DATA ASSIMILATION FOR NON-LINEAR SYSTEMS WITH A HYBRID NON-LINEAR PARTICLE FILTER

by

***Meng-Ge ZHOU*[a]*, Xiao-Qun CAO*[a,b*]*, Yan CHEN*[a]*, Yu-Chen LUO*[a]*, and Jia-Le YAO*[a]**

[a]College of Meteorology and Oceanography, National University of Defense Technology, Changsha, China
[b]College of Computer, National University of Defense Technology, Changsha, China

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The proposed methodology utilizes a novel data assimilation technique based on hybrid non-linear particle filters, a framework that has demonstrated efficacy in non-linear and non-Gaussian scenarios within the domain of Earth sciences. In numerical sensitivity experiments conducted on a non-linear dynamical system (Lorenz 63), the new method prevents filter divergence using only 10 particles for both dense and sparse observation networks. A comparison of the newly developed hybrid non-linear method with the local ensemble transform Kalman filter (LETKF) reveals the merits of the former in data assimilation applications analogous to geophysical data. Specifically, the newly developed filter exhibits significant advantages over the LETKF, particularly when the observation network consists of densely spaced measurements that are non-linearly related to the model state, akin to remote sensing data frequently employed in atmospheric analyses.

Keywords: *data assimilation, non-linear, particle filter, proposal densities*

Introduction

The field of data assimilation in geoscience, including applications such as weather forecasting and ocean prediction, has evolved into a progressively mature domain of study [1-4]. However, contemporary methodologies, such as the 4-D variational method (4-DVar), have proven ineffective in generating precise uncertainty estimates and require the implementation of efficient preconditioners. However, ensemble Kalman filters (EnKF) approximate the error distributions of observations and model forecasts using Gaussian probabilities, implicitly assuming linear models since non-linear dynamics can transform Gaussian distributions into non-Gaussian ones. While the integration of variational techniques with ensemble Kalman filtering signifies a substantial advancement, practical implementations continue to rely significantly on localization and inflation strategies. To summarize, it is evident that both variational methods and Kalman filter-like approaches encounter significant challenges when confronted with non-linear problems.

Particle filters (PF) present a fully non-linear alternative to EnKF, with the objective of supplanting them [5-8]. Probabilistic functions have the capacity to facilitate entirely non-linear data assimilation without imposing any assumptions regarding prior distributions or likelihood functions. However, these filters have been observed to encounter the so-called

* Corresponding author, e-mail: caoxiaoqun@nudt.edu.cn

curse of dimensionality [9], which restricts their wide applications to high-dimensional models without specific adjustments. In essence, if the ensemble size does not scale exponentially with the system's dimensionality, the ensemble tends to collapse into a single member.

In recent years, several strategies have been proposed to address the dimensionality challenges faced by PF in high-dimensional systems. The primary and most prevalent approach entails enhancing the flexibility of the proposal density. This objective is accomplished by manipulating the distribution of particles within the state space to ensure more uniform and balanced weights [10]. For instance, the equal-weights particle filter introduced by van Leeuwen [11] and the implicit particle filter proposed by Chorin *et al.* [12] both aim to reduce weight degeneracy by optimizing the proposal density mechanisms. The second strategy entails the resolution of an optimal transport problem, which facilitates the conversion of prior particles into posterior particles, either through a single step or *via* a more gradual transformation process. The proposed method aims to address the stochastic sampling component inherent in PF. For a more thorough examination of this topic, please refer to the work of Reich [13].

