

A NEW EULERIAN MONTE CARLO METHOD FOR THE JOINT VELOCITY-SCALAR PDF EQUATIONS IN TURBULENT FLOWS

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Abstract. *In a previous article [1], a new Eulerian Monte Carlo (EMC) method was proposed to solve the joint PDF of turbulent reactive scalars. EMC methods are based on stochastic Eulerian fields, which evolve from stochastic partial differential equations (SPDE), statistically equivalent to the PDF equation.*

In this article, EMC methods [1] are extended in order to solve the joint velocity-scalar PDF. Besides, an alternative EMC method for the scalar PDF is also derived as a special case of the full velocity-scalar method.

The principal idea is to transform the stochastic ordinary differential equations (SODE) used in Lagrangian Monte Carlo (LMC) methods into SPDEs. This transformation is similar to the one used in classical hydrodynamics, when going from a Lagrangian to a Eulerian formulation of the Navier-Stokes equations. However, in our case, the transformation is not applied to the Navier-Stokes equations, but to stochastic modelled equations. In particular, the stochastic velocity does not respect an instantaneous continuity constraint, but only a mean one. As a consequence, one must introduce a stochastic density, different from the physical density.

1 INTRODUCTION

In the field of turbulent combustion, Lagrangian Monte Carlo (LMC) methods [2] have become an essential component of the probability density function (PDF) approach. LMC methods are based on stochastic particles, which evolve from prescribed stochastic ordinary differential equations (SODEs). They are used to compute the one-point statistics of the quantities describing the state of a turbulent reactive flow: namely, the velocity field and the reactive scalars (species mass fractions and temperature).

Numerous publications document the convergence and accuracy of LMC methods. They have been used in many complex calculations (including LES), and for several

years now, they have been implemented in commercial CFD codes. Nonetheless, the development of a new Eulerian Monte Carlo (EMC) method is useful and stimulating, since the competition between LMC and EMC methods could push both approaches forward.

EMC methods have already been proposed in [1] and in [3], in order to compute the one-point PDF of turbulent reactive scalars. EMC methods are based on stochastic Eulerian fields, which evolve from prescribed stochastic partial differential equations (SPDE) statistically equivalent to the PDF equation. The extension of EMC methods to include velocity still remains to be done.

Thus, the purpose of this article is to derive SPDEs allowing to compute a modeled one-point joint velocity-scalar PDF. To achieve this objective, we start from existing Lagrangian stochastic models. The latter are described by SODEs, which can be considered as modeled Navier-Stokes equations written in Lagrangian variables. Then, the idea is to transform these Lagrangian SODEs into Eulerian SPDEs, in the same way one transforms the Lagrangian Navier-Stokes equations into Eulerian equations, in classical hydrodynamics.

However, our case differs from the classical one. Indeed, the stochastic velocity does not respect an instantaneous continuity constraint, but only a mean one. To account for this difference between the stochastic and the physical system, one must introduce a stochastic density, different from the physical density.

As a result of this procedure, we eventually obtain hyperbolic conservative SPDEs giving the evolution of a stochastic velocity, of stochastic scalars, and of a stochastic density.

In order to simplify our derivation, we will consider, in the second section, the case of a constant density flow, and limit ourselves to deriving SPDEs modeling the velocity field. Then, in the third section, the more general case of Low Mach number reacting flows will be considered and SPDEs for the turbulent reacting scalars will be derived. The paper ends with a description of how the results obtained here for the joint velocity-scalar PDF can be applied to solve scalar PDFs. We obtain an alternative – but equivalent – formulation to the one proposed in [1]. In particular, the SPDEs are in conservative form.

2 EMC METHOD FOR SOLVING THE VELOCITY PDF IN A CONSTANT DENSITY FLOW

In the present section, our attention is limited to the one-point PDF $f_{\mathbf{U}}$ of a velocity field \mathbf{U} governed by the incompressible Navier-Stokes equations. The density ρ is constant.

From the incompressible Navier-Stokes equations and by using standard techniques [4, 2], it is possible to derive an exact transport equation for the PDF $f_{\mathbf{U}}$. In this equation, the advection process is treated exactly, while the effects of the pressure gradient and of the viscous stresses are unclosed.

In this work, we will consider that these two processes are represented by the Generalized Langevin model [5, 6]. As a result, we obtain the following Fokker-Planck equation

for the modeled one-point PDF :

$$\frac{\partial f_{\mathbf{U}}}{\partial t} + U_j \frac{\partial f_{\mathbf{U}}}{\partial x_j} = - \frac{\partial}{\partial U_j} \left(\left[-\frac{1}{\rho} \frac{\partial \langle P \rangle}{\partial x_j} + G_{ij} (U_j - \langle U_j \rangle) \right] f_{\mathbf{U}} \right) + \frac{1}{2} C_0 \langle \epsilon \rangle \frac{\partial^2 f_{\mathbf{U}}}{\partial U_j \partial U_j} \quad (1)$$

with initial conditions:

$$f_{\mathbf{U}}(U; x, t = 0) = f_0(U; x) \quad (2)$$

The symbol $\langle \cdot \rangle$ denotes the average operation. For instance:

$$\langle U \rangle (x, t) = \int V f_{\mathbf{U}}(V; x, t) dV \quad (3)$$

In equation (1), P is the pressure and $\langle \epsilon \rangle$ is the mean turbulent dissipation. C_0 is a constant and G_{ij} is a second-order tensor which can depend on the Reynolds stress tensor, the mean velocity gradient and the mean dissipation. Equation (1) must also be completed by the mean continuity equation :

$$\text{div} \langle \mathbf{U} \rangle = 0 \quad (4)$$

This equation gives the normalization condition for the PDF $f_{\mathbf{U}}$ and determines the mean pressure $\langle P \rangle$.

Our objective is to derive SPDEs for computing the Fokker-Planck PDF equation (1). It is well known that there exists a connection between Fokker-Planck equations and stochastic diffusion processes [7]. This connection is precisely used in LMC methods in order to derive SODEs for computing equation (1). As our derivation is partly based on LMC methods, we will first start by recalling the diffusion processes that are used in LMC methods, as well as their corresponding statistics. We will also introduce a quantity that plays a central role in converting Lagrangian statistics to Eulerian statistics, namely the stochastic density.

