Mean Field Equations in PDF Particle Methods for Turbulent Reactive Flows

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FDA 97-06

June 1997

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1 INTRODUCTION

In the last two decades, several different particle-mesh methods have been proposed to solve different modelled PDF equations for turbulent reactive flows. In these methods, the particles contain information equivalent to the joint PDF considered; but there are usually one or more mean fields that are determined separately, by a partial differential equation (PDE) which is solved on the mesh. An important distinction between the different methods is the mean field equations that are solved, and how these mean fields (and also those estimated from the particles) are used.

The purpose of this paper is to identify the important issues in this context, to classify previous approaches, and to suggest promising approaches for future investigation.

2 PDF2DS

We illustrate the issues involved by considering a specific method, namely the hybrid velocity-composition PDF/k-ε finite-volume method used in the code *pdf2ds* (Correa and Pope 1992). This code has also been used by Chang (1996), Tsai and Fox (1996), Wouters et al. (1996) and Nau et al. (1996).

As shown in Fig. 1, the particle properties are density, ρ, velocity, $\mathbf{U}$, and composition, $\boldsymbol{\phi}$. From these particle properties, various mean fields can be estimated. We refer to these as "particle fields" to distinguish them from the mean fields obtained from PDEs. Examples of the particle fields that can be obtained are the mean density $\langle \rho \rangle$, the mass-weighted mean velocity and composition $\tilde{\mathbf{U}}$ and $\tilde{\boldsymbol{\phi}}$, and second moments such as Reynolds stresses $\widetilde{u_i'' u_j''}$ and scalar fluxes $\widetilde{u_i'' \phi_\alpha''}$.

In this method, mean field equations are solved for $\tilde{\mathbf{U}}$, the mean pressure $\langle p \rangle$, as well as for the turbulence model quantities k and ε.

The interconnection between the mean field equations and the particle equations is determined by the mean fields used in each of these. The mean field equations use the mean density $\langle \rho \rangle$ obtained from the particles. In the particle equations, the particle field $\tilde{\boldsymbol{\phi}}$ is used (in the IEM mixing model); and also used are the mean fields $\tilde{\mathbf{U}}$, $\langle p \rangle$, k and ε.

Some fields are represented both as mean fields and as particle fields. In *pdf2ds*, the "duplicate fields" are $\tilde{\mathbf{U}}$ and $\widetilde{u_i'' u_j''}$. This obviously raises questions

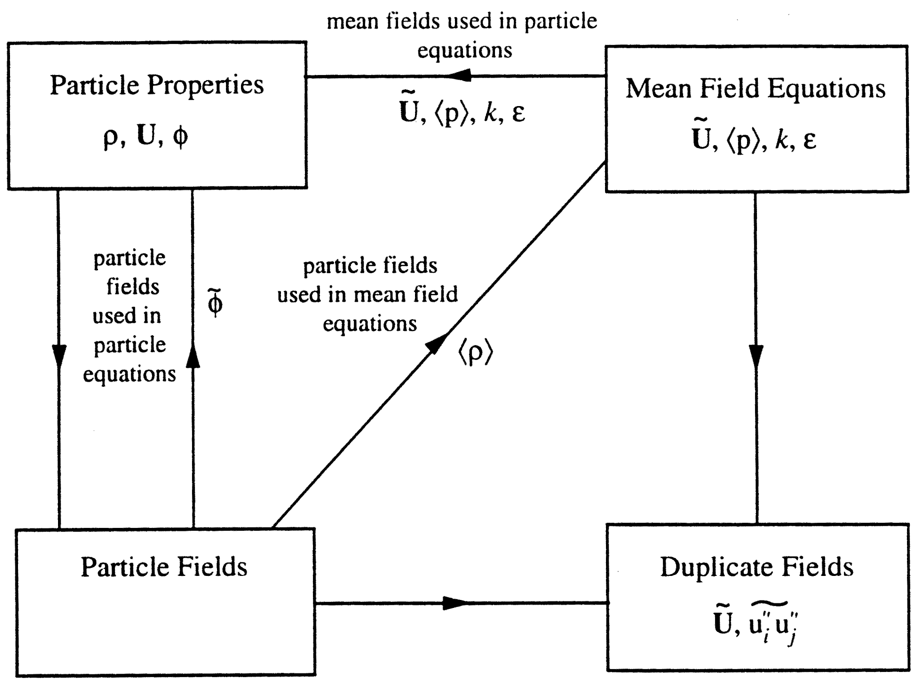

Figure 1: Fields used in *pdf2ds*.

of consistency, some of which are considered by Pope (1994) and Wouters et al. (1996).

This discussion identifies the following as important considerations:

1. the particle properties represented—which determines the *level* of the PDF model
2. the particle equations (i.e., the specific models used)—which determines the mean fields required in the solution of the particle equations
3. the particle fields used in the particle equations
4. the mean fields used in the particle equations
5. the mean field equations solved
6. the particle means used in the mean field equations

7. the duplicate fields—those that are represented both as particle fields and as mean fields.