Despite the fact that these methodologies have exhibited deficiencies in high-dimensional contexts, they are intrinsically well-suited for localization. Furthermore, smoother multi-step transition variants appear capable of avoiding degeneracy issues without necessitating localization, representing an intriguing new development in the field. The third approach involves incorporating localization into PF. The notion of performing local computations on particle weights was first introduced by Bengtsson *et al.* [14] and van Leeuwen [15], and was subsequently elaborated upon in van Leeuwen [8]. Despite the initial implementations proving unsatisfactory, subsequent iterations have attained substantial success. For instance, the local particle filter (LPF) proposed by Penny and Miyoshi [16] employs a state-block domain localization method and mitigates discontinuities through weight smoothing techniques. Furthermore, the efficacy of locally adaptive particle filters has been assessed within the framework of global operational numerical weather prediction systems [17]. Furthermore, the localized mixture coefficients particle filter (LMCPF) has been implemented within the global ICON numerical weather prediction model framework, operated by the Deutscher Wetterdienst [18]. The fourth strategy involves the integration of pure PF with EnKF. It is imperative to differentiate this approach from those that incorporate EnKF within the proposal density. Filters based on this concept include the hybrid PF, which was introduced by Majda *et al.* [19], and the hybrid particle-EnKF, which was proposed by Slivinski *et al.* [20]. Furthermore, Frei and Kunsch [21] developed a filter that integrates the theories of particle filtering and Kalman filtering. The method under consideration alternates between the EnKF and the PF. When the likelihood of filter degeneracy increases, the EnKF component is assigned a greater weight.

This study proposes a novel filtering approach for PF, demonstrating its efficacy for common data assimilation tasks within the field of geosciences. The approach utilizes a local ensemble transform Kalman filter (LETKF) to adjust particle values, subsequently calculating the proposal density to establish the aggregate weights. By extending these weights to vector formats, the method imposes limitations on the spatial impact of observations on the weights. In order to evaluate the method feasibility and validity, data assimilation experiments are implemented on the Lorenz 63 system, fig. 1. The findings indicate that the localization approach effectively addresses the challenges posed by filter degeneracy. The novel filter demonstrates superior performance in comparison to the LETKF approach in both linear and non-linear contexts.

