Lagrangian particles with mixing. II. Sparse-Lagrangian methods in application for turbulent reacting flows

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Both parts of this work present a more detailed and specific analysis of ideas introduced in the previously published letter [Phys. Fluids **19**, 031702 (2007)]. In Paper I [Phys. Fluids **19**, 065101 (2009)], we show that the continuous scalar transport and diffusion can be accurately specified by means of mixing between randomly walking Lagrangian particles with scalar properties. Here, in Paper II, we deal with the situation where the number of particles is not sufficient to resolve all scales in turbulent flows and Lagrangian particles with mixing become an approximate model rather than a stochastic framework for solving exact scalar transport equations. We consider sparse-Lagrangian methods that use relatively small numbers of particles compared to the number of Eulerian grid points and discuss similarities and differences with conventional large eddy simulations—filtered density function (LES-FDF) methods. Special attention is paid to multiple mapping conditioning (MMC) formulation for sparse-Lagrangian simulations. Physical and simulated equations for joint FDFs of reactive scalars are compared and analyzed. The efficiency of the MMC-LES approach that was demonstrated in several recent publications is explained from a methodological perspective. © *2009 American Institute of Physics*. [DOI: 10.1063/1.3147927]

I. INTRODUCTION

The models utilizing Lagrangian particles with mixing[1,2] appeared decades ago as an effective tool in simulating probability density functions (PDFs) in turbulent reacting flows. In turbulent flows the dissipative influence of diffusion is much more significant compared to spatial transport by molecular diffusion. This brought mixing into consideration as a distinct process responsible for modeling of the scalar dissipation. At the time when direct numerical simulations (DNSs)/large eddy simulations (LESs) of multiple reactive scalars was a computationally infeasible luxury, the Lagrangian PDF methods gave an opportunity to model joint distributions of all reactive species, which are needed for accurate evaluation of the chemical source terms, at a more moderate (although still significant) computational cost.

Rapid computer progress in the past decades opened new possibilities that involved LES of realistic chemical kinetics with many reactive species.[3] Performance of LES in reacting flows was good in many respects although neglecting subgrid fluctuations in LES caused noticeable errors in evaluation of the chemical source terms.[4] These errors would have been tolerable if they were encountered in a low-cost model but, for highly expensive LES simulations, existence of these errors required modifications of the approach. The LES resolve large-scale fluctuations while chemical reactions often depend on the smallest scales in turbulence.

The natural response to the problem was combining LES and other approaches [flamelet, conditional moment closure (CMC), PDF] that can simulate subgrid behavior of reactive species (see review in Ref. 3). The combination of LES and PDF approaches introduced in Ref. 4 was named filtered density function (FDF). The FDF approach effectively represents a PDF method applied to subgrid fluctuations in LES. Each Eulerian LES cell usually contains between 20 and 100 Lagrangian particles. This approach did produce very good results but at a very high computational cost due to superposition of LES and PDF computational expenses.[5] This high cost precluded applying LES-FDF to complex realistic chemical kinetics and raised questions whether LES-FDF demands computational resources that may be sufficient for refined LES and whether refined LES would be a simpler (if not better) option for simulating reacting flows. The term refined LES or under-resolved DNS can be used for simulations which are close to resolving all scales but do not achieve the resolution required in proper DNS.

The view of the author of this work is that, in the conventional combination of LES and FDF, the FDF approach is dominated by the LES methodology: FDF is allowed to function only on LES subgrid scales and has difficulties in fully displaying its best qualities under these restricted conditions. The approach suggested in Ref. 6 and further elaborated here introduces FDF that are allowed to simulate LES supergrid fluctuations. The FDF method in this case becomes a Lagrangian LES on its own and is not restricted to servicing the needs of the conventional Eulerian LES. This new understanding of FDF is now called sparse-Lagrangian simulations.[7,8]

While general properties of Lagrangian particles with scalar properties and mixing are considered in Paper I of this work,[9] this article is concerned with the situation when it is impossible or impractical to introduce the number of particles that would be sufficient to resolve all scales in a turbulent flow. If the high-frequency range of fluctuations is not resolved then Lagrangian particles with scalar properties and

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mixing become not a numerical method of solving exact transport equations but an approximate model. We consider the main features of sparse-Lagrangian models that allow for quality simulations at affordable computational cost and, specifically, we analyze the multiple mapping conditioning (MMC) approach in conjunction with sparse-Lagrangian simulations. This approach, called MMC-LES, was first described in Ref. 6 and implemented in Refs. 7 and 8.