Table 1 summarizes the attributes of different methods (discussed below) with respect to these considerations.

3 USE OF PARTICLE FIELDS AND MEAN FIELDS

It may be seen from Table 1 (from the last three rows in particular) that, for a given PDF model, several different choices can be made about which PDEs are solved for mean fields, and which fields are used in the particle equations. The fundamental considerations are:

1. the particle fields contain statistical errors (that appear as "noise")
2. time-averaging and different smoothing techniques can be used to reduce—but not remove—the statistical error
3. the use of particle fields in the particle equations can lead to bias (Xu and Pope 1997)
4. the use of particle fields in the field equations can lead to difficulties with convergence (because of the noise)
5. the solution of PDEs for mean fields requires additional algorithms and coding beyond the particle-mesh method
6. the existence of duplicate fields raises issues of consistency
7. the interconnection between the particles, the particle fields and the mean fields can potentially lead to numerical instabilities that are extremely difficult to analyse.

Table 1: Attributes of different PDF solution algorithms

Method	Particle Properties	Particle Fields used in Particle Equations	Mean Fields used in Particle Equations	Particle Fields used in Mean Field Equations	Mean Field Equations	Duplicate Fields
Composition jpdf (Pope 1981, Pope 1985)	ρ, ϕ	$\tilde{\phi}$	$\tilde{\mathbf{U}}$, Γ_T, $\tilde{\omega}$	$\langle\rho\rangle$	$\tilde{\mathbf{U}}$, $\langle p\rangle$, k, ε	-
Composition jpdf (Jaberi et al. 1997)	ρ, ϕ, $z(\phi)$	$\tilde{\phi}$	$\tilde{\mathbf{U}}$, Γ_T, $\tilde{\omega}$	$\tilde{\tilde{z}}$, $\widetilde{\mathbf{u}''z''}$	$\tilde{\mathbf{U}}$, $\langle p\rangle$, $\tilde{z}$, k, ε, $\langle\rho\rangle$	$\tilde{z}$
Velocity-composition jpdf, minimal particle properties (*pdf2ds*)	ρ, $\mathbf{U}$, ϕ	$\tilde{\phi}$	$\tilde{\mathbf{U}}$, k, ε, $\langle p\rangle$	$\langle\rho\rangle$	$\tilde{\mathbf{U}}$, $\langle p\rangle$, k, ε	$\tilde{\mathbf{U}}$, $\widetilde{u_i''u_j''}$
Velocity-composition jpdf, maximal particle properties (Anand et al. 1989, Haworth and El Tahry 1991)	ρ, $\mathbf{U}$, ϕ	$\tilde{\phi}$, k	$\tilde{\mathbf{U}}$, ε, $\langle p\rangle$	$\langle\rho\rangle$, $\widetilde{u_i''u_j''}$	$\tilde{\mathbf{U}}$, $\langle p\rangle$, ε	$\tilde{\mathbf{U}}$
Velocity-frequency-composition jdpdf *pdf2dv*	ρ, $\mathbf{U}$, ω, ϕ	$\tilde{\mathbf{U}}$, $\widetilde{u_i''u_j''}$, $\tilde{\omega}$, Ω, $\tilde{\phi}$	$\langle p\rangle$	$\langle\rho\mathbf{U}\rangle$	$\langle p\rangle$	-
Velocity-frequency-composition jpdf SPH (Welton and Pope 1996)	ρ, $\mathbf{U}$, ω, ϕ, p	$\tilde{\mathbf{U}}$, $\widetilde{u_i''u_j''}$, $\tilde{\omega}$, $\tilde{\phi}$, $\langle p\rangle$	-	-	-	-
Velocity-frequency-composition jpdf (proposed)	ρ, $\mathbf{U}$, ω, ϕ, $z(\phi)$	$\widetilde{u_i''u_j''}$, $\tilde{\omega}$, Ω, $\tilde{\phi}$	$\tilde{\mathbf{U}}$, $\langle p\rangle$	$\widetilde{u_i''u_j''}$, $\tilde{\tilde{z}}$, $\widetilde{\mathbf{u}''z''}$	$\tilde{\mathbf{U}}$, $\langle p\rangle$, $\tilde{z}$, $\langle\rho\rangle$	$\tilde{\mathbf{U}}$, $\tilde{z}$

4 DISCUSSION OF DIFFERENT METHODS

Some of the methods shown in Table 1 are now discussed in relation to the above considerations.

4.1 JDPF of Composition I

The model equation for the joint PDF of compositions can be solved by either an Eulerian or a Lagrangian algorithm. The Eulerian algorithm (developed by Pope 1981) has been used by Roekaerts (1991), Hsu et al. (1994). Jones and Prasetyo (1996), Biagioli (1997), Tatschl et al. (1997) and Zurbach et al. (1997). The Lagrangian algorithm (Pope 1985) has been used by Tsai and Fox 1996, Tolpadi et al. (1996) and Colucci et al. (1997).