2.1 LMC METHODS

2.1.1 Lagrangian Equations

In the framework of LMC methods [6], a diffusion process, described by the following SODEs, is used to solve PDF equation (1) :

$$d\mathcal{U}_j^+(t) = - \left. \frac{1}{\rho} \frac{\partial \langle P \rangle}{\partial x_j} \right|^+ dt + G_{ij} (\mathcal{U}_j - \langle U_j \rangle)^+ dt + \sqrt{C_0 \langle \epsilon \rangle^+} dW_j \quad (5)$$

$$dx_j^+(t) = \mathcal{U}_j^+ dt \quad (6)$$

$$\begin{cases} \mathbf{x}^+(0) = \mathbf{x}_0 \\ \mathbf{u}^+(0) = \mathbf{u}_0 \end{cases} \quad (7)$$

$\mathbf{u}^+(t)$ is the stochastic Lagrangian velocity. Its value is taken along the Lagrangian trajectory $\mathbf{x}^+(t)$. The W_j are independent standard Wiener processes, and the dW_j are their time increments. It is important to stress that, in the current implementation of LMC methods, the Wiener processes are also independent for different Lagrangian particles (i.e. having different initial conditions).

The Eulerian mean velocity $\langle U_j \rangle$ appearing in equations (5)- (6) is determined from the joint Lagrangian PDF of \mathbf{u}^+ and \mathbf{x}^+ (see eq. (21)).

The initial condition of \mathbf{x}^+ is \mathbf{x}_0 and the initial condition of \mathbf{u}^+ is \mathbf{u}_0 . \mathbf{x}_0 and \mathbf{u}_0 are independent from the Wiener processes. At initial time, the positions and velocities are distributed with a probability f_{0UX} :

$$f_{0UX}(\mathbf{U}_0, \mathbf{X}_0) = \langle \delta(\mathbf{x}_0 - \mathbf{X}_0) \delta(\mathbf{u}_0 - \mathbf{U}_0) \rangle \quad (8)$$

where the average is performed over the realizations of the initial conditions \mathbf{x}_0 and \mathbf{u}_0 .

SODEs (5)-(6), with initial conditions specified by (8), are the only equations used in the framework of LMC methods. As shown in [2] and as recalled in section 2.1.3, it is sufficient to solve them in order to determine PDF (1).

2.1.2 Stochastic density

SODEs (5)-(6) can be considered as modeled Navier-Stokes equations written in a Lagrangian form. The transformation from Lagrangian equations to Eulerian equations includes the replacement of the Lagrangian variables, depending on time and initial position (\mathbf{X}_0, t) , by Eulerian variables, depending on time and current position (\mathbf{X}, t) .

To perform this replacement for SODEs (5)-(6), we run against a major difficulty. Indeed, an essential difference exists between the stochastic and the physical system. Namely, the velocity defined by SODEs (5)-(6)) does not obey an instantaneous continuity constraint, as opposed to the physical velocity, which is divergence free. As a result, the density transported by the stochastic velocity is not constant, as opposed to the physical density.

We will call *stochastic density* the density transported by the stochastic velocity and note it \mathbf{r}^+ . This stochastic density is defined by SODEs (5)-(6). Indeed, one can assign an arbitrary mass to each trajectory. \mathbf{r}^+ is then given by the mass present in an infinitesimal volume, divided by this volume. This definition does not require the introduction of a supplementary equation : it is sufficient to know the position repartition to compute \mathbf{r}^+ . The stochastic density is thus contained implicitly in system (5)-(6).

It is possible to give the evolution of this stochastic density \mathbf{r}^+ by specifying an instantaneous continuity equation, linked to the instantaneous stochastic velocity \mathbf{u}^+ . As it will be shown in the next section, such an equation is not needed in LMC methods : to compute Lagrangian statistics consistent with PDF equation (1), it is sufficient to only specify a mean continuity equation (eq. (22)). This property is a consequence of the closure assumption used in the Langevin model, which only imposes a continuity constraint on the mean velocity field, but not on its instantaneous value.

Nonetheless, despite being useless in the framework of LMC methods, the instantaneous conservation of mass plays a crucial role for making the conversion between Lagrangian and Eulerian statistics. For our purpose, it is thus essential to give the main properties of \mathbf{r}^+ .

In a Lagrangian framework, the conservation of mass is expressed by the relation:

$$\mathbf{r}^+ d^3x^+ = \mathbf{r}_0 d^3x_0 \quad (9)$$

where \mathbf{r}_0 is the value of the stochastic density at initial time. \mathbf{r}_0 is an arbitrary function of the initial position \mathbf{x}_0 . In section 2.2, it will be shown that, for consistency reasons, one must take the mean of \mathbf{r}_0 proportional to the initial mean density. For a constant density flow, one can take \mathbf{r}_0 constant, equal to the physical density ρ , for instance.

From equation (9), one can see that \mathbf{r}^+ is directly linked to the Jacobian $j^+(t)$ of the current position $\mathbf{x}^+(t)$ of the trajectories with respect to their initial position:

$$j^+(t) = \text{Det}[j_{ik}], \text{ with } j_{ik} = \frac{\partial x_i^+}{\partial x_{0k}} \quad (10)$$

From this definition and from equation (9), one can deduce that \mathbf{r}^+ and j^+ are related by:

$$\mathbf{r}^+ = \frac{\mathbf{r}_0}{j^+} \quad (11)$$

This relation between \mathbf{r}^+ and j^+ gives the reason why \mathbf{r}^+ plays an important role when converting Lagrangian statistics to Eulerian statistics. Indeed, in a Lagrangian framework, the evolution of the stochastic velocity is computed along Lagrangian trajectories. Each trajectory is characterized by the initial position, so that the computed positions and velocity values are functions of \mathbf{x}_0 : $\mathbf{x}^+(t) = \mathbf{x}^+(t|\mathbf{x}_0)$ and $\mathcal{U}^+(t) = \mathcal{U}^+(t|\mathbf{x}_0)$. A Eulerian description, on the other hand, requires the velocity values to be explicitly known as functionals of the current positions $\mathbf{x}^+(t)$. Thus, to make the Lagrangian-Eulerian connection, one needs to know how to transform initial positions to current positions, or in other words to express \mathbf{x}_0 as $\mathbf{x}_0(\mathbf{x}^+)$. This transformation is precisely given by the Jacobian $j^+(t|\mathbf{x}_0)$. As a consequence, to go from a Lagrangian to a Eulerian framework, one needs to determine j^+ , and this can be done by computing the stochastic density \mathbf{r}^+ since both quantities are linked by equation (11). Thus, \mathbf{r}^+ is a key quantity for doing a Lagrangian-Eulerian transposition.

