A Hybrid DG-Monte Carlo FDF Simulator

Shervin Sammak^{a,*}, Michael J. Brazell^b, Peyman Givi^a, Dimitri J. Mavriplis^b

^a*Department of Mechanical Engineering and Materials Science, University of Pittsburgh,
Pittsburgh, PA 15261, USA*

^b*Department of Mechanical Engineering, University of Wyoming, Laramie, WY 82701,
USA*

Abstract

A new computational scheme is developed for large eddy simulation (LES) of turbulent reacting flows via the filtered density function (FDF) subgrid scale closure. This is a hybrid scheme, combining the discontinuous Galerkin (DG) Eulerian solver with a Lagrangian Monte Carlo FDF simulator. The methodology is shown to be suitable for LES, as a larger portion of the resolved energy is captured as the order of spectral approximation increases. The consistency and the overall performance of the DG-FDF solver and the realization of the simulated results are demonstrated via LES of a temporally developing mixing layer under both non-reacting and reacting conditions.

Keywords: Large eddy simulation, Filtered density function, Monte Carlo methods, Turbulent reacting flows

1. Introduction

The filtered density function (FDF) is now widely recognized as a viable tool for large eddy simulation (LES) of turbulent flows [1–7]. It is also commonly believed that the Lagrangian Monte Carlo (MC) methods provide the most
5 convenient means of solving the transported FDF equation [8–10]. In MC, the physical domain is discretized in standard formats *e.g.* finite difference (FD), finite volume (FV), finite element (FE) or others; and the FDF is represented by

*Corresponding author

Email address: shervin.sammak@pitt.edu (Shervin Sammak)

an ensemble of *particles*. Each of these particles carry information pertaining to the physical field. For stable simulations, the MC solver must be coupled with an Eulerian base flow solver of the transport variables [11–14]. The coupling must be done in such a way that the overall accuracy of the solver is maintained. It is also desired that the influence of the subgrid scale (SGS) quantities decrease with the increase of the resolution and/or the order of accuracy of the discretization procedure.

In this work, we develop a new computational methodology which is capable of meeting all of the aforementioned criteria. For that, we use the discontinuous Galerkin (DG) method as the base flow solver. This method combines the versatility of FV discretization with the accuracy of spectral approximation and is shown to be particularly suitable for coupling with the MC simulator. The novelty of the new LES solver is that it supports curved mixed-element meshes, variable discretization order, and non-conforming mesh element refinement. These features enable the flow solver to support combined $h - p$ refinement which can result in optimal solution accuracy for a given computational cost [15, 16]. The resulting DG-MC solver is tested for LES of a three-dimensional temporally developing mixing layer under both non-reacting and reacting conditions. The consistency of this procedure is assessed by comparing the first two moments of the FDF with those obtained by the DG solutions of the same moments’ transport equations. The overall predictive capability of the simulator is established via comparisons with previous direct numerical simulation (DNS) data [17, 18].

2. Formulation

We start with the basic transport equations of a chemically reactive flow, involving N_s species. In this flow, the primary transport variables are the density $\rho(\mathbf{x}, t)$, the velocity vector $u_i(\mathbf{x}, t)$ ($i = 1, 2, 3$), the pressure $p(\mathbf{x}, t)$, the total specific enthalpy $h_s(\mathbf{x}, t)$, and the species mass fractions $Y_\alpha(\mathbf{x}, t)$ ($\alpha = 1, 2, \dots, N_s$). The equations which govern the transport of these variables in space (x_i) ($i = 1, 2, 3$) and time (t) are the continuity, momentum,

conservation of enthalpy (energy) and species mass fraction equations, coupled with an equation of state. Large eddy simulation involves the spatial filtering operation [19, 20]:

$$\langle Q(\mathbf{x}, t) \rangle_\ell = \int_{-\infty}^{+\infty} Q(\mathbf{x}', t) G(\mathbf{x}', \mathbf{x}) d\mathbf{x}', \quad (1)$$