As in all the methods, the particle mean $\tilde{\phi}$ is used in the IEM mixing model. Experience shows that (from a numerical viewpoint) this is entirely satisfactory: it has not been found to cause any difficulties.

The use of the noisy particle density field $\langle \rho \rangle$ in the mean field equations has been found to be a significant problem. It can hinder and even prevent the convergence of the PDE solution (see, e.g., Chang 1996).

4.2 JDPF of Composition II

This method, developed by Jaberi et al. (1997), is designed to alleviate the problem, just mentioned, of the adverse effects of noise in the particle density field.

The quantity z is defined by

$$z = \mathcal{R} \sum_{\alpha} Y_\alpha / W_\alpha, \tag{1}$$

where $\mathcal{R}$ is the universal gas constant, Y_α is the mass fraction and W_α is the molecular weight of species α. Then the ideal gas law is

$$p = \rho z, \tag{2}$$

with mean

$$\langle p \rangle = \langle \rho \rangle \tilde{z}. \tag{3}$$

Thus $\tilde{z}$ is precisely the quantity needed to relate $\langle p \rangle$ to $\langle \rho \rangle$ in the mean equation of state. (Note that z has dimensions of specific energy.)

For each particle, z is determined by the particle composition ϕ, and so its evolution is determined by that of ϕ. Let the particle evolution be written simply as

$$\frac{dz}{dt} = \dot{z}. \tag{4}$$

Then the corresponding equation for $\tilde{z}$ is

$$\frac{\partial}{\partial t}(\langle \rho \rangle \tilde{z}) + \nabla \cdot (\langle \rho \rangle \tilde{\mathbf{U}} \tilde{z}) + \nabla \cdot (\langle \rho \rangle \widetilde{\mathbf{u}'' z''}) = \langle \rho \rangle \tilde{\dot{z}}. \tag{5}$$

In this method, mean field equations are solved for (among other quantities) $\langle \rho \rangle$ and $\tilde{z}$, with $\langle p \rangle$ being obtained from the mean equation of state. (Or alternatively, in a pressure based method, a PDE is solved for $\langle p \rangle$, and $\langle \rho \rangle$ is obtained from the mean equation of state.) The fields of $\widetilde{\mathbf{u}'' z''}$ and $\tilde{\dot{z}}$ required in the equation for $\tilde{z}$ are obtained from the particles. The resulting noise in the $\langle \rho \rangle$ field is substantially reduced compared to particle field $\langle \rho \rangle$.

4.3 Velocity-Frequency-Composition JPDF (pdf2dv)

By design, the code *pdf2dv* uses particle fields throughout, except for the mean pressure field $\langle p \rangle$. While the code successfully solves the PDF equations, it has two shortcomings:

i) the pressure algorithm is complicated, it requires damping and dissipation, and may not be very accurate (on grid sizes normally used) (see e.g., Delarue 1997)

ii) it has been found that the use of the particle mean velocity field leads to substantial bias (Xu and Pope 1997).

4.4 Velocity-Frequency-Composition JPDF (Proposed)

The shortcomings just mentioned are avoided in the proposed method.

Field equations are solved for mean mass, momentum and energy conservation:

$$\frac{\partial \langle \rho \rangle}{\partial t} + \frac{\partial}{\partial x_i}(\langle \rho \rangle \tilde{U}_i) = 0, \tag{6}$$

$$\frac{\partial}{\partial t}(\langle\rho\rangle\tilde{U}_j) + \frac{\partial}{\partial x_i}(\langle\rho\rangle\tilde{U}_i\tilde{U}_j + \langle p\rangle\delta_{ij}) = -\frac{\partial}{\partial x_i}(\langle\rho\rangle\widetilde{u_i''u_j''}), \tag{7}$$

$$\frac{\partial}{\partial t}(\langle\rho\rangle\tilde{z}) + \frac{\partial}{\partial x_i}(\langle\rho\rangle\tilde{U}_i\tilde{z}) = -\frac{\partial}{\partial x_i}(\langle\rho\rangle\widetilde{u_i''z''}) + \langle\rho\rangle\tilde{\dot{z}}, \tag{8}$$

with the mean equation of state,

$$\langle p\rangle = \langle\rho\rangle\tilde{z}. \tag{9}$$

The quantities $\widetilde{u_i''u_j''}$, $\widetilde{u_i''z''}$ and $\tilde{\dot{z}}$ on the right-hand sides of the PDEs are obtained from the particles.

This set of equations is of the same structure as that usually considered in CFD, and so established techniques can be used. However, the turbulent fluxes and the source $\tilde{\dot{z}}$ are not known as functions of the dependent variables, and so exact linearizations for use in implicit methods is not possible.

The mean field $\tilde{\mathbf{U}}$ is used in the particle method, which is expected to reduce the bias substantially.

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