Eulerian Mapping Closure Approach for Probability Density Function of Concentration in Shear Flows

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Abstract. The Eulerian mapping closure approach is developed for uncertainty propagation in computational fluid mechanics. The approach is used to study the Probability Density Function (PDF) for the concentration of species advected by a random shear flow. An analytical argument shows that fluctuation of the concentration field at one point in space is non-Gaussian and exhibits stretched exponential form. An Eulerian mapping approach provides an appropriate approximation to both convection and diffusion terms and leads to a closed mapping equation. The results obtained describe the evolution of the initial Gaussian field, which is in agreement with direct numerical simulations.

Key words. uncertainty propagation, probability density function, mapping closure approximation, concentration

Subject classification. Fluid Mechanics

1. Introduction. Uncertainty in computational fluid dynamics appeals for a probabilistic description of output [1, 2]. The probabilistic description is usually achieved by either moments or PDFs. However, both moment and PDF approaches suffer the closure problems: there are some unknown terms in their transport equations which have to be modeled. In turbulence modeling, the closure problems can be addressed by Kolmogorov’s universal theory of small scale motions. Unfortunately, such a sound theory does not exist on uncertainty problems. Therefore, we have to use some assumptions a priori. For example, the log-normal assumption is made in the moment approach [3] and the conditional dissipation is modeled in the PDF approach [4]. Recently, mapping closure approximation has been developed to calculate moments and PDFs without any ad hoc models. The main idea of the mapping closure approximation is to keep track of the evolution of an unknown random field by using a known reference field and a mapping function. The known reference field is usually chosen to be a Gaussian random field, because we understand the properties of the Gaussian closure. The dynamical evolution of the PDF is described by an evolution equation of the mapping function; the latter is obtained directly from the original governing equation under the Gaussian closure. This approach can be used to calculate evolution of unknown random fields in a fashion of successive approximation, resulting in a good statistical description.

In this paper, the Eulerian mapping closure approach is developed to calculate the uncertainty propagation through stochastical dynamical systems. The chosen example is the concentration of species advected by random shear flows. This problem is also very interesting to the turbulence community. Recent studies [5] – [13] on passive scalars have shown under some circumstances that large scale PDFs of the passive scalar could be non-Gaussian. If the velocity fields are isotropic Gaussian and the passive scalars have zero mean gradients, the scalar of initial homogeneous Gaussian distribution in a periodic box remain to be near Gaussian while its derivatives are non-Gaussian. Noting that fluctuations of the scalar at a certain location exhibit large scale behaviors and its derivatives exhibit small scale behaviors. Therefore, in this case, the large scale PDFs are near Gaussian and small scale PDFs are non-Gaussian. Holzer and Siggia [5], and
Pumir [6] have found that the large scale scalars with non-trivial mean gradients are non-Gaussian. Ching and Tu [7] found that non-periodic boundary conditions can also induce non-Gaussianity of large scale scalar. Kimura and Kraichnan [13] have shown that large scale PDFs of the scalar with non-zero mean gradient initial conditions are exponential. The next and natural question is whether or not anisotropy of the velocity field changes statistics of large scale scalars.

The simplest anisotropic velocity field is shear flow: the velocity has spatial variation in one direction. Majda [9] and Maclaughlin and Majda [10] use the path integration to analytically calculate the moments of scalar for a simple random shear velocity field. They found that the flatnesses of both passive scalar and its derivatives are larger than the ones of Gaussian distribution. Therefore, the PDFs are non-Gaussian. In the present paper, we will investigate the case for a periodic random shear velocity field. The PDFs of the scalar, such as concentration, are calculated using Direct Numerical Simulation (DNS) and the mapping closure approach. The prominent characteristics of non-Gaussianity are longer tails of the PDFs. In this paper, we will explore how shear induces long tails and non-Gaussianity of the concentration PDFs.

2. Direct numerical simulations. The concentration $T$ advected by the periodic random shear flows is governed by the following equation:

$$\frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} = \kappa \nabla^2 T.$$  

Here, the velocity field is the periodic random shear flow:

$$u = 0, \quad v = \gamma(t)|x|,$$

where $\gamma(t)$ is Gaussian noise with $\delta$ time correlation. Bronski and Maclaughlin [11] consider another form of the periodic random shear flow: $v = \gamma(t)x$, which is discontinuous in the boundary.

