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Numerical Issues of Monte Carlo PDF for Large Eddy Simulations of Turbulent Flames

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Abstract

Monte Carlo simulations of joint PDF approaches have been extensively developed in the past largely with Reynolds Averaged Navier Stokes (RANS) equations. Current interests are in the extension of PDF approaches to Large Eddy Simulation (LES). As LES intends to resolve the large scales of turbulence in time, the coupling between Monte Carlo simulation and the flow field becomes an important issue. It is crucial to ensure some sort of coherency between the scalar field solution obtained via finite-volume methods and that from the stochastic solution of the PDF. In this paper, we first review the advantages and disadvantages of Eulerian and Lagrangian approaches. In order to clarify the coherency feature of a solution method, we introduce the concept of stochastic convergence for hybrid methods. Secondly, we present some preliminary results of an ongoing study with the Eulerian approach that reveals the numerical issues needing to be resolved. Results are presented for simulations of a pure mixing jet and Sandia Flame D using a steady-state flamelet model.

Introduction

Large Eddy Simulation (LES) allows resolving the large scales of turbulence. The small scales can be modeled according to base principles, which should inherently have universal applicability to all types of flow. The extension of non-reactive, three-dimensional LES to the case of low Mach number combustion, such as jet flames, and opposed jet flames, must proceed through the modeling of the turbulent combustion process. In the past twenty years, methods based on the solution of a transport equation for the velocity-scalar joint PDF, or for the scalars joint PDF alone, have received increasing attention due to their promise for a more accurate description of the coupling between turbulent transport, chemistry and molecular diffusion. Unfortunately, the resulting equation is multidimensional, its' dimensionality scaling proportionally to the number of reactive scalars. A numerical integration strategy based on finite discretization methods would require too much memory and computational time. The only feasible option is to solve the PDF transport equation via stochastic methods. In this framework, it is crucial to assure some coherency between the flow field solution obtained via finite discretization methods, and the stochastic solution of the PDF. In this paper, we first review the advantages and disadvantages of Eulerian and Lagrangian approaches. Also, we introduce the concept of stochastic convergence for hybrid methods. Secondly, we present some preliminary results of an ongoing investigation that compares solutions from a 1st-order upwind finite-volume method and Eulerian Monte Carlo PDF method of the same space-time accuracy. We solve for the mixture fraction both directly via finite-volume and through an Euler-based Monte Carlo simulation. Some preliminary results are presented for a simulation conducted on pure mixing jet and Sandia flame D with a steady-

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state flamelet model. Comparisons reveal numerical issues needing to be resolved before stochastic methods can be used in LES in a numerically coherent fashion.

Eulerian and Lagrangian Monte Carlo PDF Methods

Monte Carlo simulations of joint PDF approaches have been extensively developed in the past largely with Reynolds Averaged Navier Stokes (RANS) equations (e.g. Pope, 1985, Chen et al., 1989, Pope, 1990). Much of the past effort focused on development of physical models, such as mixing models and reduced chemistry. As current interests are in the extension of PDF approaches to Large Eddy Simulation (LES), the numerical accuracy of present stochastic schemes needs to be greatly improved so that they are compatible with LES. Also, a deeper understanding of the issues involved in the use of hybrid methods (finite-volume methods combined with stochastic methods) must be gained. For these scalars that can be solved for using both methods, we would expect the statistical averages to match. Furthermore, their values should match at any instant as closely as possible in order to capture all the important flow features, exploiting the full potential of LES. Let us start by considering the transport equation for the joint scalar PDF, $\widetilde{P}_\phi$, for high Reynolds turbulent flames has the following form.

$$\begin{aligned}\bar{\rho}\frac{\partial \widetilde{P}_\phi}{\partial t} + \bar{\rho}\widetilde{\boldsymbol{\upsilon}}\cdot\nabla\widetilde{P}_\phi + \nabla\cdot(\bar{\rho} < \boldsymbol{\upsilon}'' \mid \phi_i = \psi_i > \widetilde{P}_\phi) = \\ -\frac{\partial}{\partial \psi_\alpha}(\bar{\rho}S_\alpha(\psi)\widetilde{P}_\phi) - \sum_{i=1}^{N}\sum_{j=1}^{N}\frac{\partial^2}{\partial\psi_i\partial\psi_j}\left[\bar{\rho} < \varepsilon_{ij} \mid \phi_i = \psi_i > \widetilde{P}_\phi\right]\end{aligned} \tag{1}$$

