Applied Filtered Density Function

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ABSTRACT

An overview is presented of recent advances in the filtered density function (FDF) modeling and simulation of turbulent combustion. The review is focused on the developments that have facilitated the FDF to be broadly applied in large eddy simulation (LES) of practical flows. These are primarily the development of a new Lagrangian Monte Carlo solver for the FDF, and the implementation of this solver on Eulerian domains portrayed by unstructured grids. With these developments, it is now much easier to apply FDF for predictions of reacting flows in complex geometrical configurations.

1. INTRODUCTION

The filtered density function (FDF); including its mass weighted form, the filtered mass density function (FMDF), is now considered as one of the most effective means of conducting large eddy simulation (LES) in turbulent combustion Givi (2006). The FDF is essentially the counterpart of the probability density function (PDF) methods in Reynolds-averaged Navier-Stokes (RANS) simulations Pope (2013). In its *stand-alone* form, the FDF must account for the joint statistics of all of the relevant physical variables. The most sophisticated FDF closure available to-date is the frequency-velocity-scalar FMDF (FVS-FMDF) Sheikhi *et al.* (2009). A simpler version (VS-FMDF) that does not include the subgrid-scale (SGS) frequency also exists (Sheikhi *et al.* 2003, 2007). Hydrodynamic closure in incompressible, non-reacting flows has been successfully achieved via the velocity-FDF (V-FDF) Gicquel *et al.* (2002). The scalar FDF (S-FDF and S-FMDF) is the most widely used form and considers only the scalar field. This is the most elementary form of the FDF that we first introduced (Colucci *et al.* 1998; Garrick *et al.* 1999; Jaberi *et al.* 1999). The first LES of a hydrocarbon flame, namely the Sandia-Darmstadt piloted diffusion flame (Barlow and Frank 1998; Sandia National Laboratories 2013), has been conducted via both S-FMDF (Sheikhi *et al.* 2005) and VS-FMDF (Nik, Yilmaz, Givi *et al.* 2010; Nik, Yilmaz, Sheikhi *et al.* 2010). The FDF has also been successful in predicting the more complex field of the bluff-body Sandia-Sydney flame Dally *et al.* (1998, 2003) and a premixed Bunsen burner Chen *et al.* (1996) as reported in Drozda *et al.* (2007) and Yilmaz *et al.* (2010), respectively.

The original work of Colucci *et al.* (1998) provides the first demonstration of a *transported* FDF. Since then, this methodology has experienced widespread usage, and is now regarded as one of the most effective and popular means of LES worldwide. Some of the most important contributions to the FDF by others are in its basic implementation (Afshari *et al.* 2008; Carrara and DesJardin 2006; Chen 2007; Drozda *et al.* 2008; Heinz 2003b; James *et al.* 2007; Jones and Navarro-Martinez 2007; Jones *et al.* 2007; McDermott and Pope 2007; Mustata *et al.* 2006; Raman and Pitsch 2005, 2007; Raman *et al.* 2005; van Vliet *et al.* 2005; Zhou and Pereira 2000), fine-tuning of its sub-closures (Cha and Trouillet 2003; Heinz 2007; Réveillon and Vervisch 1998) and its validation via laboratory experiments (Rajagopalan and Tong 2003; Tong 2001; van Vliet *et al.* 2005; Wang and Tong 2002, 2005; Wang *et al.* 2004). For a review of the state of progress in FDF modeling we refer to Ansari *et al.* (2011). For a comprehensive understanding of the FDF, we refer serious readers to several dissertations (Ansari 2012; Colucci 1998; Drozda 2005; Gicquel 2001; Nik 2012; Pisciuneri 2008; Sheikhi 2005; Yilmaz 2008).

In this article, we provide a review of recent developments which facilitate FDF to be applied to LES of complex turbulent reacting flows. The phrase "complex"

refers to both the chemical kinetics and the geometrical flow configuration. These developments are: (1) construction of an "irregularly portioned" Lagrangian Monte Carlo FDF simulator, and (2) implementation of the Monte Carlo simulator on Eulerian domains portrayed by unstructured grids. The former allows efficient FDF simulations on massively parallel platforms, and the latter facilitates simulation of flows in complex configurations. With these developments, it is now much easier to conduct LES of complex turbulent reacting flows.