We performed DNS for the concentration equation (2.1) in a cube of the sides $2\pi$ with periodic boundary conditions. The initial conditions are taken as homogeneous and isotropic Gaussian field. See Fig. 4.1. The equation (2.1) is discretized spatially using finite difference. It is integrated in time using an Euler scheme for the first time step and an Adams-Bashforth scheme for all subsequent time steps. Fig. 4.2 shows the concentration contour for the frozen $\gamma(t)$. It can be seen that the initial homogeneous patchiness is stretched into the sheets in the direction of shear. The stretched sheets induce the inhomogeneity of the concentration and then non-trivial mean gradients. Thus, the PDFs of the concentration are non-Gaussian. For the $\delta$-correlated $\gamma$, we measure the concentration PDFs at a certain point and find that they have a longer tail than Gaussian, see Fig. 4.3. Therefore, the non-Gaussianity of large scale PDFs are associated with the stretched sheets.

3. Calculate the PDFs of concentration using Eulerian mapping closure approach. The numerical observation can be interpreted using the recently developed mapping closure approach [13]. Since shear induces inhomogeneity in space, we have to assume that the mapping function explicitly depends on spatial coordinates:

$$T = X(\theta_0; x, y, t),$$

where $\theta_0(x, y)$ is a known random Gaussian field. If we know the mapping function (3.1), we can obtain the PDF of the concentration using a simple transformation:
\[ P(T,x,y) = P(\theta_0) \left[ \frac{\partial X}{\partial \theta_0} \right]^{-1}. \]

The Liouville theorem then requires that the equation of motion for \( X \) be

\[ \frac{\partial X}{\partial t} + \frac{\partial X}{\partial \theta_0} \frac{\partial \theta_0}{\partial t} = -\langle u \nabla X | \theta_0 \rangle + \kappa \langle \nabla^2 X | \theta_0 \rangle. \]

It follows from (3.1) and (3.3) that

\[ \frac{\partial X}{\partial t} = \kappa \left( \frac{c_1 \theta_0}{c_0} \frac{\partial X}{\partial \theta_0} + c_1 \frac{\partial^2 X}{\partial \theta_0^2} + \frac{\partial X}{\partial x^2} + \frac{\partial^2 X}{\partial y^2} \right) + \eta(t)x \left\{ \frac{\partial^2 X}{\partial y^2} - \frac{\partial X}{\partial y} \left( \frac{\partial X}{\partial \theta_0} \right)^{-1} \left[ 2 \frac{\partial^2 X}{\partial y \partial \theta_0} - \frac{\partial X}{\partial y} \left( \theta_0 + \frac{\partial X}{\partial \theta_0} \right)^{-1} \frac{\partial^2 X}{\partial \theta_0^2} \right] \right\}, \]

where \( c_0 \) and \( c_1 \) are defined by \( c_0 = \langle \theta_0^2 \rangle, c_1 = \langle (\nabla \theta_0)^2 \rangle \). The function \( \eta(t) \) is the eddy diffusion dependent on the time scale of the velocity field:

\[ \eta(t) = \int_{t_1}^t \langle \gamma(t) \gamma(s) \rangle ds. \]

The first term on the right side of equation (3.4) corresponds to the diffusion term of equation (2.1). The second term on the right hand side of equation (3.4), corresponding to the convection term of equation (2.1), introduces nonlinearity of the mapping function’s spatial derivatives. If the nonlinear term in equation (3.4) disappears, the mapping functions are obviously a linear function of \( \theta_0 \) so that the concentration PDFs remain Gaussian. It is this nonlinear term that produces a nonlinear mapping function and distort the Gaussian field.