where $G(\mathbf{x}', \mathbf{x}) \equiv G(\mathbf{x}' - \mathbf{x})$ denotes a filter function, and $\langle Q(\mathbf{x}, t) \rangle_\ell$ is the filtered value of the transport variable $Q(\mathbf{x}, t)$. In variable-density flows it is convenient to use the Favré-filtered quantity $\langle Q(\mathbf{x}, t) \rangle_L = \langle \rho Q \rangle_\ell / \langle \rho \rangle_\ell$. We consider a positive, physically varying filter function. We apply this function to the basic conservation transport equations:

$$\frac{\partial \langle \rho \rangle_\ell}{\partial t} + \frac{\partial \langle \rho \rangle_\ell \langle u_j \rangle_L}{\partial x_j} = 0, \quad (2)$$

$$\frac{\partial \langle \rho \rangle_\ell \langle u_i \rangle_L}{\partial t} + \frac{\partial \langle \rho \rangle_\ell \langle u_j \rangle_L \langle u_i \rangle_L}{\partial x_j} = -\frac{\partial \langle p \rangle_\ell}{\partial x_i} + \frac{\partial \langle \tau_{ij} \rangle_\ell}{\partial x_j} - \frac{\partial \Sigma_{ij}}{\partial x_j}, \quad (3)$$

$$\frac{\partial \langle \rho \rangle_\ell \langle \phi_\alpha \rangle_L}{\partial t} + \frac{\partial \langle \rho \rangle_\ell \langle u_j \rangle_L \langle \phi_\alpha \rangle_L}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\left\langle \gamma \frac{\partial \phi_\alpha}{\partial x_j} \right\rangle_\ell \right) - \frac{\partial M_j^\alpha}{\partial x_j} + \langle \rho S_\alpha \rangle_\ell. \quad (4)$$

Here, the viscous stress tensor and the scalar fluxes are represented by τ_{ij} and J_j^α , respectively. The chemical reaction source terms $S_\alpha \equiv S_\alpha(\phi(\mathbf{x}, t))$ are functions of compositional scalars ($\phi \equiv [\phi_1, \phi_2, \dots, \phi_{N_s+1}]$) where $\phi_\alpha \equiv Y_\alpha, \alpha = 1, 2, \dots, N_s$, and ϕ_{N_s+1} denotes the enthalpy. $\Sigma_{ij} = \langle \rho \rangle_\ell (\langle u_i u_j \rangle_L - \langle u_i \rangle_L \langle u_j \rangle_L)$ and $M_j^\alpha = \langle \rho \rangle_\ell (\langle u_j \phi_\alpha \rangle_L - \langle u_j \rangle_L \langle \phi_\alpha \rangle_L)$ denote the SGS stresses and the mass fluxes, respectively. For a Newtonian fluids obeying the Fick's law of diffusion and the Fourier's law of heat conduction, we have:

$$\tau_{ij} = \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \frac{\partial u_k}{\partial x_k} \delta_{ij} \right), \quad J_j^\alpha = -\gamma \frac{\partial \phi_\alpha}{\partial x_j}, \quad (5)$$

where μ is the fluid dynamic viscosity, $\gamma = \mu/Sc$ denotes the thermal and mass molecular diffusivity coefficients for all the scalars, with Sc denoting the Schmidt/Lewis number. The FDF is considered for transport of all of the scalar quantities, and is denoted by F_L [21, 22]:

$$F_L(\psi, \mathbf{x}, t) = \int_{-\infty}^{+\infty} \rho(\mathbf{x}', t) \zeta(\psi, \phi(\mathbf{x}', t)) G(\mathbf{x}' - \mathbf{x}) d\mathbf{x}', \quad (6)$$

where

$$\zeta(\boldsymbol{\psi}, \boldsymbol{\phi}(\mathbf{x}, t)) = \prod_{\alpha=1}^{\sigma} \delta(\psi_{\alpha} - \phi_{\alpha}(\mathbf{x}, t)). \quad (7)$$