The main point concerning the stochastic density \mathbf{r}^+ is that it is different from the physical density. Just as the stochastic and physical velocities, the stochastic and physical densities are only related in a statistical way. The instantaneous evolution of the stochastic density has no direct physical meaning, and in particular is not constant, even if the physical density is constant in the case considered in this section.

This can be seen through the evolution equation of the stochastic density. To derive this equation, we first give the temporal evolution of the Jacobian j^+ . By differentiating

equation (10) with respect to time, we obtain :

$$dj^+ = j^+ \operatorname{div} \mathbf{u}^+ dt \quad (12)$$

The temporal evolution of \mathbf{r} is then readily obtained from (11) :

$$d\mathbf{r}^+ = -\mathbf{r}^+ \operatorname{div} \mathbf{u}^+ dt \quad (13)$$

This equation shows that the stochastic density is not constant. Indeed, by deriving equation (5) with respect to x^+ , one can see that :

$$\frac{d}{dt} (\operatorname{div} \mathbf{u}^+) = - \left. \frac{\partial \mathcal{U}_i}{\partial x_j} \frac{\partial \mathcal{U}_j}{\partial x_i} \right|^+ - \left. \frac{1}{\rho} \frac{\partial^2 \langle P \rangle}{\partial x_i \partial x_i} \right|^+ + \left. \frac{\partial}{\partial x_i} (G_{ij}(\mathcal{U}_j - \langle \mathcal{U}_j \rangle)) \right|^+ + \frac{1}{2} \sqrt{\frac{C_0}{\langle \epsilon \rangle}} \left. \frac{\partial \langle \epsilon \rangle}{\partial x_i} \right|^+ \dot{W}_i \quad (14)$$

In this equation, the independent Brownian products cannot be balanced by any other terms, because these other terms are deterministic. Besides, the divergence of the linear relaxation term $G_{ij}(\mathcal{U}_j - \langle \mathcal{U}_j \rangle)$ is in general not equal to zero. As a result, the divergence of the velocity cannot be equal to zero. Thus, the instantaneous stochastic density \mathbf{r}^+ is not constant, as opposed to the physical density ρ .

2.1.3 Lagrangian statistics

In this section, we present the statistics that are computed with SODEs (5)-(6) and establish their link with the statistics derived from PDF equation (1). We mainly follow the presentation given in [6]. We recall that the stochastic density does not influence the determination of these Lagrangian statistics, even if it will be crucial for converting them to Eulerian statistics.

The probability of obtaining a velocity \mathbf{U} and a position \mathbf{X} when \mathbf{u}^+ and \mathbf{x}^+ are governed by SODEs (5)-(6) is given by the Lagrangian velocity-position PDF. This PDF is defined by :

$$f_{UX}(\mathbf{U}, \mathbf{X}; t) = \langle \delta(\mathbf{U} - \mathbf{u}^+(t)) \delta(\mathbf{X} - \mathbf{x}^+(t)) \rangle \quad (15)$$

where averages are performed over initial conditions and over the realizations of the Wiener noises. By standard techniques (see for instance Gardiner [7]), one can show that the transport equation of f_{UX} is similar to PDF equation (1):

$$\frac{\partial f_{UX}}{\partial t} + U_j \frac{\partial f_{UX}}{\partial X_j} = - \frac{\partial}{\partial U_j} \left(\left[-\frac{1}{\rho} \frac{\partial \langle P \rangle}{\partial X_j} + G_{ij}(U_j - \langle U_j \rangle) \right] f_{UX} \right) + \frac{1}{2} C_0 \langle \epsilon \rangle \frac{\partial^2 f_{UX}}{\partial U_j \partial U_j} \quad (16)$$

Despite the similarity between their evolution equations, f_{UX} and f_U cannot be equal. Indeed, averages performed with f_{UX} are done over the entire physical domain, while f_U yields averages at a given point.

Instead, the probability of obtaining a velocity \mathbf{U} at a given position \mathbf{X} from SODEs (5)-(6) is given by the Lagrangian PDF conditioned on position. This PDF is defined by:

$$f_{U|X}(\mathbf{U}, \mathbf{X}; t) = \frac{f_{UX}(\mathbf{U}, \mathbf{X}; t)}{f_X(\mathbf{X}; t)} \quad (17)$$

where $f_X(\mathbf{X}; t) = \int f_{UX}(\mathbf{U}, \mathbf{X}; t) d\mathbf{U}$ is the Lagrangian position PDF. $f_{U|X}(\mathbf{U}, \mathbf{X}; t)$ has the same signification as a Eulerian PDF, even if it is built from Lagrangian PDFs. Thus, if a link is to be established between PDF equation (1) and SODEs (5)-(6), it has to be done through the Eulerian PDF f_U and the Lagrangian PDF conditioned on position $f_{U|X}$. The conditional mean of a quantity Q depending on \mathbf{U}^+ and \mathbf{x}^+ is noted as:

$$\langle Q | X \rangle = \int Q(\mathbf{U}, \mathbf{X}) f_{U|X} d\mathbf{U} \quad (18)$$

The evolution equation of $f_{U|X}(\mathbf{U}, \mathbf{X}; t)$ is obtained from equations (16) and (17):

$$\begin{aligned} \frac{\partial}{\partial t} (f_X f_{U|X}) + U_j \frac{\partial}{\partial X_j} (f_X f_{U|X}) = & - \frac{\partial}{\partial U_j} \left(\left[-\frac{1}{\rho} \frac{\partial \langle P \rangle}{\partial X_j} + G_{ij} (U_j - \langle U_j \rangle) \right] f_X f_{U|X} \right) \\ & + \frac{1}{2} C_0 \langle \epsilon \rangle \frac{\partial^2}{\partial U_j \partial U_j} (f_X f_{U|X}) \end{aligned} \quad (19)$$

One deduces from equation (19) that the evolution of $f_{U|X}$ is identical to that of f_U (eq. (1)) provided that the following two consistency conditions are respected :

- $f_{U|X}$ and f_U have the same initial and boundary conditions
- f_X is constant

The first consistency condition can be enforced by applying relevant boundary and initial conditions on the SODEs. The second consistency condition is linked to the evolution of f_X . By integrating equation (19) over \mathbf{U} , and supposing that f_U and $f_{U|X}$ are equal, one deduces that :

$$\frac{\partial}{\partial t} (f_X) + \frac{\partial}{\partial X_j} (f_X \langle U_j \rangle) = 0 \quad (20)$$

This equation is identical to the evolution equation of the mean density, so that f_X is proportional to the mean density provided that they have proportional initial and boundary conditions. In our case, the density is constant, and so is the mean density. Consequently, f_X is constant provided that it has initial and boundary conditions proportional to those of ρ .