The distinctive feature of MMC models is localization of mixing in the space of reference variables. These variables are introduced in MMC to emulate properties of turbulence that affect mixing process. MMC has many common features with other combustion models. The older deterministic form of MMC (Ref. 10) effectively represents CMC (Ref. 11) supplemented by a consistent closure for the mixture fraction PDF based on mapping closure.[12–14] Different versions of MMC models have appeared.[15–18] The stochastic versions of the model were originally introduced and seen as a stochastic implementation of the CMC model.[10,18] The MMC model, however, has absorbed many features that belonged to other models. MMC has many similarities with Euclidean minimum spanning tree (EMST):[19] both models introduce localized mixing and both models use the mapping closure concept. There is, however, one essential difference: EMST enforces localness directly in the composition space (this violates independence of scalars and creates problems for EMST mixing), while MMC uses reference variables to enforce localness. It is interesting that MMC is compatible with many mixing models such as Curl's[20,21] and IEM (interactions by exchange with the mean) (Ref. 22) but is not generally compatible with its closest relative—EMST. The reason behind this is that Curl's and IEM mixing do not have any localization principles on their own and are ready to take these principles from MMC while EMST has its own localization approach which is not equivalent to the localization principles used in MMC. We also note that the MMC-Curl model retains many features of Curl's or modified Curl's mixing. From the perspective of Curl's model, MMC-Curl is different from conventional Curl's model only by a new algorithm of selecting particles for mixing. If a single mixture-fraction-like reference variable is used, MMC can be viewed as enforcing CMC on Curl's or IEM mixing. When mixing time is small, MMC is very close to CMC, while large mixing time minimizes the CMC effect on the mixing model. MMC model can effectively emulate other models as its limiting cases. The IECM model[23–25] represents IEC model[22] localized in the velocity space and corresponds to a MMC-IEM model with the reference variables represented by velocity (it should be noted that the IECM model was introduced before MMC). The degree of correlation between the reactive scalars and velocities is much smaller than between the reactive scalars and mixture fraction, and it is disputable whether true MMC regime is achieved in IECM model.[26] MMC is also related to velocity-biased Curl's mixing[1] that, in fact, can be seen as partial conditioning of mixing on velocity. Although this model was implemented in Ref. 27, it is not used as widely as IECM. The MMC model also has many common features with intrinsic low-dimensional manifolds:[28] MMC mapping of reference variables into composition space effectively creates a low-dimensional manifold that is partially responsible for emulating behavior of reactive species. There are, however, differences: species are free to fluctuate around the manifold in stochastic MMC while closeness to low-dimensional intrinsic manifold is enforced by properties of chemical kinetics.

The MMC-LES approach represents a generalized version of MMC:[26] the original Markov reference variables are replaced by a generalized random process which is deemed to produce better outcomes. Specifically, MMC-LES replaces Markov reference variables by stochastic processes generated by LES. Previous publications on MMC-LES (Refs. 6–8) follow the main physical argument of Ref. 26 that LES/DNS-generated variables enforce more realistic values for first conditional moments of simulated scalars. Generalized MMC was introduced as a modification of the original MMC. Although recent successes of MMC-LES provide justification for these arguments, there is a significant gap in MMC analysis. Pope (private communication) noted that fundamental consistency of MMC and PDF approaches established for the original MMC (Ref. 10) is not applicable to generalized MMC and this consistency has to be established again. The present paper closes this gap and provides interpretation of MMC-LES model in terms of filtered transport equations, which are conventionally used in LES.

