Commun Nonlinear Sci Numer Simulat 22 (2015) 964–979

Contents lists available at ScienceDirect

Commun Nonlinear Sci Numer Simulat

journal homepage: www.elsevier.com/locate/cnsns

Atmospheric Lagrangian coherent structures considering unresolved turbulence and forecast uncertainty

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ARTICLE INFO

Article history:
Received 30 October 2013
Received in revised form 4 April 2014
Accepted 8 July 2014
Available online 18 July 2014

Keywords:
Lagrangian coherent structures
Stochastic trajectory
Stochastic FTLE field
Ensemble forecasting
Uncertainty analysis

ABSTRACT

To obtain more realistic approximations of atmospheric Lagrangian coherent structures, the material surfaces which form a template for the Lagrangian transport, two concepts are considered. First, the effect of unresolved turbulent motion due to finite spatiotemporal resolution of velocity field data is studied and the resulting qualitative changes on the FTLE field and LCSs are observed. Stochastic simulations show that these changes depend on the probabilistic distribution of position of released virtual particles after backward or forward time integration. We find that even with diffusion included, the LCSs play a role in structuring and bifurcating the probability distribution. Second, the uncertainty of the forecast FTLE fields is analyzed using ensemble forecasting. Unavoidable errors of the forecast velocity data due to the chaotic dynamics of the atmosphere is the salient reason for errors of the flow maps from which the FTLE fields are determined. The common practice for uncertainty analysis is to apply ensemble forecasting and here this approach is extended to FTLE field calculations. Previous work has shown an association between LCS passage and fluctuations in microbial populations and we find that ensemble FTLE forecasts are sufficient to predict such passages one day ahead of time with an accuracy of about 2 h.

1. Introduction

The notion of hyperbolic Lagrangian coherent structures (LCSs) provide a framework for understanding transport and mixing phenomena especially in the case of passive particles in fluid systems [1–3]. These structures are codimension 1 manifolds (or material surfaces) which effectively separate two regions of fluid with different qualitatively different past histories or fates. Several such critical material surfaces are present in any given geophysical flow and may aid in understanding Lagrangian transport patterns. In the atmosphere, they persist from a few hours to a few days.

The present study is motivated by the role of atmospheric LCSs in aerial transport of microorganisms and the statistical correlation between sudden changes in aerobiota density and passage of LCS features over a fixed location [4–10]. Considering that role, if one can predict the LCSs to a good degree of accuracy and reliability, then important knowledge about the front propagation of microorganisms would be available.

Considering this fact, in a previous study, forecast LCSs were compared with reanalysis (pastcast) results to ascertain the accuracy and reliability of the forecasts [11,12]. Based on that study we infer the need for including more realistic considerations of atmospheric flows such as (i) finite spatiotemporal resolution of the available fluid velocity data, (ii) the accuracy of the fluid velocity data and (iii) the uncertainty of the forecast velocity fields. There have been studies about each of these

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http://dx.doi.org/10.1016/j.cnsns.2014.07.011

concerns. For example, Griffa et al. [13] and Ozgokmen et al. [14] studied the predictability of Lagrangian trajectories and Kahl and Samson [15] considered the uncertainty in trajectory calculations due to low resolution data. In addition Wilson and Sawford [16] and Stohl [17] studied different models for generating Lagrangian stochastic trajectories and Palmer [18] and Ehrendorfer [19] reviewed the concepts of predictability and uncertainty of atmospheric forecasts. Also Kalnay [20] represented various approaches for data assimilation, ensemble forecasting and uncertainty analysis. Regarding LCSs, Haller [21] discussed the errors of approximate velocity field and their effect on hyperbolic LCS features and Lermusiaux et al. [22] described the uncertainty of oceanic LCSs and their numerical studies indicated that the more intense FTLE ridges are usually more certain. Moreover, Olcay et al. [23] studied the role of flow field resolution and random errors on LCS identification. Finally, Turbulent dispersion velocity at length scales smaller than wind data grid was considered by Peng and Peterson [24] and it was shown that attracting LCS structures coincide with the regions of high particle concentration. In that study, finite time Lyapunov exponent (FTLE) fields and the associated LCSs were calculated by using deterministic atmospheric flow map and the volcanic ash particles' dispersion was calculated by adding random walk and deposition velocities to the background velocity field.