2. FDF FORMULATION AND MODELING

The primary transport variables in reactive flows are the fluid density $\rho(\mathbf{x},t)$, the velocity vector $u_i(\mathbf{x},t)$, $i = 1,2,3$ along the x_i direction, the specific enthalpy $h(\mathbf{x},t)$, the pressure $p(\mathbf{x},t)$, and the mass fractions of N_s species, $Y_\alpha(\mathbf{x},t)$ ($\alpha = 1,2,\ldots,N_s$), where $\mathbf{x} \equiv x_i (i = 1,2,3)$ and t denote space and time, respectively. Implementation of LES involves the use of the spatial filtering operation (Geurts 2004; Sagaut 2010)

$$\langle Q(\mathbf{x},t) \rangle = \int_{-\infty}^{+\infty} Q(\mathbf{x}',t) \mathcal{H}(\mathbf{x}',\mathbf{x}) d\mathbf{x}', \qquad (1)$$

where $\mathcal{H}$ denotes the filter function of width $\Delta_{\mathcal{H}}$, and $\langle Q(\mathbf{x},t) \rangle$ represents the filtered value of the transport variable $Q(\mathbf{x},t)$. In reacting flows, it is convenient to consider the Favre filtered quantity, $\langle Q(\mathbf{x},t) \rangle_L = \langle \rho Q \rangle / \langle \rho \rangle$. We consider spatially invariant and localized filter functions, $\mathcal{H}(\mathbf{x}',\mathbf{x}) \equiv \mathcal{H}(\mathbf{x}' - \mathbf{x})$ with the properties (Ghosal and Moin 1995) $\mathcal{H}(\mathbf{x}) = \mathcal{H}(-\mathbf{x})$, and $\int_{-\infty}^{\infty} \mathcal{H}(\mathbf{x}) d\mathbf{x} = 1$. We consider *positive* filter functions Vreman *et al.* (1994) for which all the moments $\int_{-\infty}^{\infty} x^m \mathcal{H}(x) dx$ exist for $m \geq 0$. The transport variables satisfy the conservation equations of mass, momentum, energy and species mass fractions Williams (1985). The filtered form of these equations are:

$$\frac{\partial \langle \rho \rangle}{\partial t} + \frac{\partial \langle \rho \rangle \langle u_i \rangle_L}{\partial x_i} = 0, \qquad (2)$$

$$\frac{\partial \langle \rho \rangle \langle u_j \rangle_L}{\partial t} + \frac{\partial \langle \rho \rangle \langle u_i \rangle_L \langle u_j \rangle_L}{\partial x_i} = \\ - \frac{\partial \langle p \rangle}{\partial x_j} + \frac{\partial \langle \tau_{ij} \rangle}{\partial x_i} - \frac{\partial T_{ij}}{\partial x_i}, \qquad (3)$$

$$\frac{\partial \langle \rho \rangle \langle \phi_\alpha \rangle_L}{\partial t} + \frac{\partial \langle \rho \rangle \langle u_i \rangle_L \langle \phi_\alpha \rangle_L}{\partial x_i} = \\ - \frac{\partial \langle J_i^\alpha \rangle}{\partial x_i} - \frac{\partial M_i^\alpha}{\partial x_i} + \langle \rho S_\alpha \rangle, \qquad (4)$$

where τ_{ij} and J_i^α denote the viscous stress tensor and the scalar fluxes, respectively. In Eq. (4), S_α denotes the source term, and this equation represents transport of the species mass fractions and enthalpy in a common form with $\phi_\alpha \equiv Y_\alpha$, $\alpha = 1,2,\ldots,N_s$, $\phi_\sigma \equiv h$, $\sigma = N_s + 1$. The SGS closure problem is associated with $T_{ij} = \langle \rho \rangle \left(\langle u_i u_j \rangle_L - \langle u_i \rangle_L \langle u_j \rangle_L \right)$, $M_i^\alpha = \langle \rho \rangle \left(\langle u_i \phi_\alpha \rangle_L - \langle u_i \rangle_L \langle \phi_\alpha \rangle_L \right)$, and $\langle \rho S_\alpha \rangle$. The FDF provides an effective means for this closure. For the scalars'

array $\phi(\mathbf{x},t)$ and the velocity field, $u(\mathbf{x},t)$, the SGS statistical information is included in the joint velocity-scalar filtered mass density function (VS-FMDF), denoted by $\mathcal{F}(v,\psi,\mathbf{x},t)$, where (v,ψ) denote the probability-space for the (u,ϕ) fields. The exact transport equation for this FDF is (Sheikhi *et al.* 2007):

$$\frac{\partial \mathcal{F}}{\partial t} + \frac{\partial (v_k \mathcal{F})}{\partial x_k} = \frac{\partial}{\partial v_k} \left[\left\langle \frac{1}{\rho} \frac{\partial p}{\partial x_k} \,\middle|\, v,\psi \right\rangle \mathcal{F} \right] \\ + \frac{\partial}{\partial \psi_\alpha} \left[\left\langle \frac{1}{\rho} \frac{\partial J_j^\alpha}{\partial x_j} \,\middle|\, v,\psi \right\rangle \mathcal{F} \right] \\ - \frac{\partial}{\partial v_k} \left[\left\langle \frac{1}{\rho} \frac{\partial \tau_{kj}}{\partial x_j} \,\middle|\, v,\psi \right\rangle \mathcal{F} \right] \\ - \frac{\partial}{\partial \psi_\alpha} \left[S_\alpha(\psi) \mathcal{F} \right], \qquad (5)$$