Generalized MMC with reference variables generated by tracing Lagrangian particles in LES simulations has strong connections with DNS/LES type of modeling. As shown in Refs. 6 and 9, MMC-LES/DNS and other sparse-Lagrangian models can be considered as LES/DNS tools on their own. This possibility of converging simulations to DNS under conditions of very large number of particles used in simulations effectively guarantees the success of this methodology (although this success based on introducing large number of particles may come at a very high computational cost). It was expected[6] and demonstrated[7,8] that, in practical simulations, the MMC-LES model may require a much smaller (in fact very small) number of particles to achieve high quality simulations. Different models must be compared on the basis of their performance per actual or nominal (i.e., number of particles in the reacting region of the flow) computational cost. The approach of the best quality at any computational cost already has its well-known solution—DNS—and improvements in performance may be related to approaching the DNS regime rather than to using a better mixing model. The MMC-LES model also has direct links with one of the oldest combustion models—the flamelet model.[29,30] Indeed, stretching the metrics of physical space to ensure better resolution across isoscalar lines of constant mixture fraction[6] has similarities with the flamelet transformation.[29,30] Although there is an underlining similarity that ensures efficiencies of MMC-LES and flamelet models, it must be noted that MMC-LES is a full-scale FDF model with DNS capabilities and its area of applicability is incomparably wider than that of the flamelet model. The fact that MMC modeling occupies the very central place in combustion modeling, which unifies nearly all existing models in the area, is probably the main underlying feature of MMC that ensures its impressive efficiency.[7,31]

Sections II–IV introduce major equations and discuss distinctive features of sparse-Lagrangian models. Sections V–VII deal with MMC-LES model and its major properties. Conclusions are given in Sec. VIII.

II. JOINT SCALAR FDF EQUATION

Filtering operation is conventionally used in LES. The filtered quantity $\bar{\varphi}$ is introduced by applying the following filtering operation:[4,32]

$$\bar{\varphi}(\mathbf{x}) = \int_{\infty} \varphi(\mathbf{x}^{\circ}) \Psi_{r_f}(\mathbf{x} - \mathbf{x}^{\circ}) dx^{\circ} \tag{1}$$

to any fully resolved field $\varphi(\mathbf{x})$ where the filter kernel Ψ_{r_f} is characterized by the filtering scale r_f. The variations of φ at the scales smaller than r_f are filtered out. The subfilter fluctuations of the reactive scalar variables

$$\rho \frac{\partial Y^{(\alpha)}}{\partial t} + \rho \mathbf{U} \cdot \nabla Y^{(\alpha)} - \nabla \cdot (\rho D \nabla Y^{(\alpha)}) = \rho W^{(\alpha)} \tag{2}$$

are characterized by filtered mass density function F where $F = \rho \delta(\mathbf{Y} - \mathbf{Y}^{\circ})$ is the fine-grained mass-weighted density joint distribution function of the n_s scalars $Y^{(1)}, \ldots, Y^{(n_s)}$, ρ is density, $W^{(\alpha)} = W^{(\alpha)}(\mathbf{Y})$ represent chemical source terms and δ is Dirac's delta function. Applying the filtering operation to F results in a filtered mass density function[32] that is referred to here as mass-weighted FDF. This FDF satisfies the following equation:[4,32,3]

$$\frac{\partial \bar{F}}{\partial t} + \nabla \cdot (\bar{\mathbf{U}}_Y \bar{F}) + \frac{\partial (W^{(\alpha)} + \overline{J_Y^{(\alpha)}}) \bar{F}}{\partial Y^{(\alpha)}} = 0, \tag{3}$$

where $J^{(\alpha)} = \rho^{-1} \nabla \cdot (\rho D \nabla Y^{(\alpha)})$, the subscript Y is used to denote conditional filtering, for example,

$$\bar{\varphi}_Y = \frac{\overline{\varphi F}}{\bar{F}} \tag{4}$$

for any φ and sum is evaluated over repeated indices. If the differential diffusion effects are neglected, the FDF governing equation can be rewritten in the form

$$\frac{\partial \bar{F}}{\partial t} + \nabla \cdot (\bar{\mathbf{U}}_Y \bar{F}) + \frac{\partial W^{(\alpha)} \bar{F}}{\partial Y^{(\alpha)}} + \frac{\partial^2 \bar{N}_Y^{(\alpha\beta)} \bar{F}}{\partial Y^{(\alpha)} \partial Y^{(\beta)}} = \nabla \cdot \overline{\rho D \nabla (F \rho^{-1})}, \tag{5}$$

where $N^{(\alpha\beta)} = D \nabla Y^{(\alpha)} \cdot \nabla Y^{(\beta)}$ is the dissipation tensor. These equations are exact but not closed since conditional filtered averages in these equations remain unknown. A significant advantage of these equations is that the chemical terms appear there in a closed form (provided all reacting scalars are considered).