If the two consistency conditions are respected then we obtain:

$$f_{U|X} = f_U \quad (21)$$

In that case, we note that $\langle U_j \rangle^+$ can be replaced by $\langle \mathcal{U}_j | X = \mathbf{x}^+ \rangle$ in SODE (5) and by $\langle U_j | X \rangle$ in PDF equation (19). Besides, the mean continuity equation (4) is replaced by:

$$\text{div} \langle \mathbf{U} | X \rangle = 0 \quad (22)$$

2.2 EMC methods

In this section, we derive, from SODEs (5)-(6) and (13), two equivalent SPDEs governing the evolution of a stochastic Eulerian velocity \mathbf{u} and of a stochastic Eulerian density \mathbf{r} . Then we show that these SPDEs allow to solve PDF (1). Finally, we establish a correspondence between Lagrangian and Eulerian PDFs.

2.2.1 Eulerian equations

Following [1], SODEs (5)-(6) and (13) can be interpreted as the characteristics of the following first order hyperbolic SPDEs:

$$\frac{\partial \mathbf{r}}{\partial t} + \mathbf{u}_j \frac{\partial \mathbf{r}}{\partial x_j} = -\mathbf{r} \frac{\partial \mathcal{U}_j}{\partial x_j} \quad (23)$$

$$\frac{\partial \mathcal{U}_i}{\partial t} + \mathbf{u}_j \frac{\partial \mathcal{U}_i}{\partial x_j} = -\frac{1}{\rho} \frac{\partial \langle P \rangle}{\partial x_i} + G_{ij} (\mathcal{U}_j - \langle U_j \rangle) + \sqrt{C_0 \langle \epsilon \rangle} \dot{W}_j \quad (24)$$

$$\mathbf{r}(\mathbf{x}, t = 0) = \mathbf{r}_0(\mathbf{x}) \quad (25)$$

$$\mathbf{u}(\mathbf{x}, t = 0) = \mathbf{U}_0(\mathbf{x}) \quad (26)$$

SPDEs (23) and (24) are strictly equivalent to SODEs (5)-(6) and (13), and can be viewed as modeled Navier-Stokes equations in a Eulerian form. This system of hyperbolic SPDEs can be rewritten under a conservative form:

$$\frac{\partial \mathbf{r}}{\partial t} + \frac{\partial}{\partial x_j} (\mathbf{r} \mathcal{U}_j) = 0 \quad (27)$$

$$\frac{\partial}{\partial t} (\mathbf{r} \mathcal{U}_i) + \frac{\partial}{\partial x_j} (\mathbf{r} \mathcal{U}_j \mathcal{U}_i) = -\frac{\mathbf{r}}{\rho} \frac{\partial \langle P \rangle}{\partial x_i} + \mathbf{r} G_{ij} (\mathcal{U}_j - \langle U_j \rangle) + \mathbf{r} \sqrt{C_0 \langle \epsilon \rangle} \dot{W}_j \quad (28)$$

$$\mathbf{r}(\mathbf{x}, t = 0) = \mathbf{r}_0(\mathbf{x}) \quad (29)$$

$$\mathbf{u}(\mathbf{x}, t = 0) = \mathbf{U}_0(\mathbf{x}) \quad (30)$$

As it will be seen later (eq. (36)), $\langle U_j \rangle$ in equation (28) is determined from the Eulerian PDF of \mathbf{u} .

2.2.2 Eulerian PDF

The Eulerian PDF of the stochastic velocity \mathbf{u} is defined by :

$$f_{\mathbf{u}}(\mathbf{U}; \mathbf{x}, t) = \langle \delta(\mathbf{U} - \mathbf{u}(\mathbf{x}, t)) \rangle \quad (31)$$

In section 2.1.2, it was shown that the density \mathbf{r} associated with \mathbf{u} is variable. For a variable density flow, one usually does not work with unweighted (Reynolds) statistics

but with density weighted (Favre) statistics. We proceed here in the same way and introduce the PDF of the stochastic velocity \mathbf{u} weighted by the stochastic density :

$$f_{u:r}(\mathbf{U}; \mathbf{x}, t) = \frac{\langle \mathbf{r} \delta(\mathbf{U} - \mathbf{u}(\mathbf{x}, t)) \rangle}{\langle \mathbf{r} \rangle} = \frac{\langle \mathbf{r} | \mathbf{U} \rangle}{\langle \mathbf{r} \rangle} f_u(\mathbf{U}; x, t) \quad (32)$$

The mean of a quantity Q depending on \mathbf{u} and weighted by the stochastic density by will be noted as:

$$\langle Q \rangle_r = \int Q(\mathbf{U}) f_{u:r} d\mathbf{U} \quad (33)$$

By using standard techniques [7], one can show that the transport equation for $f_{u:r}$ is :

$$\begin{aligned} \frac{\partial}{\partial t} (\langle \mathbf{r} \rangle f_{u:r}) + U_j \frac{\partial}{\partial x_j} (\langle \mathbf{r} \rangle f_{u:r}) = & - \frac{\partial}{\partial U_j} \left(\left[-\frac{1}{\rho} \frac{\partial \langle P \rangle}{\partial x_j} + G_{ij} (U_j - \langle U_j \rangle) \right] \langle \mathbf{r} \rangle f_{u:r} \right) \\ & + \frac{1}{2} C_0 \langle \epsilon \rangle \frac{\partial^2}{\partial U_j \partial U_j} (\langle \mathbf{r} \rangle f_{u:r}) \end{aligned} \quad (34)$$