The terms on the left hand side represent the physical transport of adjacent fluids to the local location through turbulent mean and fluctuating velocities. The terms on the right hand side are due to chemical reactions and mixing at the molecular level. When stochastic simulations are used to solve for these processes, two main sources of error must be considered. Due to obvious constraints, the PDF is represented by a finite ensemble of *N* stochastic particles within each finite volume cell. Using a finite number of stochastic particles to present the PDF leads to stochastic or statistical errors. Additionally, every time a differential equation is discretized, truncation errors are introduced. The overall numerical errors associated with current stochastic schemes are then due to both these sources. Nevertheless, it can be argued that if a hybrid scheme is "well constructed", as the number of stochastic particles is increased, stochastic errors should tend to zero. As the number of particles increases, we expect the stochastic solution to converge (in a numerical sense) to the solution obtained via classic discrete methods (in our case, FV methods). We establish such concept of instantaneous-local coherence (i.e. at the level of space-time fluctuations resolved by the scheme), by defining the notion of stochastic convergence of the hybrid scheme.

For the joint scalar PDF, two approaches have been developed in the past: Eulerian and Lagrangian Monte Carlo methods. Both approaches are coupled to FV methods forming hybrid algorithms. In the Eulerian approach, stochastic particles are held fixed at each finite volume cell, while their properties evolve in time to simulate the different processes. An update equation can be written as Eq. (2) below

$$\widetilde{P}(t+\Delta t) = (I+\Delta tCD)\cdot(I+\Delta tM)\cdot(I+\Delta tR)\cdot\widetilde{P}(t) \tag{2}$$

where *CD* represents the transport process (convection by turbulent mean and fluctuating velocities), *M* stands for the molecular mixing, and *R* identifies the contribution due to chemical reaction. Discretization schemes identical to these used in typical FV schemes are used in developing the operator splitting updates for Eulerian algorithms. As such, the Eulerian algorithm displays the stochastic convergence property defined above.

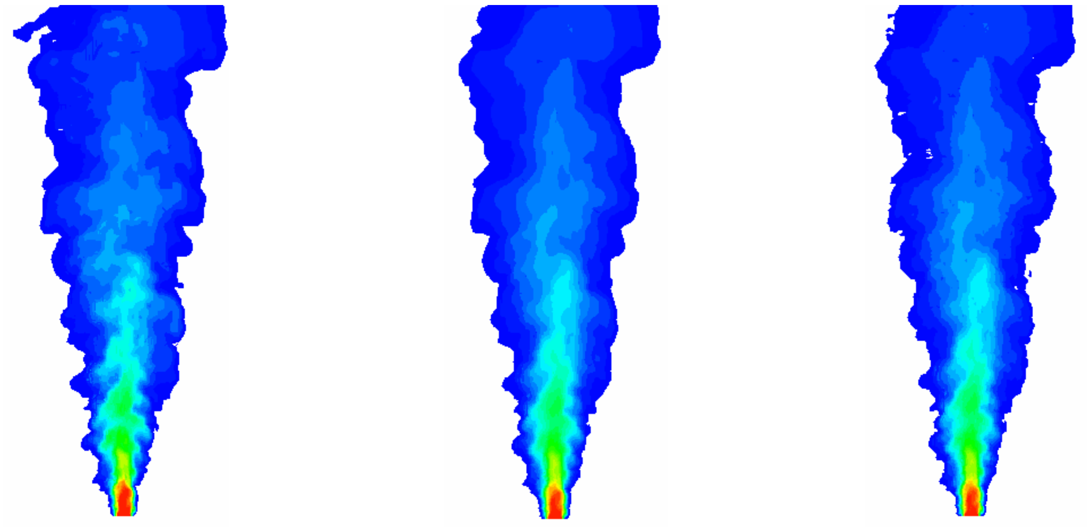
The particles in the Lagragian method move through the computation domain according to their respective stochastic equation for each process. For example, to simulate the turbulent convection and diffusion, the locations of particles move according to the following stochastic equation

$$\underline{X}^{(p)}(t+\Delta t) = \underline{X}^{(p)}(t) + \Delta t \cdot \underline{U} + (2\Delta t D_{eff})^{1/2} \cdot \underline{\xi} \tag{3}$$