The term on right-hand side (rhs) of Eq. (5) represents transport by molecular diffusion and it is small in high-Reynolds flows where the diffusion coefficient D is small. This term can be written simply as $D \nabla^2 \bar{F}$ when ρ and D are constant. It must be noted that, in turbulent flows, the dissipation term $\bar{N}_Y^{(\alpha\beta)}$ remains significant even if D is very small. This term is responsible for reduction in scalar variance and is simulated by mixing. It is easy to see that the direct effect of the dissipation term does not change the mean values of the scalars and, thus, does not involve spatial scalar transport.

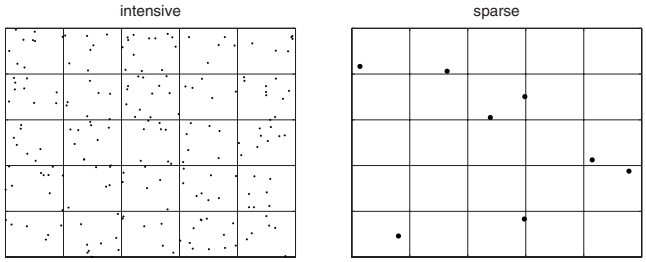

FIG. 1. Illustrative example for random particle distributions on Eulerian grid for intensive (200 particles) and sparse (eight particles) conditions.

The process of diffusion is linked to two main effects: scalar transport by diffusion and scalar dissipation. In general these effects are closely related to each other and this corresponds to combining these two effects in one term $\overline{J_Y^{(\alpha)}}$. However, in high-Reynolds turbulent flows the effects of transport by molecular diffusion and dissipation are separated: the former appears to be small while the later is always significant. Idealized mixing can be defined as dissipation that does not have any spatial transport components; mixing occurs between two (or more) fluid particles at the same location while fluctuations of particle positions due to diffusional random walk involve spatial transport. Consideration of mixing distinct from diffusional transport appeared first in modeling of turbulent flows.[1,2]

III. SPARSE-LAGRANGIAN METHODS

Simulations of reactive scalars in turbulent flows can be performed using Lagrangian particles.[1,2] In practical simulations the number of particles is insufficient to resolve the smallest details of the scalar fields. We label these particles as a "Lagrangian grid" and the scalar fluctuations, which are not resolved due to a limited number of particles, are called Lagrangian subgrid fluctuations. Velocity is evaluated on the conventional Eulerian grid. Modeling under conditions when the number of Lagrangian particles is much smaller than the number of Eulerian grid points is referred to as sparse-Lagrangian modeling.[6–8] The opposite case of having many particles in every Eulerian cell is called here intensive Lagrangian modeling. Figure 1 illustrates sparse and intensive distributions of particles on an Eulerian grid. If r_L is the scale that characterizes the Lagrangian grid (i.e., r_L represents distance between particles) and r_E characterizes Eulerian grid (representing distance between nodes) then $r_L > r_E$ in sparse-Lagrangian models. To avoid confusion related to multiple grids, in several points of our analysis we may assume that the fully resolved Eulerian velocity field is available in simulations—we are most concerned with modeling Lagrangian subgrid fluctuations, which are the largest unresolved quantities in sparse-Lagrangian simulations.

The obvious advantage of sparse models is in significant reduction in the computational cost since the large number of reactive scalars can be evaluated at relatively few points.

Fewer particles, however, provide less information about the structure of the scalar field. If there is a hundred particles in a selected control volume, this allows us to determine mean values, variances and maybe some of the joint characteristics related to different scalars. While the mean values can be determined with a stochastic error of $100^{-1/2}=10\%$, the accuracy of determining joint characteristics of the scalars from 100 particles is much lower. If we have only one particle in the control volume, we cannot possibly determine any average characteristics but this does not mean that these characteristics do not exists. The scalar values assigned to the particle are denoted by $Z^{(\alpha)}$, $\alpha=1,2,\ldots,n_s$—the same as $Z^{(\alpha)}$ in Ref. 9 but in this paper we assume for simplicity that all particles have equal weights (i.e., $Z^{(0)}=1$). Unlike in Ref. 9, in this work values $Y^{(\alpha)}$ are used to denote the real physical values of the scalars as defined by Eq. (2). The scalars $Z^{(\alpha)}$ are used for modeling of the physical scalars (as interpreted further in this section) and do not necessarily coincide with $Y^{(\alpha)}$. The values $Z^{(\alpha)}$ are random values that posses means, variances and joint PDFs $P(\mathbf{Z},\mathbf{x};t)=P(Z^{(1)},Z^{(2)},\ldots,\mathbf{x};t)$, which account for particle random walk but not for fluctuations of the simulated velocity field. These PDFs are the same as the single particle PDF P_Z or P_1 in Ref. 9. The PDF $P(\mathbf{Z},\mathbf{x};t)$ satisfies the equation