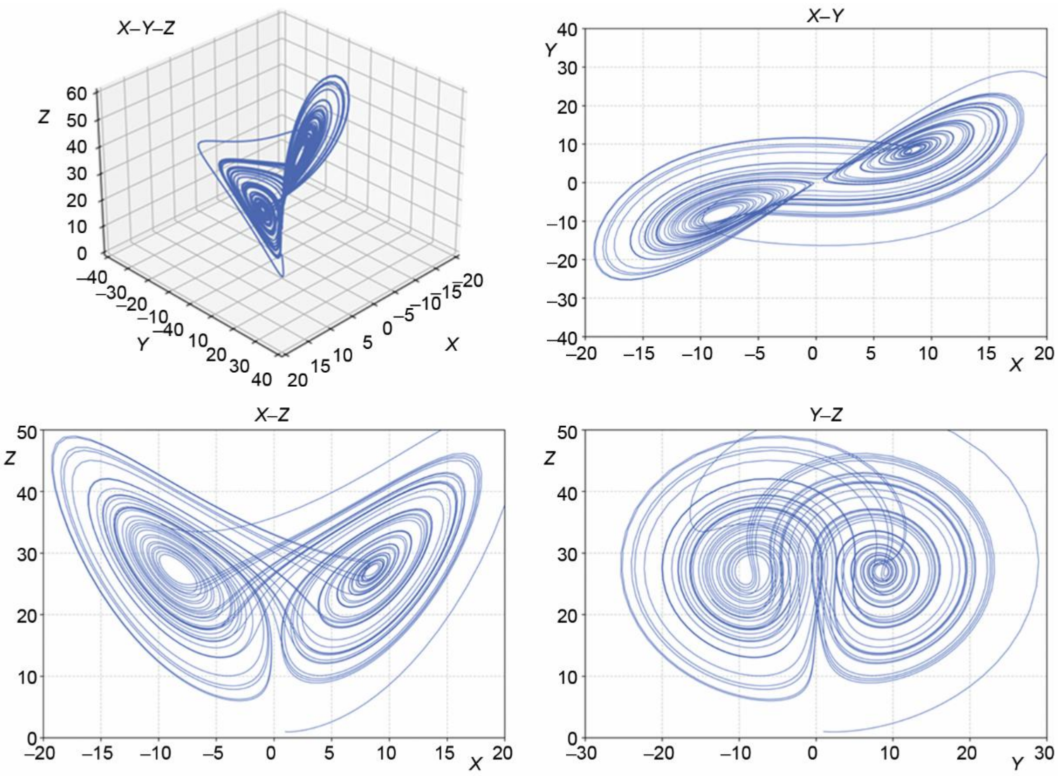

Figure 1. Simulation of the Lorenz-63 System

A new hybrid non-linear particle filter

Bayes' theorem facilitates the update of the prior density by integrating the likelihood, resulting in the posterior probability density function (PDF). By introducing a proposal density PDF, we can formulate the posterior PDF of the model variable at time step n given the observations, particularly for Markovian systems with independent observational errors across time steps:

$$p(\mathbf{x}^n \mid \mathbf{y}^{1:n}) = \frac{p(\mathbf{y}^n \mid \mathbf{x}^n)}{p(\mathbf{y}^n)} \int \frac{p(\mathbf{x}^n \mid \mathbf{x}^{n-1})}{q(\mathbf{x}^n \mid \mathbf{x}^{n-1}, \mathbf{y}^n)} q(\mathbf{x}^n \mid \mathbf{x}^{n-1}, \mathbf{y}^n) p(\mathbf{x}^{n-1} \mid \mathbf{y}^{1:n-1}) \, \mathrm{d}x^{n-1} \tag{1}$$

Instead of sampling from the original transition density $p(\mathbf{x}^n| \, \mathbf{x}^{n-1}, \mathbf{y}^n)$, particles are drawn from the proposal density $q(\mathbf{x}^n| \, \mathbf{x}^{n-1}, \mathbf{y}^n)$. This approach leads to the representation of the posterior PDF as shown in:

$$p(\mathbf{x}^n \mid \mathbf{y}^{1:n}) = \frac{1}{N} \sum_{i=1}^{N} \frac{p(\mathbf{y}^n \mid \mathbf{x}_i^n)}{p(\mathbf{y}^n)} \frac{p(\mathbf{x}_i^n \mid \mathbf{x}_i^{n-1})}{q(\mathbf{x}_i^n \mid \mathbf{x}_i^{n-1}, \mathbf{y}^n)} \delta(\mathbf{x}^n - \mathbf{x}_i^n) = \sum_{i=1}^{N} w_i \delta(\mathbf{x}^n - \mathbf{x}_i^n) \tag{2}$$

In this framework, each particle $\mathbf{x}_i$ represents a state within the model space, and its corresponding weight w_i signifies its relative importance in the posterior distribution. The weight w_i is decomposed into two components: the likelihood weight w_i^o and the proposal weight w_i^*:

$$w_i^o = p(\mathbf{y}^n \mid \mathbf{x}_i^n)$$
$$w_i^* = \frac{p(\mathbf{x}_i^n \mid \mathbf{x}_i^{n-1})}{q(\mathbf{x}_i^n \mid \mathbf{x}_i^{n-1}, \mathbf{y}^n)} \tag{3}$$

Consequently, the overall weight is determined by the product of these two factors

$$w_i = w_i^o \; w_i^* \tag{4}$$

This paper introduces a new hybrid non-linear particle filter, which employs the LETKF as the proposal density to generate proposed particles and proposal weights. Thus, the analysis results from LETKF are designated as proposed values. For resampling, the accumulated weights w_ℓ^{ac}, are defined by $w_0^{ac} = 0, \, w_\ell^{ac} = w_{\ell-1}^{ac} + w_\ell, \, \ell = 1, \ldots, L.$ the transformation matrix for the particles is defined:

$$\breve{\mathbf{W}}_{i,\ell} = \begin{cases} 1, & \text{if } R_\ell \in \left(w_{\ell-1}^{ac}, w_\ell^{ac} \right] \\ 0, & \text{otherwise} \end{cases} \tag{5}$$

By applying the properties of the trace, we obtain:

$$\rho = \frac{\mathbb{E}\left[\mathbf{d}_{o-b}^{\mathrm{T}} \mathbf{d}_{o-b} \right] - Tr\left(\mathbf{R}\right)}{Tr\left(\mathbf{H}\mathbf{P}^b\mathbf{H}^{\mathrm{T}}\right)} \tag{6}$$

Resampling can lead to a decline in filter performance, where just a small number of particles capture most of the weights. To address this issue, a regeneration phase is typically introduced. This phase involves pseudo-randomly sampling in the vicinity of the retained particles within the ensemble space to create new particles during the resampling process.