Here, δ denotes the Dirac delta function, and $\boldsymbol{\psi}$ represents the scalar array in the sample space. The term ζ is the “fine-grained” density [23, 24], and Eq. (6) defines FDF as the spatially filtered value of the fine-grained density. With the condition of a positive filter kernel [25], F_L has all the properties of a mass density function [24]. Defining the “conditional filtered value” of $Q(\mathbf{x}, t)$ as

$$\langle Q | \boldsymbol{\psi} \rangle_{\ell} \equiv \frac{\int_{-\infty}^{+\infty} Q(\mathbf{x}', t) \rho(\mathbf{x}', t) \zeta(\boldsymbol{\psi}, \boldsymbol{\phi}(\mathbf{x}', t)) G(\mathbf{x}' - \mathbf{x}) d\mathbf{x}'}{F_L(\boldsymbol{\psi}, \mathbf{x}, t)}, \quad (8)$$

40 the FDF is governed by the exact transport equation [7]:

$$\begin{aligned} \frac{\partial F_L}{\partial t} + \frac{\partial[\langle u_j(\mathbf{x}, t) | \boldsymbol{\psi} \rangle_{\ell} F_L]}{\partial x_j} &= -\frac{\partial}{\partial \psi_{\alpha}} [S_{\alpha}(\boldsymbol{\psi}) F_L] \\ &+ \frac{\partial}{\partial \psi_{\alpha}} \left[\left\langle \frac{1}{\rho(\boldsymbol{\phi})} \frac{\partial J_j^{\alpha}}{\partial x_j} \middle| \boldsymbol{\psi} \right\rangle_{\ell} F_L \right]. \end{aligned} \quad (9)$$

This equation indicates that the effect of chemical reaction (the first term on RHS) appears in a closed form. The unclosed nature of SGS convection and mixing is shown via the conditional filtered values in the other two terms. For closure of these terms, we use a gradient diffusion model for convection, and the linear mean square estimation (LMSE) model [26, 27] for the molecular mixing. These are given in terms of the stochastic differential equations (SDE's) [19, 23]:

$$dX_i^+(t) = \left[\langle u_i \rangle_L + \frac{1}{\langle \rho \rangle_{\ell}} \frac{\partial(\gamma + \gamma_t)}{\partial x_i} \right] dt + \sqrt{2(\gamma + \gamma_t) / \langle \rho \rangle_{\ell}} dW_i(t), \quad (10)$$

$$d\phi_{\alpha}^+ = -\Omega_m (\phi_{\alpha}^+ - \langle \phi_{\alpha} \rangle_L) dt + S_{\alpha}(\boldsymbol{\phi}^+) dt. \quad (11)$$

where dW_i is the Wiener-Levy process [28] and, X_i^+ and ϕ_{α}^+ are probabilistic representations of the position and the scalar variables, respectively. In the model, $\Omega_m = C_{\phi}(\gamma + \gamma_t) / (\langle \rho \rangle_{\ell} \Delta^2)$ is the SGS mixing frequency and $C_{\phi} = 4$

is a model constant. The Fokker-Planck equation corresponding to this model
 45 is [29]:

$$\frac{\partial F_L}{\partial t} + \frac{\partial[\langle u_j \rangle_L F_L]}{\partial x_j} = \frac{\partial}{\partial x_j} \left[(\gamma + \gamma_t) \frac{\partial(F_L / \langle \rho \rangle_\ell)}{\partial x_j} \right] + \frac{\partial}{\partial \psi_\alpha} [\Omega_m(\psi_\alpha - \langle \phi_\alpha \rangle_L) F_L] - \frac{\partial[S_\alpha F_L]}{\partial \psi_\alpha}. \quad (12)$$

Equation (12) represents the modeled FDF transport equation. This equation may be integrated to obtain transport equations for the SGS moments. Since the FDF is involved only for the scalar variable, all of the hydrodynamic SGS terms need to be modeled by other means. For those, we employ the
 50 standard Smagorinsky model [30, 31]:

$$\Sigma_{ij} - \frac{2}{3} \langle \rho \rangle_\ell C_{\nu_2} \Delta^2 S^2 \delta_{ij} = -2\mu_t \left(\langle S_{ij} \rangle_L - \frac{1}{3} \langle S_{kk} \rangle_L \delta_{ij} \right), \quad M_j^\alpha = -\gamma_t \frac{\partial \langle \phi_\alpha \rangle_L}{\partial x_j}. \quad (13)$$