Consequently, we deduce that $f_{u:r}$ is identical to f_u , provided that the following consistency conditions are verified :

- $f_{u:r}$ and f_u have the same initial and boundary conditions
- $\langle \mathbf{r} \rangle$ is constant

The second consistency condition is linked to the evolution of $\langle \mathbf{r} \rangle$. Supposing that $f_{u:r}$ and f_u are equal, this evolution is given by :

$$\frac{\partial \langle \mathbf{r} \rangle}{\partial t} + \frac{\partial}{\partial x_j} (\langle \mathbf{r} \rangle \langle U_j \rangle) = 0 \quad (35)$$

This equation is identical to the transport equation of the mean physical density, so that $\langle \mathbf{r} \rangle$ is proportional to the mean physical density provided that they have proportional initial and boundary conditions. In our case, the physical density is constant, and so is the mean physical density. Consequently, $\langle \mathbf{r} \rangle$ is constant provided that it has initial and boundary conditions proportional to those of ρ .

When the two consistency conditions are verified then we have:

$$f_{u:r} = f_u \quad (36)$$

In that case, $\langle U_j \rangle = \langle \mathcal{U}_j \rangle_r$, and we note that $\langle U_j \rangle$ can be replaced by $\langle \mathcal{U}_j \rangle_r$ in SPDE (28) and in PDF equation (34). Besides, the mean continuity equation (4) is replaced by:

$$\text{div} \langle \mathbf{u} \rangle_r = 0 \quad (37)$$

As a conclusion, we showed that SPDEs (27)-(28) allow to solve PDF equation (1).

2.2.3 Link between Lagrangian and Eulerian statistics

To link Lagrangian and Eulerian statistics, we first introduce the mass m defined by:

$$m(\mathbf{x}_0) = \frac{\mathbf{r}_0(\mathbf{x}_0)}{f_{X_0}(\mathbf{x}_0)} \quad (38)$$

The mass $m(\mathbf{x}_0)$ can be interpreted as the mass transported along the individual trajectory originating from \mathbf{x}_0 . In the case of a constant density flow, f_{X_0} is constant, and it is also possible to choose \mathbf{r}_0 constant, so that we will suppose here that m is also a constant. The generalization to the case when m is variable can easily be done.

With the same techniques as in [1], it is possible to show that the following relation exists between Lagrangian and the Eulerian PDFs:

$$mf_X(\mathbf{X})f_{U|\mathbf{X}}(\mathbf{U}, \mathbf{X}) = \langle \mathbf{r} \rangle f_{U:\mathbf{x}}(\mathbf{U}; \mathbf{X}, t) \quad (39)$$

This equality can be split into two parts. By integrating equation (39) over velocity, one obtains:

$$mf_X = \langle \mathbf{r} \rangle \quad (40)$$

so that :

$$f_{U|\mathbf{X}} = f_{U:\mathbf{x}}(\mathbf{U}; \mathbf{x}, t) \quad (41)$$

Thus, the Eulerian weighted statistics are equivalent to the conditioned Lagrangian statistics. This equivalence shows that $f_{U|\mathbf{X}}$ is not a Eulerian PDF, i.e. the PDF of a Eulerian stochastic field. It is instead the PDF of a stochastic Eulerian velocity, weighted by a stochastic density. Besides, it is observed that the consistency conditions for the Lagrangian and Eulerian Monte Carlo are expressed in terms of equivalent quantities, i.e. f_X and $\langle \mathbf{r} \rangle$.

3 EMC METHOD FOR SOLVING THE VELOCITY-SCALAR PDF IN A LOW MACH NUMBER REACTING FLOW

We now turn our attention to the joint one-point PDF $f_{\mathbf{U}c}$ of a velocity field \mathbf{U} governed by the Navier-Stokes equations and of a scalar c governed by an advection-diffusion-reaction equation. For the sake of clarity, only one scalar is considered here, but all the subsequent reasonings can be straightforwardly extended to the case of multiple scalars. We will suppose that the reactive source term in the scalar equation, noted S , only depends on the reactive scalar c and on the density ρ : $S = S(c, \rho)$.

For variable density flows, it is a common practice to work with Favre statistics, it is to say with statistics weighted by the physical density ρ . Favre statistics are defined with

respect to the Reynolds (i.e. unweighted) statistics as follows: if $f_{\mathbf{U}c}$ is the unweighted one-point velocity-scalar PDF, then the Favre one-point PDF $\tilde{f}_{\mathbf{U}c}$ is defined by:

$$\tilde{f}_{\mathbf{U}c}(\mathbf{U}, c) = \frac{\langle \rho | \mathbf{U}, c \rangle}{\langle \rho \rangle} f_{\mathbf{U}c}(\mathbf{U}, c) \quad (42)$$

where $\langle \rho | \mathbf{U}, c \rangle$ represents the average of ρ conditioned on the velocity and scalar. The Reynolds average and Reynolds fluctuation of a quantity Q are respectively noted $\langle Q \rangle$ and $Q' = Q - \langle Q \rangle$. Its Favre average and Favre fluctuation are respectively noted \tilde{Q} and $Q'' = Q - \tilde{Q}$. From the definition of the Favre velocity-scalar PDF (eq. (42)), we recover, for Q depending on \mathbf{U} and c , the well known relation: $\tilde{Q} = \langle \rho Q \rangle / \langle \rho \rangle$.

In this work, we will restrict ourselves to low Mach number flows. As a consequence, the physical density can be approximated by a function of the reactive scalar c : $\rho = \rho(c)$. The source term is then be approximated by a function of c , $S = S(c)$, and the definition of the Favre PDF reduces to

$$\tilde{f}_{\mathbf{U}c}(\mathbf{U}, c) = \frac{\rho(c)}{\langle \rho \rangle} f_{\mathbf{U}c}(\mathbf{U}, c) \quad (43)$$

From the Navier-Stokes equations and from the evolution equation of c , it is possible to derive [4, 2] an exact transport equation for the Favre PDF $\tilde{f}_{\mathbf{U}c}$. In this equation, the advection and chemical reaction processes are treated exactly, while the effects of the pressure gradient, of the viscous stresses and of the scalar diffusion are unclosed.