where $\langle | \rangle$ denotes the conditional filtered values. As Eq. (5) shows, the effects of SGS convection and combustion are in *closed* forms. However, all of the terms involving conditional filtered values require closure. The marginal FMDF of the scalar (S-FMDF) field, $\mathcal{F}_\phi(\psi,\mathbf{x},t)$, is obtained by integration of the VS-FMDF over the velocity domain:

$$\frac{\partial \mathcal{F}_\phi}{\partial t} + \frac{\partial \left[\langle u_i(\mathbf{x},t) | \psi \rangle \mathcal{F}_\phi \right]}{\partial x_i} \\ = \frac{\partial}{\partial \psi_\alpha} \left[\left\langle \frac{1}{\rho} \frac{\partial J_j^\alpha}{\partial x_j} \,\middle|\, \psi \right\rangle \mathcal{F}_\phi \right] \\ - \frac{\partial}{\partial \psi_\alpha} \left[S_\alpha(\psi) \mathcal{F}_\phi \right]. \qquad (6)$$

Again, the effects of chemical reaction appear in a closed form. However, in this case, the SGS convection (second term on the left-hand side) requires closure. This approach has been the most popular among other investigators using FDF (Afshari *et al.* 2008; Carrara and Des-Jardin 2006; Cha and Trouillet 2003; Chen 2007; Drozda *et al.* 2008; Heinz 2003b; James *et al.* 2007; Jones and Navarro-Martinez 2007; Jones *et al.* 2007; McDermott and Pope 2007; Mustata *et al.* 2006; Raman and Pitsch 2005, 2007; Raman *et al.* 2005; Réveillon and Vervisch 1998; van Vliet *et al.* 2005; Zhou and Pereira 2000).

The SGS closures have been primarily based on modeled stochastic differential equations (SDEs) for each of the transport variables. These SDEs must account for all of the physics of turbulent combustion; including scalar mixing, chemistry, exothermicity, dilatation, and dissipation. It is straightforward to realize the capability of the FDF in that it accounts for all of the processes involving direct correlations of the transported variables. For example, there is no need for additional closures for turbulent-chemistry interactions and/or velocity-scalar correlations. A system of modeled SDEs (Gikhman and Skorokhod 1972; Karlin and Taylor 1981) based on the stochastic diffusion process (Stratonovich 1963) has proven effective for the FDF closure. The coefficients in the modeled Langevin equation will be set in such a way that the resulting Fokker-Planck equation Risken (1989) defines the modeled FDF transport equation, and thus the SGS closures. In particular, the generalized Langevin model (GLM) (Dreeben and Pope 1997; Haworth and

Pope 1986; Pope 1994a,b) combined with the linear mean square estimation (LMSE) (Borghi 1988; Dopazo 1994) has proven to be effective. This is described by Sheikhi *et al.* (2007):

$$dx_i^+ = u_i^+ \, dt + \sqrt{\frac{2\mu}{\langle \rho \rangle}} \, dW_i, \tag{7a}$$

$$
\begin{aligned}
du_i^+ = &-\frac{1}{\langle \rho \rangle} \frac{\partial \langle p \rangle}{\partial x_i} \, dt \\
&+ \frac{2}{\langle \rho \rangle} \frac{\partial}{\partial x_j} \left(\mu \frac{\partial \langle u_i \rangle_L}{\partial x_j} \right) dt \\
&+ \frac{1}{\langle \rho \rangle} \frac{\partial}{\partial x_j} \left(\mu \frac{\partial \langle u_j \rangle_L}{\partial x_i} \right) dt \\
&- \frac{2}{3} \frac{1}{\langle \rho \rangle} \frac{\partial}{\partial x_i} \left(\mu \frac{\partial \langle u_j \rangle_L}{\partial x_j} \right) dt \\
&+ G_{ij} \left(u_j^+ - \langle u_j \rangle_L \right) dt \\
&+ \sqrt{C_0 k \omega} \, dW_i' \\
&+ \sqrt{\frac{2\mu}{\langle \rho \rangle}} \frac{\partial \langle u_i \rangle_L}{\partial x_j} \, dW_j, \tag{7b}
\end{aligned}
$$

$$
\begin{aligned}
d\phi_\alpha^+ = &-C_\phi \omega \left(\phi_\alpha^+ - \langle \phi_\alpha \rangle_L \right) dt \\
&+ S_\alpha(\phi^+) \, dt, \tag{7c}
\end{aligned}
$$