The filtered strain rate tensor is $\langle S_{ij} \rangle_L = \frac{1}{2} \left[\frac{\partial \langle u_i \rangle_L}{\partial x_j} + \frac{\partial \langle u_j \rangle_L}{\partial x_i} \right]$. With that, the SGS viscosity is modeled by $\mu_t = \langle \rho \rangle_\ell [C_{\nu_1} \Delta]^2 S$, where $C_{\nu_1} = 0.2$, $C_{\nu_2} = 0.18$, $\gamma_t = \mu_t / S c_t$, $S c_t = 1$, $S = \sqrt{2 \langle S_{ij} \rangle_L \langle S_{ij} \rangle_L}$. The parameter Δ denotes the characteristic filter size and is taken as $\Delta = K_P \times (\Delta_x \Delta_y \Delta_z)^{\frac{1}{3}}$, where K_P
 55 estimated to be $\frac{1}{2(P+1)}$ with p denoting the polynomial order of approximation of the DG elements.

3. The Coupled DG-MC FDF Simulator

The DG flow solver provides high-order approximations of the filtered transport equations with the flexibility to deal with complex geometries. To im-
 60 plement this solver, the domain is discretized into a number of structured or unstructured elements. Each of these elements are mapped from the physical space to the computational space ($\mathbf{x} \rightarrow \eta$). Within this space, the transport variable are represented via spectral approximations. The eigenfunctions of the appropriate Sturm-Liouville problem are used for this approximation. Here
 65 the Legendre polynomials are employed in conjunction with Gauss quadrature points [32]. The number of Gauss quadrature points is given by $ngp = p + 1$.

Unlike FE schemes, DG methods are discontinuous at the element interfaces, which makes them suitable for advection dominated problems. This property allows for flux calculation via approximate Riemann solvers as done here. Appendix A provides an error estimate study to demonstrate the accuracy of the DG solver.

The FDF is represented by an ensemble of MC particles, each with a set of scalars $\phi_\alpha^n(t) = \phi_\alpha^n(X^{(n)}(t), t)$ and Lagrangian position vector $X^{(n)}$. This information is updated via temporal integration of the SDEs. By doing so, the position of the MC particles are updated due to convection and (random walk) diffusion; and their compositions are modified due to mixing and chemical reaction.

The DG-MC simulator as developed in this way has several advantages over more conventional methods (like FV, FD and FE). A significant advantage is that DG allows convergence to the DNS limit via p -refinement. Based on the close to exponential convergence of this refinement, the procedure is much more efficient than the conventional approaches of refining the grid (reducing h) as is the typical practice. Another advantage is that the DG variables can easily be evaluated at the MC particle's locations since these variables are represented by simple polynomials within each element. Hence, there is no loss of accuracy due to the use of a lower order interpolation method as is typically used in conventional approximations. Moreover, due to the high order polynomial approximation, the DG mesh elements are typically much larger than the cells in conventional discretizations. This implies that the FDF particles will remain much longer within one element as compared to those in conventional schemes, and thus the computational effort for the particle tracking algorithm is reduced significantly.

The MC statistics are constructed by consideration of an ensemble of N_p particles within a hexahedral domain of size Δ_E . This is illustrated in Fig. 1(a) for a domain discretized by unstructured tetrahedral elements. For reliable statistics with minimal numerical dispersion, it is desired to minimize the size of the ensemble domain and maximize the number of the MC particles N_p . To

Figure 1: (a) Ensemble averaging on unstructured mesh. (1): hexahedral with $\Delta_E = \Delta$. (2): hexahedral with $\Delta_E = \Delta/2$. (b) Schematic distribution of MC particles within a tetrahedral cell. The solid circles denote the MC particles and the solid squares denote the quadrature points.

maximize the statistical accuracy with finite number of particles, a variant of the basis function method is implemented [33].