As in section 2, we model the pressure and viscous terms with a Generalized Langevin model [5, 6]. As for the effects of the molecular diffusion of the scalars, we choose to model them with the IEM model [8]. By applying these models to the exact transport equation of the Favre one-point velocity-scalar PDF $\tilde{f}_{\mathbf{U}c}$, one obtains the following modeled equation:

$$\begin{aligned} \frac{\partial}{\partial t} (\langle \rho \rangle \tilde{f}_{\mathbf{U}c}) + \frac{\partial}{\partial x_j} (\langle \rho \rangle U_j \tilde{f}_{\mathbf{U}c}) = & - \frac{\partial}{\partial U_j} \left(\langle \rho \rangle \left[-\frac{1}{\rho} \frac{\partial \langle P \rangle}{\partial x_j} + G_{ij} (U_j - \tilde{U}_j) \right] \tilde{f}_{\mathbf{U}c} \right) \\ & + \frac{1}{2} C_0 \langle \rho \rangle \tilde{\epsilon} \frac{\partial^2 \tilde{f}_{\mathbf{U}c}}{\partial U_j \partial U_j} \\ & - \frac{\partial}{\partial c} \left(-\langle \rho \rangle \langle \omega_c \rangle (c - \tilde{c}) \tilde{f}_{\mathbf{U}c} + \langle \rho \rangle S \tilde{f}_{\mathbf{U}c} \right) \end{aligned} \quad (44)$$

The first two terms on the right-hand side correspond to the Generalized Langevin model, which has already been described in section 2. The last term on the right-hand side correspond to the IEM model and to the chemical source term. $\langle \omega_c \rangle$ is the mean scalar frequency.

Our objective in this section is to derive SPDEs for computing PDF equation (44). These SPDEs will govern the evolution of a stochastic velocity field noted \mathcal{U} and of a stochastic scalar field noted θ .

To achieve this objective, we follow exactly the same path as the one described in section 2. This leads us to introduce again a stochastic density noted \mathbf{r} , and to work with statistics weighted by this stochastic density.

We finally obtain that the following set of hyperbolic conservative SPDEs allows to compute the Favre PDF equation (44):

$$\frac{\partial \mathbf{r}}{\partial t} + \frac{\partial}{\partial x_j} (\mathbf{r} \mathcal{U}_j) = 0 \quad (45)$$

$$\frac{\partial}{\partial t} (\mathbf{r} \mathcal{U}_i) + \frac{\partial}{\partial x_j} (\mathbf{r} \mathcal{U}_j \mathcal{U}_i) = -\frac{\mathbf{r}}{\rho} \frac{\partial \langle P \rangle}{\partial x_i} + \mathbf{r} G_{ij} (\mathcal{U}_j - \langle \mathcal{U}_j \rangle_{\mathbf{r}}) + \mathbf{r} \sqrt{C_0 \epsilon} \tilde{W}_j \quad (46)$$

$$\frac{\partial}{\partial t} (\mathbf{r} \theta) + \frac{\partial}{\partial x_j} (\mathbf{r} \mathcal{U}_j \theta) = -\mathbf{r} \langle \omega_c \rangle (\theta - \langle \theta \rangle_{\mathbf{r}}) + \mathbf{r} S \quad (47)$$

As previously, the notation $\langle Q \rangle_{\mathbf{r}}$ refers to the mean of a quantity Q weighted by the stochastic density \mathbf{r} . We write in these SPDEs $\langle \mathcal{U}_j \rangle_{\mathbf{r}}$ (resp. $\langle \theta \rangle_{\mathbf{r}}$) instead of \tilde{U}_j (resp. $\tilde{\theta}$) since it will be proved later that those means are equal (eq. (51)).

Let us introduce $f_{\mathcal{U}\theta}$, the Eulerian PDF of \mathcal{U} and θ and let us define $f_{\mathcal{U}\theta;\mathbf{r}}$ as the Eulerian PDF of \mathcal{U} and θ weighted by the stochastic density \mathbf{r} :

$$f_{\mathcal{U}\theta;\mathbf{r}}(\mathcal{U}, \theta) = \frac{\langle \mathbf{r} | \mathcal{U}, \theta \rangle}{\langle \mathbf{r} \rangle} f_{\mathcal{U}\theta}(\mathcal{U}, \theta) \quad (48)$$

It can be shown that the transport equation of $f_{\mathcal{U}\theta;\mathbf{r}}$ is equation (44), provided that the following condition is verified :

$$\langle r \rangle = \langle \rho \rangle \quad (49)$$

The mean equation for \mathbf{r} is:

$$\frac{\partial \langle \mathbf{r} \rangle}{\partial t} + \frac{\partial}{\partial x_j} (\langle \mathbf{r} \rangle \langle \mathcal{U}_j \rangle_{\mathbf{r}}) = 0 \quad (50)$$

Thus, it is sufficient to take the same initial and boundary conditions for $\langle \mathbf{r} \rangle$ and $\langle \rho \rangle$ to ensure the consistency condition (49).

When consistency condition (49) is verified and when $\tilde{f}_{\mathbf{U}c}$ and $f_{\mathcal{U}\theta;\mathbf{r}}$ have the same initial and boundary conditions then:

$$\tilde{f}_{\mathbf{U}c} = f_{\mathcal{U}\theta;\mathbf{r}} \quad (51)$$

Finally, we would like to stress that the unweighted PDF $f_{\mathcal{U}\theta}$ has no direct physical meaning. The Favre PDF $\tilde{f}_{\mathbf{U}c}$ is given by the weighted PDF $f_{\mathcal{U}\theta;\mathbf{r}}$, and from equations (43) and (51), it is deduced that the Reynolds PDF $f_{\mathbf{U}c}$ is given by:

$$f_{\mathbf{U}c}(\mathbf{U}, c) = \frac{\langle \rho \rangle}{\rho(c)} \tilde{f}_{\mathbf{U}c}(\mathbf{U}, c) = \frac{\langle \mathbf{r} | \mathbf{U}, c \rangle}{\rho(c)} f_{\mathcal{U}\theta}(\mathbf{U}, c) \quad (52)$$