where $x_i^+, u_i^+, \psi_\alpha^+$ are probabilistic representations of position, velocity vector and scalar variables, respectively. μ denotes the fluid dynamic viscosity. The W terms denote the Wiener-Lévy processes in the physical (without the prime) and the velocity (with prime) spaces Gardiner (1990). The terms G_{ij} and $k = T_{ii}/2\langle \rho \rangle$ denote the kernel of GLM and the SGS kinetic energy, respectively. The mixing frequency ω is defined as: $\omega = C_f k^{1/2}/\Delta_{\mathcal{H}}$. The constants: C_0, C_ϕ and C_f are model parameters and are chosen as suggested in the literature Pope (1994a). The corresponding Fokker-Planck equation, or effectively the modeled VS-FMDF transport equation becomes:

$$
\begin{aligned}
\frac{\partial \mathcal{F}}{\partial t} + \frac{\partial v_i \mathcal{F}}{\partial x_i} = &\frac{1}{\langle \rho \rangle} \frac{\partial \langle p \rangle}{\partial x_i} \frac{\partial \mathcal{F}}{\partial v_i} \\
&- \frac{2}{\langle \rho \rangle} \frac{\partial}{\partial x_j} \left(\mu \frac{\partial \langle u_i \rangle_L}{\partial x_j} \right) \frac{\partial \mathcal{F}}{\partial v_i} \\
&- \frac{1}{\langle \rho \rangle} \frac{\partial}{\partial x_j} \left(\mu \frac{\partial \langle u_j \rangle_L}{\partial x_i} \right) \frac{\partial \mathcal{F}}{\partial v_i} \\
&+ \frac{2}{3} \frac{1}{\langle \rho \rangle} \frac{\partial}{\partial x_i} \left(\mu \frac{\partial \langle u_j \rangle_L}{\partial x_j} \right) \frac{\partial \mathcal{F}}{\partial v_i} \\
&- G_{ij} \frac{\partial \left[\left(v_j - \langle u_j \rangle_L \right) \mathcal{F} \right]}{\partial v_i} \\
&+ \frac{\partial}{\partial x_j} \left(\mu \frac{\partial (\mathcal{F}/\langle \rho \rangle)}{\partial x_j} \right) \\
&+ \frac{\partial}{\partial x_j} \left(\frac{2\mu}{\langle \rho \rangle} \frac{\partial \langle u_i \rangle_L}{\partial x_j} \frac{\partial \mathcal{F}}{\partial v_i} \right) \\
&+ \frac{\mu}{\langle \rho \rangle} \frac{\partial \langle u_i \rangle_L}{\partial x_k} \frac{\partial \langle u_j \rangle_L}{\partial x_k} \frac{\partial^2 \mathcal{F}}{\partial v_i \partial v_j} \\
&+ \frac{1}{2} C_0 k \omega \frac{\partial^2 \mathcal{F}}{\partial v_i \partial v_i} \\
&+ C_\phi \omega \frac{\partial \left[\left(\psi_\alpha - \langle \phi_\alpha \rangle_L \right) \mathcal{F} \right]}{\partial \psi_\alpha}
\end{aligned}
$$

$$- \frac{\partial [S_\alpha(\psi) \mathcal{F}]}{\partial \psi_\alpha}. \tag{8}$$

3. LAGRANGIAN FDF SIMULATOR

For the FDF to be practical, it must be implemented in a computationally efficient manner, especially if it is to be employed for the prediction of complex flows. For example, some of the current LES methods require up to several months of computing time for a moderately sized domain! In many cases, this is simply due to inefficient usage of a computer's resources. With petascale computing becoming a reality, one must take advantage of the enormous opportunities it provides for FDF simulations.

An effective way to solve the FDF numerically is via Lagrangian Monte Carlo (MC) methods (Grigoriu 1995; Kloeden *et al.* 1997). These methods have been the primary means of solving the PDF in RANS and, thus far, the most effective choice for solving the FDF in LES (including all of the previous works cited in §1). There have been some efforts to resurrect Eulerian PDF solvers (Chen 2007; Sabel'nikov and Soulard 2005), but they have not shown any particular advantages over Lagrangian methods. See Madnia *et al.* (2006) for a complete discussion. In the Lagrangian setting, the physical domain is discretized in standard formats (via finite difference, finite volume, spectral, or other methods), and the FDF is represented by an ensemble of *particles*. Each of these particles carry information pertaining to the physical field (*i.e.* each of the EPFVS variables) and also the position vector. This is shown in Fig. 1 in which the MC particles are overlaid on grid points, and the transport properties are identified by the colors of the particles. These properties are updated via temporal integration of the modeled SDEs.
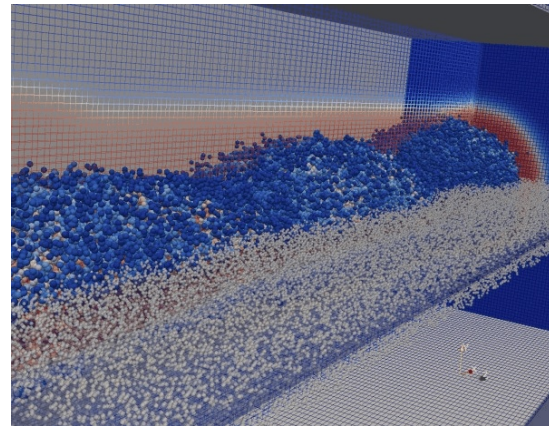