Numerical solution of the SDEs (Eq. (10)) requires the input of the filtered velocity, the diffusion coefficient and gradients of the scalars field at the particle locations. These are provided by the DG solution, and subsequent evaluation at the particle locations. This procedure is called projection. Figure 1(b) provides a schematic of a tetrahedral cell showing its quadrature points with inclusion of the MC particle. Let 1, 2, 3, 4 denote the quadrature points. An estimate of the scalar values at the particle location (ϕ_p) is obtained by summing over all polynomial degrees in the linked element and taking into account the Legendre basis functions:

$$\phi_p = \sum_{j=1}^{ngp} \phi_j \mathcal{L}_j(p), \quad (14)$$

100 Similar to that observed in other hybrid approaches, with this coupled DG-MC algorithm, several of the transport variables are calculated repeatedly [5]. This “redundancy” is very important to establish consistency as will be demonstrated below.

4. Demonstration

105 Simulations are conducted on a three-dimensional, temporally developing mixing layer, similar to those in previous DNS [17, 25]. The layer consists of two parallel streams traveling in opposite directions with the same speed. In the representation below, x , y and z denote the stream-wise, the cross-stream and the span-wise flow directions respectively (Fig. 2). The velocity components in
 110 these directions are denoted by u , v and w . The filtered stream-wise velocity is initialized with a hyperbolic tangent profile with $\langle u \rangle_L = 1$ on the top stream and $\langle u \rangle_L = -1$ on the bottom stream. All of the Reynolds-averaged values are time-dependent and are determined by ensemble averaging over the homogeneous $x - z$ planes. These are denoted by an overbar.

Figure 2: Structured hexahedral mesh for the temporal mixing layer and the distribution of Monte-Carlo particles within the domain at an initial time. The particles are colored by their scalar values.

115 The simulations are conducted on a cube box, $0 \leq x \leq L$, $-L/2 \leq y \leq L/2$ and $0 \leq z \leq L$. The box length L is specified such that $L = 2^{n_p} \lambda_u$, where n_p is the desired number of successive vortex pairings and λ_u is the wavelength of the most unstable mode corresponding to the mean stream-wise velocity profile imposed at the initial time. The flow variables are normalized with respect to

120 the half initial vorticity thickness, $L_r = [\delta_v(t=0)/2]$; $\delta_v = \Delta U / |\partial \langle \overline{u} \rangle / \partial y|_{max}$,
 where $\langle \overline{u} \rangle$ is the Reynolds averaged value of the filtered stream-wise velocity and
 ΔU is the velocity difference across the layer. The reference velocity is $U_r =$
 $\Delta U/2$. The Reynolds number based on the reference velocity and length scales
 is $Re = 50$. The formation of the large scale vortical structures are expedited
 125 by harmonic forcing of the layer. This includes 2D and 3D perturbations with a
 random phase shift between the 3D modes [25]. This results in the formation of
 two successive vortex pairings and strong three dimensionality caused by growth
 of secondary instabilities.

Both non-reacting and reacting layers are considered. In the former, the
 130 trace of a passive scalar ϕ is considered. This is again initialized as a hyperbolic
 tangent profile with $\langle \phi \rangle_L = 1$ and 0 on the top and bottom streams, respectively.
 In the reacting case, an irreversible, second-order reaction scheme of type $\mathcal{A} +$
 $\nu \mathcal{B} \rightarrow (\nu + 1) \mathcal{P}$ is considered. The reactant conversion is governed by $S_A =$
 $k_r AB$, where k_r is the reaction rate constant; and A, B denote the mass fractions
 135 of the two reactants. In this case, the reactants are initialized such that $A \equiv \phi$
 (as described above), and $B = 1 - A$. The stoichiometric coefficient is unity. The
 temperature in both streams is kept constant at $T = T_\infty$, and the combustion
 exothermicity ($-\Delta H$) is parameterized via the heat release parameter $\mathcal{Q} =$
 $\frac{-\Delta H}{C_p T_\infty} = 0.1$, where C_p denotes the specific heat value at constant pressure.
 140 The rate of reactant conversion is parameterized by the Damköhler number,
 $Da = k_r L_r / U_r$. Simulations are conducted with relatively slow ($Da = 10^{-2}$),
 moderate ($Da = 1$) and relatively fast ($Da = 10^2$) reactions.