In this study we connect notions such as unresolved turbulence and uncertainty of flow field to the atmospheric LCSs. For this aim we consider two concepts. First we use a Lagrangian particle dispersion model (LPDM) which approximately represents the effects of unresolved turbulence. Accordingly, we study the FTLE scalar field and the resultant LCSs in the presence of stochastic diffusion by adding the stochastic component of displacement to the deterministic flow map (note, we will often refer to FTLE-derived LCSs as FTLE-LCSs). As a result, the trajectories will be stochastic and non-differentiable instead of deterministic and smooth. We observe significant changes in the (probabilistic) position of particles and the associated FTLE fields. We show that the spatiotemporal dependence of the stochastic velocity component to the time-varying deterministic background velocity field [25–27] plays an important role in the determination of the probabilistic distribution of the end-position of released virtual particles and consequently on the stochastic FTLE fields. We should note that Peng and Peterson [24] just considered the dispersion velocity for the ash particles and the FTLE-LCSs were calculated by deterministic velocity field.

Second, we study the quantification of uncertainty and reliability of the FTLE-LCS when forecast velocity data are used to generate flow maps. The effects of forecast velocity data on the accuracy of forecast FTLE-LCSs have previously been observed [11]. In that paper we compared FTLE-LCSs from forecast velocity data with archive based FTLE-LCSs. Results of that study show the sensitivity of FTLE-LCS forecasting to different parameters such forecast lead time, but because we used a deterministic forecast velocity field (NAM-218 data set) we were not able to measure the uncertainty of the forecast FTLE-LCS results. In the present study we propose a practical approach to measure uncertainty of forecast FTLE-LCSs by using ensemble forecasting concepts and considering the distribution of local FTLE values. In addition, we study the ensemble-based distribution of forecast LCS passage times over a fixed geographical location, which provides a measure of reliability of the LCS forecasts.

2. Effects of unresolved turbulence on the FTLE field; stochastic FTLE field

In this section we show how including the stochastic component of unresolved turbulent velocity changes the FTLE field.

In atmospheric applications, the spatial resolution of archived operational data could vary from the order of 10 km to more than 250 km and the temporal resolution is usually of the order of 3 to 12 h. For example, in the operational model NAM-218, which we use, the spatial resolution is about 12 km and the temporal resolution is 6 h (a short term forecast at each intermediate 3 h is also available). As a result of this coarse resolution, important *unresolved motions* with significant effects on the particle flow map and the resultant FTLE field could exist. To investigate this, we use a particle dispersion model to calculate the stochastic turbulent velocity component of the flow field. These components are functions of turbulent diffusivity [25,26].

Considering the Lagrangian frame, a fluid particle trajectory $\mathbf{x}(t)$ is governed by the stochastic differential equation,

$$\frac{d\mathbf{x}}{dt} = \mathbf{v}[\mathbf{x}(t)], \tag{1}$$

where the velocity of the particle is composed of the deterministic grid scale velocity, $\bar{\mathbf{v}}(\mathbf{x}, t)$, and the stochastic turbulent fluctuation component, $\mathbf{v}_t(\mathbf{x}, \bar{\mathbf{v}}, t)$, respectively,

$$\mathbf{v}(\mathbf{x}, t) = \bar{\mathbf{v}}(\mathbf{x}, t) + \mathbf{v}_t(\mathbf{x}, \bar{\mathbf{v}}, t). \tag{2}$$

Using the Langevin equation and assuming a Markovian process [28,29], one can parameterize the turbulent component of velocity as,

$$dv_{t_i} = a_i(\mathbf{x}, \mathbf{v_t}, t)dt + \sum_{j=1}^{3} b_{i,j}(\mathbf{x}, \mathbf{v_t}, t)dW_j, \tag{3}$$

where drift (a_i) and diffusion $(b_{i,j})$ are functions of time, position and turbulent velocity and v_{t_i} represents the ith component of $\mathbf{v}_t(\mathbf{x}, \bar{\mathbf{v}}, t)$ [30,16,17,31]. Moreover, dW is the standard white noise Wiener process.

There are different methods for estimating the drift and diffusion terms with respect to the available data and turbulent regime of the flow field. In this study we follow the work of Thomson [30], Fay et al. [26], Legg and Raupach [27], Stohl et al. [31] and Draxler and Hess [25].