LPF. Gray, purple, green, and red boxes represent the components of LETKF,
670 a similar component as in the LETKF, the components of the LPF, and a unique component of the LPFGM, respectively.
Subroutines, source files, and computational complexities are also described in boxes, where *n*, *m*, *p*, and *p'* denote the model dimension, ensemble size, number of observations, and number of local observations at analysis grid points, respectively.







Figure 4: Observing networks for (a) REG2 and (c) RAOB experiments. Small black dots and red crosses represent model

675 grid points and observing points, respectively.







Figure 5: Time-mean background RMSEs (solid lines) and ensemble spreads (dashed lines) for T (K) at the fourth model level (~500 hPa) as a function of RTPS parameter *α* averaged over three months of the third year (February-April) with REG2
observations. Magenta, red, blue, and green lines are LPF experiments with horizontal localization scales of 700, 600, 500, and 400 km, respectively. Dashed lines represent RMSE of LETKF (0.1257 K) with adaptive multiplicative inflation instead of RTPS.









Figure 6: Time series of globally-averaged background (a) RMSEs (solid lines) and ensemble spreads (dashed lines) for T (K) and (b) effective particle size N_{eff} at the fourth model level (~500 hPa) with REG2 observations. Black lines show the LETKF. Red, blue, and green lines are the LPF experiments with localization scales of 600, 500, and 400 km, respectively. RTPS parameter α is set to 1.00 in all three LPF experiments. The abscissa shows month/day.







Figure 7: Similar to Figure 5, but for the LPFGM with REG2 and 600-km localization scale. Magenta, red, blue, and green lines show the cases with $N_0 = 40$, 10, 5, and 2, respectively. Dashed lines represent RMSE of LETKF (0.1257 K). Panels (a) and (b) show the LPFGM with and without succeeding weights (i.e., $\tau = 0.0$ and 1.0), respectively.







Figure 8: Similar to Figure 6, but showing the LPFGM experiments with REG2 and 600-km localization scale. Magenta, red, blue, and green lines are LPFGM experiments with $N_0 = 40$, 10, 5, and 2, respectively. Forgetting factor τ is 1.0. The RTPS parameter is set to 1.00 in the experiment with $N_0 = 40$ (i.e., all-time resampling) and to 0.50 for in other experiments.







Figure 9: Spatial patterns of background RMSE for T (K) at the fourth model level (~500 hPa) for (a) LETKF, (b) LPF, and
(c) LPFGM with optimal localization scale and RTPS parameter, averaged over February-April with REG2 and 600-km localization scale. Panels (d) and (e) show the differences LETKF–LPF and LETKF–LPFGM, respectively. The warm (cold) color indicates that the LPF or LPFGM is better (worse) than the LETKF.







Figure 10: Similar to Figure 5, but showing the LPFGM experiments with the RAOB and 1100-km localization scale. Magenta, red, blue, and green lines are the LPFGM experiments with $N_0 = 40$, 10, 5, and 2, respectively. Forgetting factor τ is fixed at 1.0. Dashed black lines represent the RMSE of the LETKF (0.4762 K). (b) enlarges (a) for the range of the RMSE of 0.25–0.45.







Figure 11: Similar to Figure 8, but showing the LPFGM experiments with the RAOB and 1100-km localization scale. Magenta, red, blue, and green lines are LPFGM experiments with $N_0 = 40, 10, 5, \text{ and } 2$, respectively. Forgetting factor τ is 1.0.







Figure 12: Spatial patterns of background RMSE for T (K) at the fourth model level (~500 hPa) for (a) LETKF and (b) LPFGM, averaged over February-April with RAOB and 1100-km localization scale. Panel (c) shows the difference between
LETKF and LPFGM. Warm (cold) color indicates that the LPFGM is better (worse) than the LETKF.







Figure 13: Spatial distributions of the background (a, b) Kullback–Leibler divergence and (c, d) ensemble spread for T (K), at the fourth model level (\sim 500 hPa) averaged over February-April with RAOB and 1100-km localization scale. (a, c) and (b, d) show the LETKF and LPFGM, respectively.









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Figure 14: Time-mean background RMSEs for T (K) at the fourth model level (~500 hPa) as a function of RTPS parameter α averaged over three months of the third year (February-April). (a) shows REG2 with 600-km localization scale, and (b) shows RAOB with 1100-km localization scale. Red, blue, and green lines are LPFGM experiments with being γ =2.5, 1.5, and 0.5, respectively. Black dashed lines represent RMSE of LETKF (0.1257 K) with adaptive multiplicative inflation instead of RTPS. Other parameters are set to be optimal: $N_0 = 2$ and $\tau = 1.0$.