where $\underline{U}$ is the filtered velocity, and D_{eff} is the effective turbulent diffusivity, and $\underline{\xi}$ is a standardized joint normal random vector. Most importantly, the numerical solutions from the Lagrangian algorithm have been found inconsistent with the FV methods. For instance, in the Lagrangian approach, each particle is assigned a mass. The actual PDF is recovered by sampling the particles falling into all of the FV cells and by determining a mean density for each cell. However, such mean density is not guaranteed to be the same as that obtained from the FV method as the particles move with the mean velocity and some random motions. Similarly, when the joint scalar-velocity PDF is solved, the mean value of fluctuating velocity is likely to deviate from zero; the expected correct value. Correction algorithms are needed to maintain a correct spatial distribution of particles so that the consistency between the FV solutions and the stochastic solutions can be maintained at the numerical level. Several studies have been devoted to this difficult numerical issue (e.g., Muradoglu et al, 1999, 2001; Zhang and Haworth, 2004). So far, these correction algorithms are at best 2nd-order accurate in space and they are far from perfect. More critically, these correction algorithms only ensure consistency for statistical averages but not at any instant, a requirement that is not only highly desirable but perhaps mandatory for LES applications. Hence, Lagrangian hybrid method do not naturally display stochastic convergence in the sense defined above. Tracking and sorting particles consume the majority of computational time. In addition, the CPU time used for such corrections can be significant. Past experiences with the RANS applications revealed that the Eulerian Monte Carlo approach is computationally faster (by roughly a factor of 10) and easier to implement than the corresponding Lagrangian method (Mobus et al 2001; Wilmes et al 2004). Furthermore, for practical geometries, extending the Lagrangian approach to unstructured grids is a challenging task (e.g., Subramanian and Howard 2000) but this extension is straightforward using the Eulerian approach. Finally, creating adaptive Lagrangian schemes appears as a daunting task, given the impossibility of controlling the location of the stochastic particles in the flow field. As a consequence of all of the observations above, the solutions obtained from Lagrangian hybrid algorithms not only do not display the property of stochastic coherence, but they are also rich in implementation difficulties.

Eulerian approach with LES

Applications of the Eulerian approach to LES are explored in this paper. The following exploring study using the Eulerian approach in LES for jet mixing problems confirms the stochastic convergence property of the hybrid method encompassing an Eulerian stochastic method with FV algorithm. Figure 1 shows a comparison of computed instantaneous mixture fraction contours from (a) 2nd-order FV method, (b) 1st-order upwind FV and (c) the Eulerian approach for a jet mixing problem. Comparisons of the two right plots reveal that the solutions from the Eulerian method and from the 1st-order upwind FV method are almost identical at the instantaneous level. Note, however that these two 1st-order solutions contain high level of numerical diffusion and hence, they miss many detailed features exhibited in the solution by the 2nd-order scheme (a). Figure 2 further compares the computed instantaneous values of mixture fraction along the jet centerline. To the eyes, the solutions from the 1st-order Eulerian Monte Carlo are identical to those from the corresponding FV scheme. Once again we reiterate the fact that since these two schemes are consistent at the numerical level, i.e. they adopt the same discretization scheme, the differences between the two solutions are caused only by the statistical errors that should decrease with



(a) (b) (c)

Figure 1. A comparison of computed instantaneous mixture fraction contour from (a) 2nd-order TVD FV method, (b) 1st-order upwind FV and (c) the 1st-order Eulerian approach for a jet mixing problem.

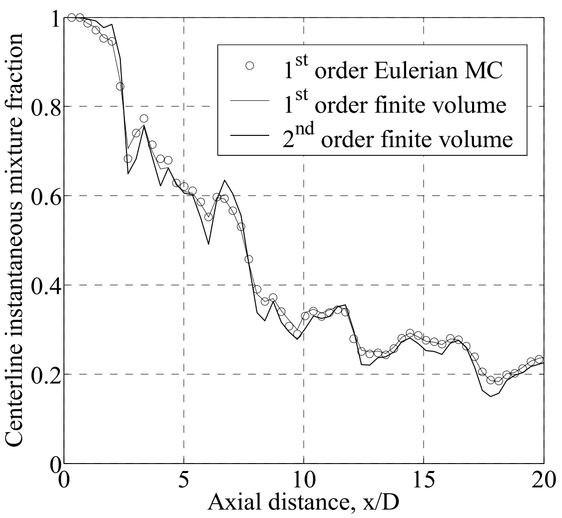


Figure 2. A comparison of finite-volume method and the Eulerian approach for jet mixing problem showing full consistency between the two solutions.