Fig. 1. Lagrangian Monte Carlo particles over structured Eulerian grids. The colors of the particles denote their transport properties. Displayed are particles on the center plane, and within a mixture fraction isosurface.

MC simulations typically require on the order of millions to billions of particles. The computational requirements can become "*monstrous*" for LES of practical flows, especially those involving complex kinetics. Therefore, scalable parallelization at the MC *particle level* is required. The major challenge in scalability is the extreme *load imbalance* associated with stiff chemistry. At any time during the simulation, different regions of the flow
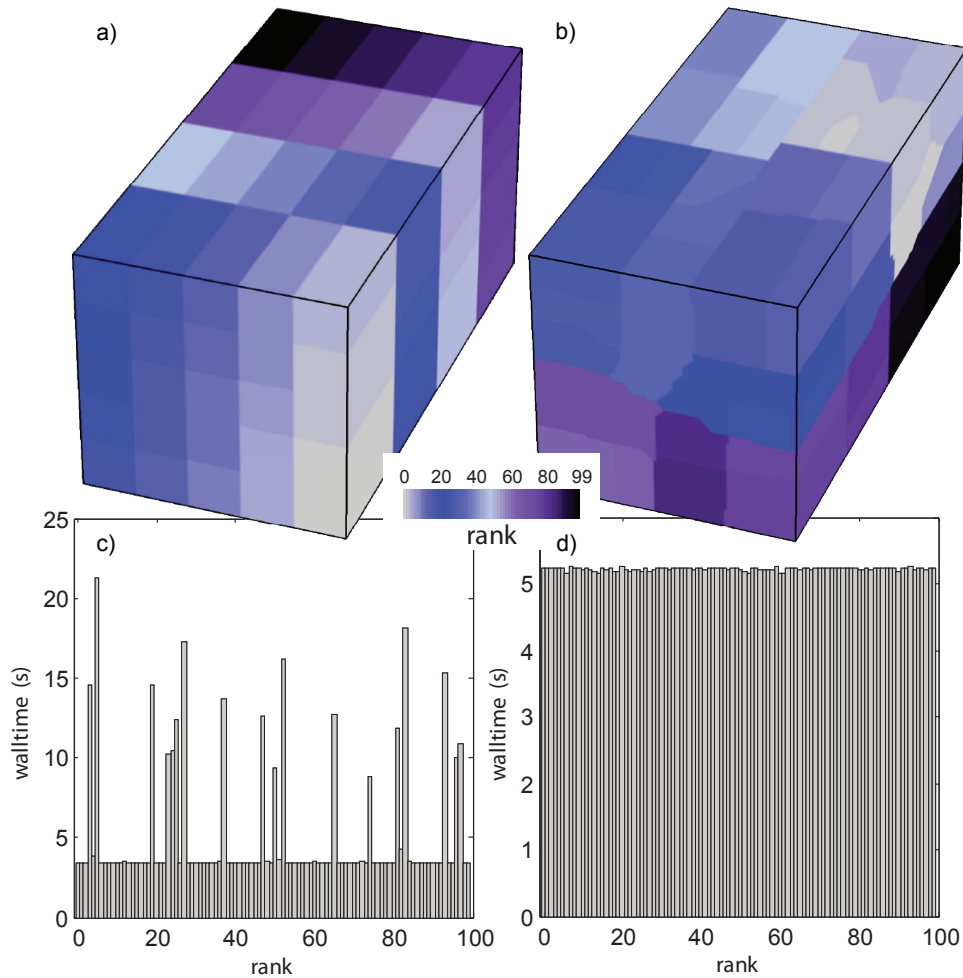
Fig. 2. Domain topology with (a) the uniform decomposition, and (b) adaptive irregular decomposition. Non-idle CPU times per time step for each rank for subsequent time steps with (c) uniform decomposition, and (d) adaptive irregular decomposition.

experience different stages of chemical reactions. Even though the particle number density is statistically uniform spatially, the computational load per particle varies significantly.