$$\frac{\partial P}{\partial t}+\nabla\cdot(\mathbf{U}P)-\nabla\cdot\rho D\,\nabla\,(P\rho^{-1})+\frac{\partial W^{(\alpha)}P}{\partial Z^{(\alpha)}}=\left[\frac{dP}{dt}\right]_{\mathrm{mix}},\quad(6)$$

derived in Ref. 9. Whether we have many or few particles in the flow, this does not alter the probabilistic nature of the Lagrangian simulations. We can use convergence with intensification (r_m remains fixed), as discussed in the last section of Ref. 9, and increase the number of particles without altering the model to extent that allows evaluation of the PDF in every small volume. This, however, would impose a large computational cost on the simulations.

If relatively few particles are used in the simulations, the average distance between closest particles is not small and mixing between these particles generates significant numerical diffusion $D_m\sim r_m^2/\tau$ where r_m is the mixing distance indicative of localization of mixing and τ is the mixing dissipation time as discussed in Refs. 6 and 9. In practical simulations, the mixing distance cannot be smaller than the distance between closest particles. This means that all fluctuations of scale smaller than r_m are effectively filtered out and are not directly reproduced in these simulations. As in any numerical method, the mixing scale r_m must be small compared to the macroscale of the problem under consideration to avoid the direct influence of numerical diffusion on marcoparameters. The scale r_m is always presumed to belong to the inertial interval of turbulence, although in sparse-Lagrangian simulations r_m can be noticeably larger than the conventional Eulerian grid size. If r_m is smaller than the Kolmogorov scale, τ is sufficiently small and the velocity field is fully resolved, then our Lagrangian simulations approach DNS.[6,9]

We note that the scalars fluctuate around their average values

$$\langle Z^{(\alpha)}\rangle\equiv\int Z^{(\alpha)}P d\mathbf{Z}.\quad(7)$$

As in Ref. 9, angular brackets are used to denote averaging over the ensemble of particles (with turbulent velocity field being given) and not the averages over the ensemble of realizations of turbulent flows. In the case of convergence to DNS, the variance $\langle(z^{(\alpha)})^2\rangle$, $z^{(\alpha)}\equiv Z^{(\alpha)}-\langle Z^{(\alpha)}\rangle$ is interpreted as representing stochastic errors indicating incomplete convergence, but in sparse-Lagrangian methods we treat these fluctuations as representing the high-frequency components of the fields that are filtered out in simulations and can be called Lagrangian subgrid fluctuations. This interpretation corresponds to FDF approaches. The FDF simulations are not intended to reproduce all details of the scalar field, instead, these simulations are focused on emulating equivalent statistics. Reproducing realizations of the fields can be called strong simulations while emulating equivalent statistics can be called weak simulations, in accordance with commonly adopted mathematical terminology.[7]

We now nominate the function that represents a model for $\bar{F}$ in Eq. (5). The filtering operation applied to P produces a new distribution function $\bar{P}$ and we assume that $\bar{F}=\bar{P}M_0$ where M_0 is a normalization constant that can be interpreted as the total mass present in the domain under consideration. The filtered PDF $\bar{P}$ satisfies the equation

$$\frac{\partial\bar{P}}{\partial t}+\nabla\cdot(\bar{\mathbf{U}}_Z\bar{P})+\frac{\partial W^{(\alpha)}\bar{P}}{\partial Z^{(\alpha)}}-\overline{\left[\frac{dP}{dt}\right]}_{\mathrm{mix}}=\nabla\cdot\overline{\rho D\,\nabla\,(P\rho^{-1})},\quad(8)$$

where

$$\bar{\varphi}_Z=\frac{\overline{\varphi P}}{\bar{P}},\quad(9)$$

conditional filtered averages evaluated for any φ and conditioned on a fixed value of Z while $W^{(\alpha)}=W^{(\alpha)}(\mathbf{Z})$ is the chemical source term in the model. This equation coincides with Eq. (5) provided the mixing term in Eq. (8) emulates behavior of the dissipation term in Eq. (5). We also expect that $\bar{\mathbf{U}}_Z$ represents a model for $\bar{\mathbf{U}}_Y$ implying local isotropy of the physical fields at the Eulerian subgrid scales.