Numerical experiments

Lorenz [22] introduced a non-linear dynamical system known as the Lorenz 1963 system. Owing to its chaotic characteristics, this model has become a widely utilized framework for evaluating and comparing various data assimilation techniques, *e. g.*, [23, 24].

The Lorenz 1963 system offers a simplified representation of thermal convection and is governed by three interconnected non-linear differential equations:

$$\frac{\mathrm{d}x_1}{\mathrm{d}t} = \sigma(x_2 - x_1)$$
$$\frac{\mathrm{d}x_2}{\mathrm{d}t} = \rho x_1 - x_2 - x_1 x_3$$
$$\frac{\mathrm{d}x_3}{\mathrm{d}t} = x_1 x_2 - \beta x_3 \tag{7}$$

In these equations, x_1, x_2, and x_3 represent the state variables, while σ, ρ, and β are the model parameters. For this study, we adopt Lorenz's recommended parameter values of $\sigma = 10$, $\rho = 28$, and $\beta = 8/3$, under which the system exhibits chaotic behavior. With these settings, the model produces the well-known butterfly-shaped attractor, fig. 1. Additionally, the variables have the following physical interpretations: x_1 indicates the intensity of convective motion, x_2 measures the temperature difference between ascending and descending currents, and x_3 reflects the distortion of the vertical temperature profile from a linear state [22].

A series of data assimilation experiments were conducted to compare the performance of the new hybrid non-linear particle filter with the LETKF under model and observational system configurations that simulate geoscientific applications. These experiments also provided an opportunity to evaluate the filters sensitivity to ensemble size and localization methods across various problem settings. Both filtering approaches employed the correlation function proposed by Gaspari and Cohn [25] for localization.

This study conducts a comparative evaluation of the new hybrid non-linear particle filter against the LETKF across various model and filter configurations. The experiments encompass three distinct forms of the measurement operator H and multiple ensemble sizes. Observational data are assimilated over 10000 cycles to generate a substantial sample for assessing the performance of both data assimilation systems. Following a 1000-cycle spin-up period, the domain-averaged prior RMSE and ensemble spread are averaged over the remaining 9000 cycles to summarize the experimental outcomes.

In the initial test, both filters assimilated observational data using ensemble sizes of 10, 20, 30, 40, 80, and 160 particles. Three distinct sets of experiments were conducted, each differing solely in the definition of the measurement operator H: the first set employed interpolation from model space to observation space for H, the second set extended H to include $|x|$, and the third set applied $|x^3|$ to the interpolated values. For a univariate random variable $x \sim N(1, 1)$, fig. 2 illustrates the impact of transforming Gaussian samples into observation space for each $H[x]$. For reference, the red dashed lines represent the Gaussian estimates of the observation-space priors, calculated based on the mean and variance of the transformed samples. These two non-linear measurement operators introduce additional non-Gaussianity, which may constrain the effectiveness of the LETKF.

Figure 3 illustrates the average posterior ensemble RMSE of the baseline method (LETKF) and the new method across various observation types and ensemble member counts. This study compares these two approaches to evaluate the effectiveness of the new method in reducing forecast errors.

As depicted in the figure, the new method (red circles – 1) consistently demonstrates lower RMSE in most scenarios, particularly with larger ensemble sizes. This suggests that the new method can more effectively capture the characteristics of the prior error distribution when managing larger ensembles, thereby enhancing forecast accuracy. In contrast, the baseline method (green circles) exhibits higher RMSE under the same conditions, highlighting its limitations in capturing complex error structures.