A popular parallelization strategy in modern CFD is via temporally invariant block decomposition, where the mesh is partitioned into equally sized boxes, and each box is assigned to a processor (Fig. 2a). This uniformity is relatively easy to implement and yields a minimal communication overhead, but for unsteady and inhomogeneous flows, it usually leads to a poor load distribution. Processors with lighter loads must wait (and remain idle) until the synchronization at the end of each time step. The local computation time of each processor for this is shown in Fig. 2(c). In this example, the idle time is about half of the total time! The load imbalance problem is resolved by development of an irregularly portioned Lagrangian Monte Carlo solver (IPLMC) Yilmaz *et al.* (2011). In this method, the Eulerian mesh is represented as an undirected graph where particle cells are the vertices of the graph and are weighted by the computational load. Each vertex is assigned a computational weight, *i.e.* a computation-load metric, which is a function of heterogeneous and homogeneous computational loads. This

weighted graph is then fed into a graph partitioning algorithm (Karypis and Kumar 1999) which subdivides the domain into clusters of particle cells on which the computational load is evenly distributed. Figure 2(d) shows the load distribution corresponding to the balanced irregular decomposition. Here, the idle time is insignificant. The transient load redistribution problem is resolved by recomputing the load metric, repartitioning the domain, and intercommunicating the local data of the partitions as the simulation proceeds. The frequency of redistribution is adjusted based on the communication cost and the extent of load imbalance.

In its current implementation, LES/FDF employs MPI for inter-domain communication, and can scale up to 1000s of segments via the adaptive partitioning as described. Further local refinement can be made at each individual domain, where ensembles of MC particles can be assigned to accelerator units for simultaneous computations. Sample results to demonstrate scalability are presented in Fig. 3. Shown on the left is the ratio of sequential wall time (t_1) to wall-time with p CPU cores (t_p), *i.e.* the *speed-up* (or *strong scaling*). On the right is the *scalability* (or *weak scaling*); that is the ratio of total computational work per time for p CPU cores (N_p/t_p) to that with
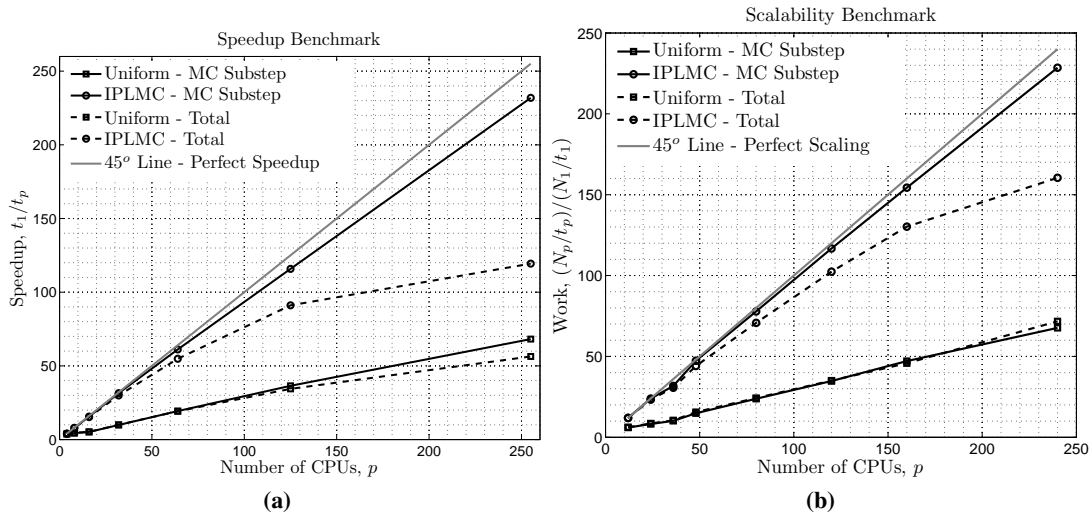
Fig. 3. Speed-up (strong scaling) and scalability (weak scaling) comparisons of the IPLMC versus uniform decomposition, based on wall-clock timings for chemistry substep and total iteration step. N_p denotes the total number of MC particles, and is increased linearly with number of CPUs (p) for the scalability benchmark.

a single core (N_1/t_1). In this analysis, the Eulerian mesh is kept fixed, but the number of MC particles per mesh point is increased in direct proportion to p. In the speed-up analysis, only p is varied for the same mesh with a fixed number of MC particles. In Fig. 3, the MC substep curves (solid) are for that subset of the computation, and message passing is done by the particle solver (including particle migration). The label 'total' (dashed) refers to these and everything else within the whole time step. As seen in both the speed-up and scalability curves, the IPLMC performs better, and is nearly perfect in scaling up-to 250 CPU cores for the MC solver. However, scaling to much larger number of CPUs is less impressive. This is not surprising, because with more CPUs no matter how well the load is balanced at the particle level, overall parallel performance is constrained by the sequential flow solver limiting the scalability as governed by Amdahl's law Amdahl (1967). The time spent on the parallel (MC) and sequential parts of the simulation are shown in Fig. 4. The MC substep time is sharply reduced in IPLMC; and after 150 or so CPU cores, the sequential parts start dominating the computation. With uniform decomposition, this ratio does not decrease nearly as much, agreeing with the observation made in Fig. 3 where the scalability characteristic of the total simulation is not very different than that in the MC substep. Future work includes the full parallelization by a similar strategy for the Eulerian solver, and aggressively reducing the sequential parts of the implementation. As demonstrated for the perfect scaling in the MC substep, this may facilitate near perfect scaling up to 1000s of CPU cores.