The sparse-Lagrangian methods are FDF simulations that directly simulate the largest fluctuations and emulate the smaller fluctuations by variations of $z^{(\alpha)}$. If the number of particles is very large, simulations can be performed under conditions of convergence with localizations approaching the regime of direct simulation of all fluctuations. Under these conditions, many mixing models will perform adequately due to convergence to DNS conditions and quality simulations are achieved at a high computational cost. Economical simulation using a relatively small number of particles is a more challenging task for a mixing model, since under sparse conditions this model handles a larger fraction of scalar fluctuations. High quality of the mixing model is of prime importance in this case. Thus, in the framework of Lagrangian simulations, quality simulations can be achieved by using a large number of particles with localized mixing, or by employing a good mixing model and a limited number of par-

ticles. Comparing two mixing models requires that compatible number of particles is used in the simulations, otherwise, this comparison is more linked to computational performance than to quality of the models. It should be noted that the minimal number of particles required in quality simulations is dependent on complexity of the problem: more complex cases need more particles to represent accessible volume in composition space.[33]

IV. FILTERED MEAN AND VARIANCE

The modeling Eq. (8) matches the FDF Eq. (5), provided that the mixing operator correctly emulates the dissipation term. This can be symbolically expressed by the following equality:

$$\rho_0 \overline{\left[\frac{dP}{dt}\right]}_{\mathrm{mix}} = \frac{\partial^2 \bar{N}_Y^{(\alpha\beta)} \bar{F}}{\partial Y^{(\alpha)} \partial Y^{(\beta)}}. \tag{10}$$

This equality, however, is difficult to satisfy exactly and this problem is well known in all mixing models as the problem of mixing. Indeed, the first moment of the rhs is zero while the first moment of lhs is not due to numerical diffusion. We, of course, can always minimize numerical diffusion by introducing more and more particles and localizing mixing but this, effectively, would convert our simulations into DNS with heavy computational costs. We qualitatively assess the major differences for filtered mean and variance that stem from surrogate nature of particle mixing under sparse conditions. In this section, for the sake of simplicity we assume constant density ρ=const and neglect the chemical source term. Here and in the rest of the paper, our analysis is applied to any scalar selected from $Y^{(\alpha)}$ $(\alpha=1,\ldots,n_s)$ and, unless this may cause a confusion, we tend to omit the superscript index α. This implies that equations under consideration are applicable to any of the scalars $Y^{(1)},\ldots,Y^{(n_s)}$. However, the superscript α is retained when a particular scalar needs to be nominated (for example, the mixture fraction). The filtered scalar transport equation takes the form

$$\frac{\partial \bar{Y}}{\partial t} + \bar{\mathbf{U}} \cdot \nabla \bar{Y} - \nabla \cdot ((D_f + D) \nabla \bar{Y}) = 0,$$

where the gradient-diffusion approximation is used $(\overline{\mathbf{U}Y} - \bar{\mathbf{U}}\bar{Y}) = -D_f \nabla \bar{Y}$ and D_f represent turbulent diffusion coefficient related to the filtering scale r_f. The equation for the resolved scalar field $\langle Z \rangle$

$$\frac{\partial \langle Z \rangle}{\partial t} + \mathbf{U} \cdot \nabla \langle Z \rangle - \nabla \cdot ((D_m + D) \nabla \langle Z \rangle) = 0 \tag{11}$$

involves the numerical diffusion effects represented by coefficient $D_m \sim r_m^2/\tau$ as discussed in Refs. 6 and 9. Here, r_m is the mixing interaction radius, which characterizes locality of mixing, and τ is the mixing time. Note that unless the number of particles is sufficient to achieve the DNS regime, D_m is likely to be dominant over D. The filtered version of this equation becomes

$$\frac{\partial \overline{\langle Z \rangle}}{\partial t} + \bar{\mathbf{U}} \cdot \nabla \overline{\langle Z \rangle} - \nabla \cdot ((D_f + D_m + D) \nabla \overline{\langle Z \rangle}) = 0, \tag{12}$$