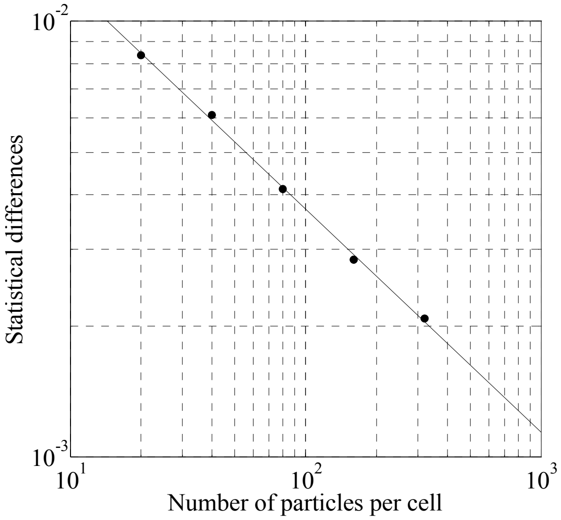


Figure 3. The differences between the FV and Eulerian stochastic solutions show a square root dependence from the number of particles.

the square root of the total of number particles per cell. Indeed, in Figure 3, the statistical differences between several solutions from the Eulerian Monte Carlo simulations with different numbers of particles per cell and the 1st-order finite-volume method show a decreasing trend with the square root of number particle. One observation on the overall accuracy of the method is necessary. As revealed in Figs. 1 and 2, the solutions obtained with a 2nd-order TVD scheme clearly show the need of improvements in the low-order schemes as they exhibit substantial numerical diffusion and hence miss many detailed features of the flow.

A consistency check has also been conducted for the Sandia piloted jet flame: Flame D. The Eulerian PDF simulation was carried out with 40 particles per cell using a steady-state flamelet model. The LES flow solver developed by Kempf et al. (2004) was used with a grid of (250 x 35 x 40, for axial x radial x azimuthal directions respectively).

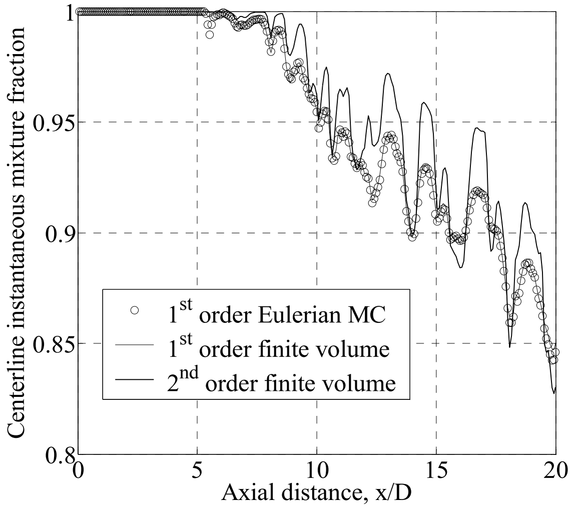


Figure 4. Predicted instantaneous mixture profiles along jet centerline for the Sandia Flame D. Results from the Eulerian PDF with 40 particles/cell are seen in consistency with the corresponding 1st-order FV method.

Figure 4 compares the computed instantaneous profiles along the centerline using the three methods. The consistency between the Eulerian method and the corresponding 1st-order FV method is again confirmed. Note that, as being more diffusive, the 1st-order methods give a slightly faster decay than the 2nd-order FV method as expected.

Conclusions

The Eulerian Monte Carlo PDF approach has been implemented into LES for predictions of turbulent mixing jet as well as a piloted jet flame. Both results show that the resulting hybrid scheme displays the stochastic convergence property as defined in this paper. Although the 1st-order Eulerian approach presented has many advantages, its major deficiency is the low numerical accuracy in treating the advection terms (see Figs 1 and 2). This low-accuracy issue needs to be resolved in order to be numerically compatible with LES. Future work will concentrate on the extension of the Eulerian method to 2nd-order accuracy, keeping the overall hybrid scheme fully consistent in light of the newly defined stochastic convergence property.

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