In the general case, $\langle \mathbf{r} | \mathbf{U}, c \rangle \neq \rho(c)$, so that :

$$f_{\mathbf{U}c} \neq f_{\mathcal{U}\theta} \quad (53)$$

4 MODIFIED EMC METHOD FOR SOLVING THE JOINT SCALAR PDF

In a previous work [1], Sabel'nikov and Soulard proposed a Eulerian Monte Carlo method for computing the Favre PDF of a turbulent reactive scalar c :

$$\frac{\partial}{\partial t} (\langle \rho \rangle \tilde{f}_c) + \frac{\partial}{\partial x_j} (\langle \rho \rangle \tilde{U}_j \tilde{f}_c) = \frac{\partial}{\partial x_j} \left(\langle \rho \rangle \Gamma_T \frac{\partial \tilde{f}_c}{\partial x_j} \right) - \frac{\partial}{\partial c} (\langle \rho \rangle [-\langle \omega_c \rangle (c - \tilde{c}) + S(c)] \tilde{f}_c) \quad (54)$$

$\Gamma_T = C_\mu \tilde{k}^2 / \tilde{\epsilon}$ is a turbulent diffusivity and models the effects of the fluctuating velocity on the scalar statistics. \tilde{k} the Favre averaged turbulent energy, $\tilde{\epsilon}$ is the turbulent dissipation and C_μ is a constant. \tilde{k} , $\tilde{\epsilon}$ and $\tilde{\mathbf{U}}$ are supposed to be known. For instance, they are computed from a RANS solver.

4.1 Derivation of SPDEs

PDF equation (54) is a limiting case of PDF equation (1): it can be formally obtained from equation (1) by letting the correlation time of the fluctuating velocity $\tau = \tilde{k} / \tilde{\epsilon}$ tend to zero, with respect to other correlation times, while keeping the diffusivity $\tilde{\epsilon} \tau^2$ proportional to Γ_T .

From this consideration, and because SPDEs (45)-(47) are statistically equivalent to PDF equation (1), we expect that, in the zero-correlation time limit, SPDEs (45)-(47) will tend to SPDEs which are statistically equivalent to PDF equation (54). This is what we show below, by deriving the limit SPDEs corresponding to equations (45)-(47).

In addition, we will also show that the equations we derive remain stochastically equivalent to PDF equation (54), even in the case of non zero-correlated velocity fields.

To facilitate our reasonings, we consider the simplified isotropic Langevin model (SLM) instead of the GLM [6]. In the SLM, the tensor G_{ij} reduces to [6]:

$$G_{ij} = \frac{1}{\tau_{rel}} \delta_{ij} \quad (55)$$

where:

$$\frac{1}{\tau_{rel}} = \left(\frac{1}{2} + \frac{3}{4} C_0 \right) \frac{\tilde{\epsilon}}{\tilde{k}} \quad (56)$$

The zero correlation time limit of \mathbf{u} corresponds to the limit $\tau_{rel} \rightarrow 0$, with the additional constraint that the diffusivity $\tilde{\epsilon} \tau_{rel}^2$ remains finite. In this limit, equation (46) reduces to :

$$r \circ \mathcal{U}_j - r \langle \mathcal{U}_j \rangle_{\mathbf{r}} + r \sqrt{C_0 \tilde{\epsilon} \tau_{rel}^2} \dot{W}_j = 0 \quad (57)$$

where the symbol \circ denotes the Stratonovitch interpretation of the stochastic product, while the absence of symbol denotes the Ito interpretation.

We note that before equation (57), stochastic products were interpreted with the Ito interpretation (see [7, 1] for a discussion on Ito versus Stratonovitch interpretations). The reason for using the Stratonovitch interpretation can be loosely explained as follows: let some stochastic process be described by a SPDE or an SODE with a rapidly fluctuating random multiplicative noise, having a small correlation time τ . Then, by definition, the asymptotic solution for $\tau \rightarrow 0$ is found by using the Stratonovitch interpretation of the multiplicative terms.

For the same reason, the limit SPDEs deduced from equations (45) and (47) for the density and the scalar are obtained with a Stratonovitch interpretation of the convection terms:

$$\frac{\partial \mathbf{r}}{\partial t} + \frac{\partial}{\partial x_j} (\mathbf{r} \circ \mathcal{U}_j) = 0 \quad (58)$$

$$\frac{\partial \mathbf{r}\theta}{\partial t} + \frac{\partial}{\partial x_j} ((\mathbf{r}\theta) \circ \mathcal{U}_j) = -\mathbf{r} \langle \omega_c \rangle (\theta - \langle \theta \rangle_{\mathbf{r}}) + \mathbf{r}S \quad (59)$$

There now remains to find a stochastic velocity \mathbf{u} satisfying equation (57). A solution to equation (57) is looked for in the form:

$$\mathbf{u} = \langle \mathcal{U} \rangle + \mathbf{u}' ; \mathbf{u}' = \sqrt{2D_T} \dot{\mathbf{W}} \quad (60)$$

with :

$$D_T = \frac{1}{2} C_0 \tilde{\epsilon} \tau_{rel}^2 = \frac{1}{2} \frac{C_0}{\left(\frac{1}{2} + \frac{3}{4} C_0\right)^2} \frac{\tilde{k}^2}{\tilde{\epsilon}} \quad (61)$$

Quite obviously, the equivalence between the stochastic equations and PDF equation (54) will require that D_T and Γ_T are equal. We will hereafter assume that the value of C_0 is chosen in order to respect this equality, so that we will have:

$$D_T = \Gamma_T \quad (62)$$

The form of solution (60) is directly suggested by equation (57). It only requires the unweighted mean velocity $\langle \mathcal{U} \rangle$ to be specified, for the solution to be complete.

However, the unweighted mean velocity $\langle \mathbf{u} \rangle$ is not directly linked to the physical system. Indeed, as mentioned in the previous sections, it is the weighted mean $\langle \mathbf{u} \rangle_{\mathbf{r}}$ which is meaningful. More precisely, we must have for consistency reasons:

$$\langle \mathbf{u} \rangle_{\mathbf{r}} = \tilde{\mathbf{U}} \quad (63)$$

Thus, if we can find a relation between $\langle \mathbf{u} \rangle$ and $\langle \mathbf{u} \rangle_{\mathbf{r}}$, then we will have found the solution to our problem.