4. UNSTRUCTURED FDF SOLVER

The FDF and its IPLMC (or other MC) simulator(s) must be coupled with a base flow solver which identifies the computational domain. A major challenge in doing so is the discretization of complex geometries. Structured grids, as are typically used, lack the required flexibility and robustness for handling such geometries. Also, the
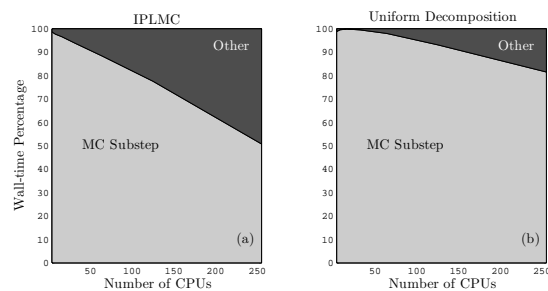

Fig. 4. Percentages of computational work for the Monte Carlo solver and the rest of the simulation for different CPU counts.

grid cells may become too skewed and/or twisted, prohibiting efficient simulations. Unstructured grids provide an excellent remedy for the problem of producing grids for complex geometries. Such grids have irregularly distributed nodes and their cells are not required to be of a specific shape. Furthermore, the connectivity of neighboring cells can vary spatially.

For LES of problems of practical interest, we have developed an unstructured grid system on which the MC simulator can be constructed Ansari *et al.* (2011). The Eulerian flow solver is based on a second order finite-volume (FV) method. The sacrifice for this lower discretization accuracy, as compared to that of high-order finite difference methods, is justified by the versatility provided by the FV method for consideration of complex configurations. The computational domain is discretized via cells of arbitrary shapes. These cells serve two purposes: (1) they identify the regions where the statistical information from the MC are obtained; (2) they are used to couple the FV and MC solvers for LES. The FV solver is primarily based on a bounded central composite normalized variable diagram (NVD) scheme Darwish (1993), and consists of a blended scheme of central differencing and a second order upwind scheme. The statistics are gener-

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ated by consideration of the MC particles within a volume centered at the point of interest. Effectively, this volume constitutes an "ensemble domain" characterized by the length scale Δ_E in which the FDF is discretely represented. For reliable statistics with minimal dispersion, it is required to maximize the number of particles and to minimize the size of the ensemble domain. In most of our work, the tetrahedral cell is taken as the ensemble domain. To maximize accuracy with a finite number of particles, a variant of the "basis function method" (Subramaniam and Haworth 2000) is considered. Solution of the modeled stochastic differential equation (7) requires the input of the filtered velocity, the diffusion coefficient and gradients of the scalars field. These are provided by the FV solution and are subsequently interpolated to the particles' locations via a piecewise linear reconstruction method (Barth and Jespersen 1989). Within the cell, the filtered values are expressed in terms of the vertex mean values. In doing so, an efficient particle tracking procedure is constructed Ansari *et al.* (2011).
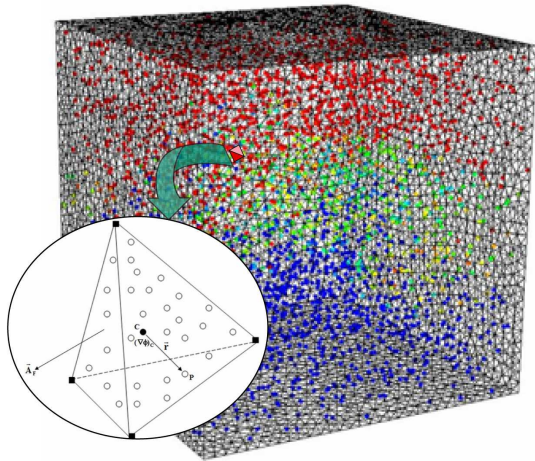

Fig. 5. Lagrangian Monte Carlo particles over unstructured Eulerian tetrahedrons for LES of a homogeneous turbulent flow Sheikhi *et al.* (2009). The colors of the particles denote their transport properties.