In fig. 3(a), where the observation operator is linear, the performance of the new hybrid non-linear particle filter becomes comparable to LETKF when the ensemble size exceeds 160 members, while overall still outperforming the baseline method.

When the observation operator is the absolute value of the system variables, fig. 3(b), the new method significantly outperforms the baseline method. The non-linearity introduced by the absolute value function invalidates the Gaussian/linear assumptions of the baseline method, and the new method shows substantial improvement over the baseline even with smaller ensemble sizes. This indicates that the new method can more accurately utilize prior information in non-linear systems or with complex observation operators, thereby enhancing filtering performance.

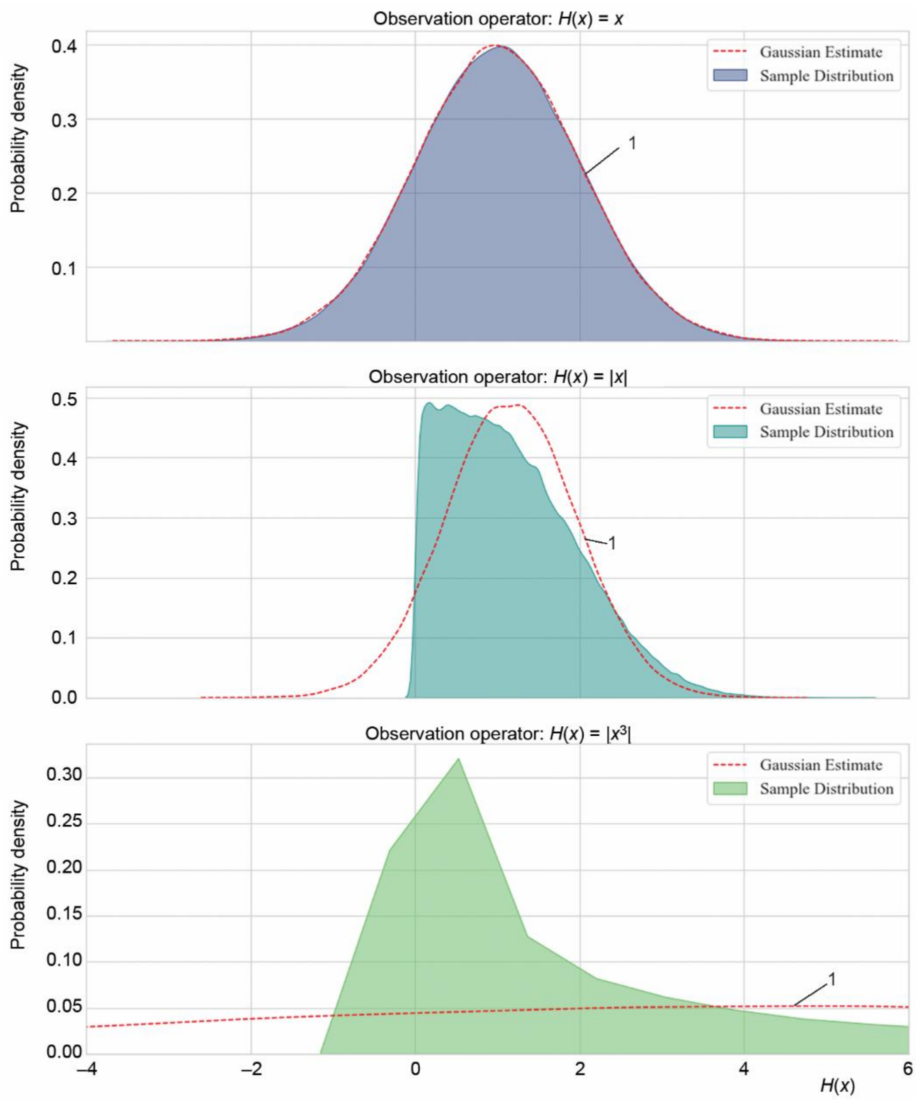

Figure 2. Probability densities demonstrating the non-Gaussian effects of three different measurement operators; the red dashed line – 1 shows a Gaussian curve using the same mean and variance as the probability densities given by the shading.