To establish the consistency and convergence of the MC solver, the gen-
 eralized first SGS moment $\langle \phi_\alpha \rangle_L$ and the SGS variance $\tau_{\alpha\alpha} \equiv \tau(\phi_\alpha, \phi_\alpha)$ are
 145 considered. These moments are obtained via integration of the modeled FDF
 transport equation (Eq. (12)), as given by:

$$\frac{\partial(\langle \rho \rangle_\ell \langle \phi_\alpha \rangle_L)}{\partial t} + \frac{\partial[\langle \rho \rangle_\ell \langle u_j \rangle_L \langle \phi_\alpha \rangle_L]}{\partial x_j} = \frac{\partial}{\partial x_j} \left[(\gamma + \gamma_t) \frac{\partial(\langle \phi_\alpha \rangle_L)}{\partial x_j} \right] + \langle \rho \rangle_\ell \langle S_\alpha \rangle_L, \quad (15)$$

$$\begin{aligned} \frac{\partial(\langle \rho \rangle_\ell \tau_{\alpha\alpha})}{\partial t} + \frac{\partial[\langle \rho \rangle_\ell \langle u_j \rangle_L \tau_{\alpha\alpha}]}{\partial x_j} &= \frac{\partial}{\partial x_j} \left[(\gamma + \gamma_t) \frac{\partial \tau_{\alpha\alpha}}{\partial x_j} \right] + 2(\gamma + \gamma_t) \left[\frac{\partial(\langle \phi_\alpha \rangle_L)}{\partial x_j} \frac{\partial(\langle \phi_\alpha \rangle_L)}{\partial x_j} \right] \\ &- 2\Omega_m \langle \rho \rangle_\ell \tau_{\alpha\alpha} + 2 \langle \rho \rangle_\ell (\langle \phi_\alpha S_\alpha \rangle_L - \langle \phi_\alpha \rangle_L \langle S_\alpha \rangle_L). \end{aligned} \quad (16)$$

These equations are identical to those which would be obtained by employing consistent closures for the SGS fluxes and the dissipation from Eq. (4). In such a direct moment formulation, however, the terms involving $\langle S_\alpha \rangle_L$ require
150 modeling.

Figure 3: Contour plots of the filtered scalar field for $p = 4$ at $t = 60$. (a) FDF, (b) DG.

The DG-MC FDF simulator is invoked in conjunction with Lax-Friedrichs [34], Roe [35] and artificially upstream flux vector splitting scheme [36] for the advective fluxes, and a symmetric interior penalty method [37, 38] for the diffusive fluxes. Temporal integration in the DG calculations is via a 4th order
155 Runge Kutta method [39]. The SDEs in the MC solver are integrated via the Euler-Marruyamma approximation [10]. The computational domain is discretized on equally spaced cells. These points are used for two purposes: (1) to identify the regions where the statistical information from the MC simulations is obtained; (2) to assess consistency of the coupled DG-MC solver (as
160 described below). Simulations are conducted on a structured hexahedral mesh with a total number of cells equal to 35,937. The MC particles are initially

Figure 4: Scatter plot of the filtered values as obtained by FDF vs. those obtained by DG for $p = 4$ at $t = 60$. (a) filtered scalar, the correlation coefficient is 0.9991. (b) second-order SGS moment, the correlation coefficient is 0.9984.