where the gradient-diffusion approximation $(\overline{\mathbf{U}\langle Z \rangle} - \overline{\mathbf{U}}\overline{\langle Z \rangle}) = -D_f \nabla \overline{\langle Z \rangle}$ is consistently applied. The direct influence of numerical diffusion is minimal if $D_f \gg D_m$ and this happens when $r_f \gg r_m$. This implies that distance between particles must always be much smaller than the integral scale of the problem under consideration and we always assume that r_m belongs to the inertial interval of turbulence. The other formulation of this restriction is that mean parameters must not change significantly within the mixing distance r_m. It must be noted that a similar restriction applies to any finite difference method, Lagrangian or Eulerian: the solution must be observed at scales much greater than the grid size. In intensive Lagrangian models particles are allowed to mix when they are within the same Eulerian cell and this generates numerical diffusion with D_m linked to the cell size. The cell size is typically much smaller than the macroscale of the problem. In sparse-Lagrangian methods, r_m is larger and we properly resolve only the largest fluctuations present in the flow. The filtering length r_f is introduced here as an observation scale—the mixing model does not depend on this scale. In extreme conditions of having a small number of particles, it may be difficult to select any reasonable value of r_f. In this case, the filtering operation specified in Eq. (1) and used in other equations should be interpreted as ensemble average. Note that Lagrangian resolved scales are always linked to the mixing distance r_m and can be linked to the characteristic distance between the closest particles r_1 only because r_m is never smaller than r_1. Perhaps Lagrangian subgrid fluctuations should be more accurately referred to as "sub-mixing-distance" fluctuations but this notation does not seem appropriate from a linguistic point of view.

The numerical viscosity also affects the variance suppressing all small-scale fluctuations of $\langle Z \rangle$ at distances below r_D where $r_D = (D_m^3/\bar{\varepsilon})^{1/4} = (D_m/D)^{3/4} r_K$ is the scale calculated on the basis of D_m and r_K is the Kolmogorov scale, assuming that $\bar{\varepsilon}$ is the average dissipation of energy and that diffusion D is the same as viscosity. The fluctuations of intensity $\Theta_m \sim (D_m/\bar{\varepsilon})^{1/2} \bar{\chi}$ are attenuated by the excessive diffusion where the scalar dissipation is approximately the same for the scalar and its model

$$\bar{\chi} = \overline{D(\nabla Y)^2} \approx \overline{D_m (\nabla \langle Z \rangle)^2}$$

due to the similarity of the large-scale structures of these fields. Hence, the resolved variance $\Theta_{\langle Z \rangle} = \overline{\langle Z \rangle^2} - \overline{\langle Z \rangle}^2$ appears to be smaller than the physical variance $\Theta_Y \equiv \overline{Y^2} - \bar{Y}^2$ by Θ_m so that $\Theta_Y - \Theta_{\langle Z \rangle} = \Theta_m$. The variance of Z also has two components the resolved $\Theta_{\langle Z \rangle}$ and unresolved (or subgrid) $\overline{\langle z^2 \rangle}$ as determined by $\Theta_Z \equiv \overline{Z^2} - \overline{\langle Z \rangle}^2 = \Theta_{\langle Z \rangle} + \overline{\langle z^2 \rangle}$ where $z \equiv Z - \langle Z \rangle$. The equations for the filtered variance can be found in Ref. 34 while the equation for $\langle z^2 \rangle$ is derived in Ref. 9. The dissipation of resolved variance $\Theta_{\langle Z \rangle}$ is given[34] by the term $2\bar{\chi}$ and the same term represents[9] generation of subgrid variance $\overline{\langle z^2 \rangle}$. The subgrid variance $\overline{\langle z^2 \rangle}$ dissipates due to mixing and its dissipation term is $\overline{[d\langle z^2 \rangle/dt]}_{\mathrm{mix}} = 2\overline{\langle z^2 \rangle}/\tau$. Under quasi-

steady conditions, generations of subgrid variance matches its dissipation so that $\overline{\langle z^2\rangle}=\bar{\chi}\tau$.