A simple perturbative analysis of equation (3.4) can be carried out as follows. For \( \eta = 0 \), the solution of equation (3.4) is a linear function of \( \theta_0 \). Thus, the concentration PDF remains to be Gaussian, in agreement with the physics of diffusion. For the small \( \eta \), the solution is assumed to have the following perturbative form

\[ X(\theta_0; x, y, t) = X_0(\theta_0; x, y, t) + \eta X_1(\theta_0; x, y, t) + \cdots. \]

Substituting equation (3.6) into equation (3.4), we find that \( X_0 \propto \theta_0 \) and \( X_1 \propto \theta_0^n, \ 1 < n \leq 3 \), for large \( \theta_0 \). Thus, the tail of the concentration PDF is proportional to \( \text{exp}(-T^{2/n}) \). Obviously, shear introduces higher order terms of \( \theta_0 \), leading to a stretched exponential form of the tail of the concentration PDF.

The general solution of equation (3.4) can be obtained by numerical integration, using the same procedure used in equation (2.1). The boundary conditions for the mapping function \( X \) are periodic in the direction of \( x \) and \( y \), and obtained by extrapolation in the direction of \( \theta_0 \). The initial conditions for \( X \) are Gaussian fields of spatial variation. The convection terms involving the velocity are treated in the conservative forms.

In Fig. 4.4, we show the behaviors of the mapping functions, at different times for a given location, with respect to the reference Gaussian field. These mapping functions are the numerical solution of the mapping equation (3.4). In Fig. 4.5, we plot the PDFs of the concentration \( T \) at the same times and location as in
In the very early stage, the mapping function is kept to be almost linear by the initial Gaussian fields and the corresponding PDF is almost Gaussian. As time passes, the nonlinear term in equation (3.4) distorts the initial linear mapping and results in a nonlinear mapping: the central section near $\theta_0 = 0$ is almost linear but the left and right sections to the central one are polynomial-like forms. Consequently, the PDF of the concentration consists of a Gaussian core and a stretched exponential tail. In other words, the convection term distorts the initial isotropic Gaussian field and drives it to an inhomogeneous and anisotropic non-Gaussian field. We compare the results obtained by the DNS and the mapping closure and find that they are in good agreement (see Fig. 4.3).

4. Conclusion. In summary, we have obtained one-point PDFs of the concentration advected by shear flow using two methods, DNS and mapping closure. The PDFs for both methods are non-Gaussian and exhibit stretched exponential tails. DNS visualizes that the initial homogeneous and isotropic patchiness are sheared into the stretched sheets in the directions of shear. By shear-induced stretches, the mapping function is distorted from the initial linear functions to the nonlinear functions. As the result of shear, the initial Gaussian concentration evolves into the exponential one. Moreover, the shear direction may induce different tails of the PDFs of the concentration's longitudinal and transversal derivatives, leading to anisotropy of small scale concentration [8]. We have demonstrated that the present approach of mapping closure can track the PDF’s evolution for the concentration in random shear flows. We believe that the mapping closure approach can be used to investigate the uncertainty propagation in computational fluid dynamics.

REFERENCES


Fig. 4.1. The initial snapshot of homogeneous and isotropic Gaussian scalar field. Grey scales indicate the magnitudes of scalar.

Fig. 4.2. The final snapshot of scalar field. Grey scales indicate the magnitudes of scalar.
FIG. 4.3. The PDFs of scalar at some given time and a certain point. Solid line: DNS; Dash line: Mapping closure; Dotted line: Gaussian.

FIG. 4.4. The mapping functions $T$ versus the reference Gaussian field $\theta_0$ for some given location $(x, y)$ at different times from bottom to top: (1) $t = 0.6$, (2) $t = 1.2$, (3) $t = 1.8$; the inset is for $t = 0.1$. 
FIG. 4.5. The PDFs of scalar for some given location \((x, y)\) at different times from inside to outside: (1) \(t = 0.1\), (2) \(t = 0.6\), (3) \(t = 1.2\), (4) \(t = 1.8\).
The Eulerian mapping closure approach is developed for uncertainty propagation in computational fluid mechanics. The approach is used to study the Probability Density Function (PDF) for the concentration of species advected by a random shear flow. An analytical argument shows that fluctuation of the concentration field at one point in space is non-Gaussian and exhibits stretched exponential form. An Eulerian mapping approach provides an appropriate approximation to both convection and diffusion terms and leads to a closed mapping equation. The results obtained describe the evolution of the initial Gaussian field, which is in agreement with direct numerical simulations.