distributed somewhat uniformly throughout the domain. The initial number of particles per cell is 40. Figure 2 shows the distribution of MC particles inside the cube with the structured mesh at an initial time. The simulated results are analyzed both instantaneously and statistically. In the former, the snapshot contours and scatter plots of the scalar variable are displayed. In the latter, the Reynolds averaged values are considered. In the presentation below, $\tau(a, b) = \langle ab \rangle_L - \langle a \rangle_L \langle b \rangle_L$ denotes the SGS stresses. The resolved stresses are expressed by $R(a, b) = \overline{\langle a \rangle_L \langle b \rangle_L} - \left(\overline{\langle a \rangle_L} \right) \left(\overline{\langle b \rangle_L} \right)$ and the total stresses are given by $r(a, b) = \overline{\langle ab \rangle} - \overline{\langle a \rangle} \overline{\langle b \rangle}$. Note that for a generic filter, $r(a, b) = R(a, b) + \tau(a, b)$.

The overall consistency of the simulator is best achieved by comparing the lower moments as obtained from FDF with those simulated directly via DG on the same mesh. The chemical source terms are evaluated solely via the MC and are then used in the DG solution of the filtered scalar equations. In this way, the filtered scalar values are obtained via both DG and MC. Figure 3 shows the instantaneous contour plots of filtered scalar ($\langle \phi_\alpha \rangle_L$) field as computed via both DG and MC where $p = 4$ and $t = 60$. This figure provides a visual demonstration of the consistency of the FDF simulation as the MC results are in agreement with those via DG. This is corroborated quantitatively by the

Figure 5: Cross-stream variation of the Reynolds averaged values for $p = 2$ and various ensemble domain size. (a) filtered scalar field, (b) SGS scalar variance.

180 scatter plots of the instantaneous filtered values in Fig. 4.

Figure 5 shows the influence of Δ_E in both filtered scalar ($\langle \phi_\alpha \rangle_L$) field and the SGS variance $\tau(\phi, \phi)$. It is indicated that, the size of the ensemble domain does not have a significant influence on the Reynolds statistics of the first filtered moments. However, for the SGS variance, the FDF and the DG solutions merge
 185 as the size of the ensemble domain decreases. The best agreement is observed with a ensemble domain size $\Delta_E = \Delta/2$. Hereinafter, unless otherwise noted, statistics are generated with consideration of $\Delta_E = \Delta/2$.

In Fig. 6 the first order moment from MC solver compared to those obtained by the DG for various polynomial degrees. Since the accuracy of the DG pro-
 190 cedure is well-established (at least for the first-order filtered quantities), such a consistency assessment provides a good means of assessing the performance of the MC solution. As shown (and somewhat expected), the first filtered values are not significantly influenced by the larger values of p . However, this is not the case for the variances as shown in Fig. 7. It is clear that as the value of
 195 p increases, the amount of SGS energy decreases. This is in accord with the expectation that with increased resolution, the influence of SGS scales becomes less pronounced. This is further demonstrated in Fig. 8 in which the profiles of the resolved variances are shown. Consistent with the philosophy of LES, as

Figure 6: Cross-stream variation of the Reynolds-averaged values of the filtered scalar field for various degree of polynomial. (a) $p = 2$, (b) $p = 3$, (c) $p = 4$.

the solution becomes more accurate, a more significant portion of the energy is resolved. In all cases, the total energy remains the same, as shown in Fig. 9. For all p values, the LES predictions are in close agreements with DNS data. This is very encouraging as it indicates that regardless of the portion of energy captured by the resolved field, the total energy is predicted well and there is no contamination of the total field due to SGS modeling.

In the reacting case, the consistency of the FDF calculations and realizability of the simulated results are investigated by considering the compositional structure of the flame in the mixture fraction domain ξ [40]. As shown in Fig. 10, when chemistry is slow the composition is close to that of pure mixing. On the opposite side of the spectrum, for very fast reactions, the composition is

Figure 7: Cross stream variation of the Reynolds averaged SGS scalar variance. The thick solid line denotes the DG data and dashed line denotes the FDF data. (a) $p = 2$, (b) $p = 3$, (c) $p = 4$.