To begin with, we must determine how $\langle \mathbf{u} \rangle_{\mathbf{r}}$ transforms when taking the zero-correlation time limit. This can be done by taking the average of equation (57), and by using the

fact that, with the Ito Interpretation, $\left\langle r \sqrt{C_0 \tilde{\epsilon} \tau_{rel}^2} \dot{W}_j \right\rangle = 0$. We obtain :

$$\langle \mathbf{r} \circ \mathcal{U}_j \rangle - \langle \mathbf{r} \rangle \langle \mathcal{U}_j \rangle_{\mathbf{r}} = 0 \Leftrightarrow \langle \mathcal{U}_j \rangle_{\mathbf{r}} = \frac{\langle \mathbf{r} \circ \mathcal{U}_j \rangle}{\langle \mathbf{r} \rangle} \quad (64)$$

Then, using the Ito-Stratonovitch correspondence [1], we may re-express $\langle \mathbf{r} \circ \mathcal{U}_j \rangle$ as :

$$\langle \mathbf{r} \circ \mathcal{U}_j \rangle = \langle \mathbf{r} \mathcal{U}_j \rangle + \frac{1}{2} \langle d\mathbf{r} \mathcal{U}_j \rangle \quad (65)$$

The stochastic density is a functional of \mathbf{U} . Its differential $d\mathbf{r}$ is deduced from equation (58):

$$d\mathbf{r} = -\frac{\partial}{\partial x_j} (\mathbf{r} \circ \mathcal{U}_j) dt \quad (66)$$

Using the properties of the Ito interpretation, we then deduce that :

$$\begin{aligned} \langle \mathbf{r} \circ \mathcal{U}_j \rangle &= \langle \mathbf{r} \rangle \langle \mathcal{U}_j \rangle - \frac{1}{2} \sqrt{\Gamma_T} \frac{\partial}{\partial x_j} \left(\langle \mathbf{r} \rangle \sqrt{\Gamma_T} \right) \\ &= \langle \mathbf{r} \rangle \langle \mathcal{U}_j \rangle - \frac{1}{2} \langle \mathbf{r} \rangle \frac{\partial \Gamma_T}{\partial x_j} - \Gamma_T \frac{\partial \langle \mathbf{r} \rangle}{\partial x_j} \end{aligned} \quad (67)$$

so that:

$$\langle \mathcal{U}_j \rangle = \langle \mathcal{U}_j \rangle_{\mathbf{r}} + \frac{1}{2} \frac{\partial \Gamma_T}{\partial x_j} + \frac{1}{\langle \mathbf{r} \rangle} \frac{\partial \langle \mathbf{r} \rangle}{\partial x_j} \quad (68)$$

Then, using the consistency conditions $\langle \mathcal{U}_j \rangle_{\mathbf{r}} = \widetilde{U}_j$ and $\langle \mathbf{r} \rangle = \langle \rho \rangle$, we finally obtain that:

$$\langle \mathcal{U}_j \rangle = \widetilde{U}_j + \frac{1}{2} \frac{\partial \Gamma_T}{\partial x_j} + \frac{1}{\langle \rho \rangle} \frac{\partial \langle \rho \rangle}{\partial x_j} \quad (69)$$

Thus, we derived the following system of SPDEs :

$$\mathcal{U}_i = \widetilde{U}_i + \Gamma_T \frac{1}{\langle \rho \rangle} \frac{\partial \langle \rho \rangle}{\partial x_i} + \frac{1}{2} \frac{\partial \Gamma_T}{\partial x_i} + \sqrt{2\Gamma_T} \dot{W}_i \quad (70)$$

$$\frac{\partial \mathbf{r}}{\partial t} + \frac{\partial}{\partial x_j} (\mathbf{r} \circ \mathcal{U}_j) = 0 \quad (71)$$

$$\frac{\partial}{\partial t} (\mathbf{r} \theta) + \frac{\partial}{\partial x_j} ((\mathbf{r} \theta) \circ \mathcal{U}_j) = -\mathbf{r} \langle \omega_c \rangle (\theta - \langle \theta \rangle_{\mathbf{r}}) + \mathbf{r} S \quad (72)$$

By deriving the PDF equation corresponding to SPDEs (70)-(72), it can be shown that this system is statistically equivalent to PDF equation (54). Besides, this remains true even in the case when τ_{rel} is not small.

4.2 Some remarks on SPDEs (70)-(72)

We note that \mathbf{u}'' , the fluctuating part of the stochastic velocity, verifies the relation:

$$\widetilde{\mathbf{u}}'' \equiv \langle \mathbf{u} - \langle \mathbf{u} \rangle_{\mathbf{x}} \rangle_{\mathbf{x}} = 0 \quad (73)$$

We also note that equations (70)-(72) are in conservative form. This may simplify the numerical integration of the method in CFD codes, which are often based on conservative numerical schemes.

The formulation (70)-(72) is different from the one proposed in [1]. First, the stochastic scalar equation in [1] is proposed in such a manner that ensemble averaging gives immediately Favre statistics. Due to this, in [1], the stochastic density (eq. (71)) is not needed, and the equation for the stochastic scalar is not in conservative form.

The formulation (70)-(72) has been validated by M. Ourliac on test cases identical to those proposed in [1]. The results were similar to those obtained with the first formulation [1].

The EMC method based on SPDEs (70)-(72) has been implemented into CEDRE, the industrial CFD code of ONERA. It is currently applied to compute a premixed methane/air flame over a backward facing step. This flame was also calculated in [9] with the formulation proposed in [1]. Results obtained with both formulations were found to be similar.

5 CONCLUSIONS

In this article, we derived SPDEs for computing the modeled one-point transport equation of the velocity scalar PDF. By using the notion of stochastic characteristic, we established SPDEs equivalent to the SODEs used in LMC methods. Then, we put forward the link between Lagrangian and Eulerian one-point statistics. This led us to introduce a stochastic density, and to consider statistics weighted by this stochastic density. As a result of these procedures, we obtained SPDEs that are hyperbolic and in conservative form.

The next step in the development of an EMC method will consist in doing a numerical analysis of the SPDEs that we derived, and in testing their applicability on simplified one-dimensional configurations. Then, we will apply it to the calculation of a practical case and compare the results against other methods, in particular against LMC methods.

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