We demonstrate the feasibility of the method by applying our S-FMDF for LES of a homogeneous turbulent flow. Figure 5 shows an instantaneous ensemble of MC particles overlaid on an unstructured grid. The inset shows the schematics of a tetrahedral cell, and the MC particles it contains. The success of this new solver is assessed by duplicating our previous results via a high-order finite difference algorithm Sheikhi *et al.* (2009). We have implemented the solver for LES of a variety of turbulent flames. The most complex case considered thus far is the PRECCINSTA experimental burner from the German Aerospace Center (DLR) Meier *et al.* (2007). This is an excellent representation of an industrial gas turbine burner. The mesh for this burner is shown in Fig. 6. It consists of 2.2 million tetrahedral unstructured mesh elements. Figure 7 shows the volume rendered, instantaneous CO mass fraction. The flame with a V-shape is located near the burner inlet and shows wrinkling in its structure. The structure of the turbulent flow field is ev-

ident in the isosurface of the second invariant of the velocity deformation tensor colored by velocity as shown in Fig. 8.

5. CONCLUDING REMARKS

The filtered density function (FDF) has proven very effective for reliable and affordable prediction of turbulent reactive flows. The primary advantage of the FDF is that it accounts for the effects of subgrid-scale (SGS) chemical reactions in an exact manner regardless of the speed of reaction. Also, it provides all the higher SGS moments of the flow; whereas most other LES strategies predict only the mean values, at best. Since its original development, the FDF has experienced widespread applications for LES of a variety of reacting flows, as reviewed in this article. The methodology has been the subject of broad coverage in modern text- and hand-books (Bilger 2000; Fox 2003; Heinz 2003a; Kuo and Acharya 2012; Minkowycz *et al.* 2006; Peters 2000; Pope 2000). It has been implemented in commercial and government combustion codes such as FLUENT/ANSYS Ansari *et al.* (2011), VULCAN Drozda *et al.* (2012), and US3D Otis *et al.* (2012), among others.

Recent developments in FDF simulation consist of (1) construction of an irregularly portioned Lagrangian Monte Carlo FDF solver and (2) implementation of (any) Monte Carlo simulator on Eulerian domains portrayed by unstructured grids. The former allows efficient FDF simulations on massively parallel platforms, and the latter facilitates discretization of flows in complex geometrical configurations. With these developments, it is now possible to apply FDF for LES of practical problems, such as gas-turbine combustors.
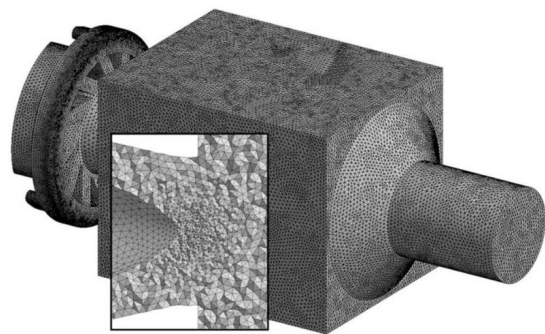
Fig. 6. Tetrahedral mesh on the PRECCINSTA burner Meier *et al.* (2007) and combustion chamber.
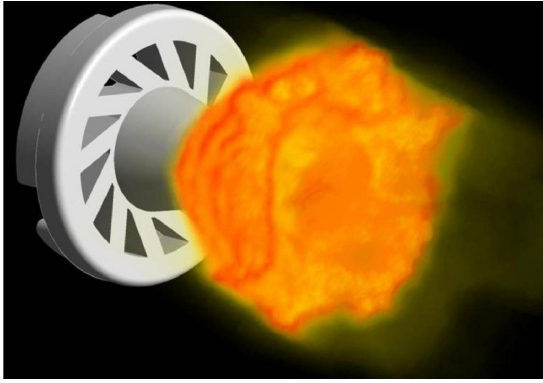
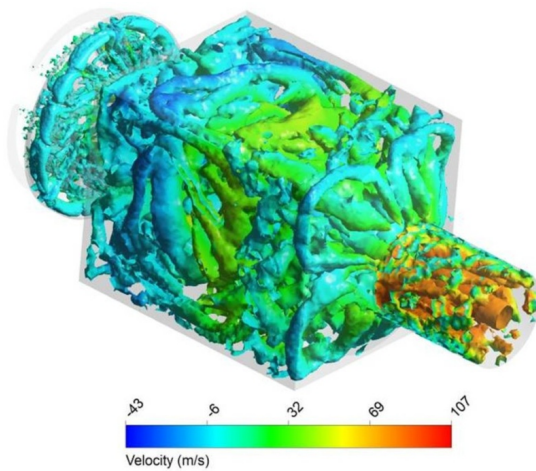**Fig. 7.** Instantaneous volume rendered plot of CO mass fraction.

Fig. 8. Flow structure for PRECCINSTA burner (Meier *et al.* 2007) visualized by the isosurface of the second invariant of the velocity deformation tensor colored by velocity.

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