close to that of the infinitely fast reaction. For the moderate chemistry, the compositional structure is similar to that of a distributed reaction zone. To demonstrate accuracy, transport of two Shvab-Zeldovich variables [41] are also considered:

$$Z_1 = \frac{A - \frac{B}{\nu} + \frac{B_\infty}{\nu}}{A_\infty + \frac{B_\infty}{\nu}}, \quad Z_2 = \frac{A + \frac{1}{Q} \left(\frac{T}{T_\infty} - 1 \right)}{A_\infty}. \quad (17)$$

where the subscript ∞ denotes the values at the free streams. Figure 11 demonstrates that the conserved scalar and the mixture fraction are nearly perfectly correlated for $Da = 10^2$. The results for the other two cases are, as expected,

Figure 8: Cross-stream variation of the Reynolds-averaged values of the resolved scalar variance for various polynomial degree at $t = 60$. (a) $p = 2$, (b) $p = 3$, (c) $p = 4$.

very similar and thus are not presented.

5. Concluding Remarks

This work shows that the merger of a high-order DG with the MC solution of the FDF, provides an excellent tool for conducting LES. The primary features of this hybrid method are summarized below:

1. The method combines the versatility of finite-volume discretization with the accuracy of spectral approximations and is shown to be particularly effective when utilized in conjunction with Lagrangian methods.

Figure 9: Cross-stream variation of the Reynolds-averaged values of the total scalar variance for various polynomial degree at $t = 60$. (a) $p = 2$, (b) $p = 3$, (c) $p = 4$.

- 225 2. The solver supports curved mixed-element meshes, variable discretization order, and non-conforming mesh element refinement. Therefore, it supports combined $h - p$ refinement which results in an optimal solution accuracy for a given computational cost.
- 230 3. Even at low p values, when the resolved energy is significantly reduced, the total energy is captured very accurately. This feature is particularly attractive when the prediction of the total energies/stresses are of the primary concern.
- 235 4. **The dense kernels of the high-order DG discretization enable superior scalability on massively parallel computer architectures [15, 42–45].** The solver is designed to scale to very large cases, and simulations involving

Figure 10: Scatter plots of the filtered composition variables versus the filtered mixture fraction for (a) $Da = 10^{-2}$, (b) $Da = 1$ and (c) $Da = 10^2$. The dashed lines denote pure mixing and infinitely fast chemistry limits.

several billion degrees of freedom on over 100,000 are within reach.

5. The superior numerical efficiency and scalability of the DG method can be leveraged by using large polynomial approximation orders $p \sim 4 - 6$. Such large polynomial orders result in very low numerical dissipation [46] which is very desired (in fact essential) in LES.
6. A significant advantage of the proposed methodology is that it will allow us to reach to DNS limit via p -refinement. Based on the close to exponential convergence of this refinement, the procedure is much more efficient than the conventional approach of refining the grid (reducing h) as is the typical practice in typical Eulerian LES.

Figure 11: Scatter plot comparing Z_2 to the mixture fraction for $Da = 10^2$.

7. A particular advantage of the approach is that the DG variables can easily be evaluated at the MC particle locations since these variables are represented by simple polynomials on each element. Hence, there is no loss of accuracy due to the use of a lower order interpolation method as is used in conventional approximations.
8. Due to the high order polynomial approximation, the DG mesh elements are typically much larger than the cells in FD or FV discretizations. This implies that the FDF particles will remain much longer in one element as compared to that in conventional approaches, and thus the computational effort for the particle tracking algorithm will be reduced significantly.

The success of the DG-MC FDF simulator as demonstrated here warrants its further extension and applications for LES of complex turbulent combustion problems.

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Appendix A

265 This appendix provides an error estimate of the DG formulation. For this
 purpose, the two-dimensional Ringleb flow [47] is considered. Simulations are
 conducted with four different mesh sizes (h), consisting of 5, 10, 20 and 40
 elements in both flow directions. The simulated results are compared with the
 exact solution. The L_2 norm of the error is presented in Fig. A1. It is shown
 270 that the error decreases in a rate proportional to h^{p+1} .

Figure A1: L_2 norm vs. h [15].

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