When the observation operator involves the absolute value raised to the third power of the system variables, fig. 3(c), the new method outperforms the baseline method with as few as ten particles and continues to maintain superiority as the number of particles increases.

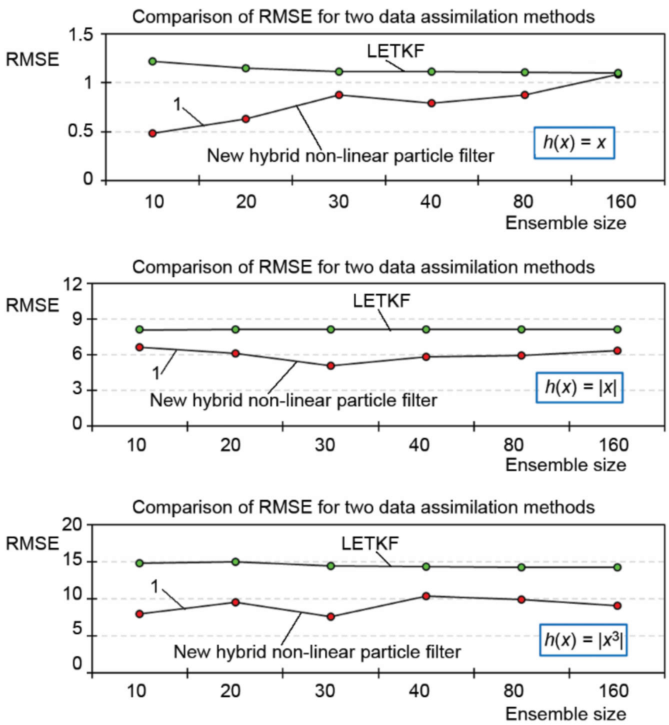

Figure 3. The average posterior RMSE over the data assimilation period using the new hybrid non-linear particle filter and LETKF as a function of ensemble size, in which the observation operators are (a) $h(x) = x$, (b) $h(x) = |x|$, and (c) $h(x) = |x^3|$

Overall, the experimental results depicted in fig. 3 demonstrate that the new method consistently achieves lower RMSE across different observation types and ensemble sizes, with particularly notable advantages in larger ensembles and non-linear observation conditions. The new method shows clear superiority over the baseline method in small ensembles. When the number of particles exceeds 40, the new method remains superior to the baseline when handling linear observation operators and continues to hold its advantage with non-linear observation operators. The baseline method exhibits certain limitations when dealing with non-linear observation operators, whereas the new method remains at least as effective as the baseline across all observation operator scenarios. Therefore, the proposed new method effectively integrates the strengths of the baseline method while mitigating its weaknesses, significantly enhancing filtering performance. This validates the new method's effectiveness in reducing forecast errors and improving filtering accuracy.

Conclusion

This paper presents a new hybrid non-linear particle filter. Compared with the traditional particle filter [26], the present filter figures out the posterior weight vectors based on how likely the observations are in the area around each model state variable. We have put the new method to work and given it a thorough going-over using the Lorenz 63 model. The new filter worked really well in experiments involving data assimilation. These experiments ran for 10000 cycles, and the filter was able to prevent filter degeneracy with as few as 10 particles. When the conditions are right for numerical weather prediction, the system shows stability and quality that are just as good as those of the EnKF. It is also been shown to handle different non-Gaussian distributions during the analysis step. These findings make us want to explore more about the potential linear measurement operators and approximately Gaussian priors. The new method always gets lower posterior RMSE compared to the LETKF. The main perk of this new method is clear in situations with a lot of observation networks and non-linear relationships between observations and model states. In these situations, the performance of the proposed method is way better than the LETKF approach, which only uses ten particles. The new hybrid non-linear particle filter is better than the LETKF in high-dimensional geophysical systems, like weather and oceanic models. This technology has a lot of potential uses, like processing satellite data, which needs non-linear measurement operators. Some examples of this kind of data are satellite radiances and radar reflectivity.

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