We, of course, wish to see that the subgrid variance $\overline{\langle z^2\rangle}$ emulates the variance component Θ_m negated by the numerical diffusion. Substituting $D_m\sim r_m^2/\tau$ into $(D_m/\bar{\varepsilon})^{1/2}\bar{\chi}\sim\bar{\chi}\tau$ results in $\tau^3=r_m^2/\bar{\varepsilon}$. This is simply the inertial interval link between time τ and distance r_m—the same estimate was previously obtained in Ref. 6 from different considerations. This link, which can be expressed by

$$\tau=C_m\left(\frac{r_m^2}{\bar{\varepsilon}}\right)^{1/3}, \tag{13}$$

where C_m is a constant, ensures that "correct" subgrid variance is generated by the model. If τ is too small, then $\overline{\langle z^2\rangle}$ is underproduced; if τ is too large, then $\overline{\langle z^2\rangle}$ exceeds Θ_m.

It should be noted that the filtered mean and variance are not the only way how surrogate (i.e., simulated) mixing affects the scalars—numerical diffusion suppresses all subgrid joint features of the scalars at small scales and these features have to be emulated by a mixing model. For a given mixing model, it is not guaranteed that these features are emulated well. In Secs. V–VIII, we consider how emulation of subgrid fluctuations of the scalars can be improved using the approach.

V. REFERENCE VARIABLES IN GENERALIZED MMC

The MMC approach is characterized by using reference variables. These variables simulate properties of turbulence that affect combustion processes. The choice of reference variables can include variables simulating mixture fraction, velocity components, dissipation, and/or other quantities. The reference variables must not coincide with the simulated reactive species, otherwise independence of simulated scalars is violated. Hence, if mixture fraction (or mixture fraction-like variable) is used as MMC reference variable, there must be another mixture fraction that is linked to simulated reacting scalars. In the original MMC,[10] the reference variables were represented by Markov processes. Here, we follow a more general understanding of MMC (Refs. 6 and 26) and allow for reference variables being simulated by a DNS (or LES) solver according to conventional transport equations

$$\rho\frac{\partial\xi^{(i)}}{\partial t}+\rho\mathbf{U}\cdot\nabla\xi^{(i)}-\nabla\cdot(\rho D_\xi\nabla\xi^{(i)})=\rho S^{(i)}. \tag{14}$$

A large class of transport equations can be written in this form, for example, if $\xi^{(i)}$ represents velocity then the source term $S^{(i)}$ must involve the pressure gradient. Note that lowercase indices i and j are consistently used to denote values related to the reference variables while the values related to simulated scalars are indexed by Greek superscripts. The MMC-LES model introduced in Ref. 6 involves only one reference variable—the LES mixture fraction. At this stage, this approach seems to be the most practical.[7,8] Here, we have many reference variables $\xi^{(1)},\xi^{(2)},\ldots,\xi^{(n_r)}$ but do not consider the differential diffusion effects so that all diffusion coefficient D_ξ are presumed to be the same. The filtered mass density function $\tilde{\Phi}=\overline{\rho\delta(\xi-\xi^*)}$ satisfies the following equation:

$$\frac{\partial\tilde{\Phi}}{\partial t}+\nabla\cdot(\tilde{\mathbf{U}}_\xi\tilde{\Phi})+\frac{\partial\overline{(S^{(i)}+J^{(i)})_\xi\tilde{\Phi}}}{\partial\xi^{(i)}}=0. \tag{15}$$

The FDF governing equation can also be written in the dissipative form

$$\frac{\partial\tilde{\Phi}}{\partial t}+\nabla\cdot(\tilde{\mathbf{U}}_\xi\tilde{\Phi})+\frac{\partial\overline{S}_\xi^{(i)}\tilde{\Phi}}{\partial\xi^{(i)}}+\frac{\partial^2\overline{N}_\xi^{(ij)}\tilde{\Phi}}{\partial\xi^{(i)}\,\partial\,\xi^{(j)}}=\nabla\cdot\overline{\rho D_\xi\nabla\,(\Phi\rho^{-1})}, \tag{16}$$

where $J^{(\iota)}=\rho^{-1}\nabla\cdot(\rho D_\xi\nabla\xi^{(i)}),N^{(ij)}=D_\xi\nabla\xi^{(i)}\cdot\nabla\xi^{(j)}$ and the subscript "ξ" is used to denote conditional density weighted filtering

$$\bar{\varphi}_\xi=\frac{\overline{\varphi\Phi}}{\tilde{\Phi}} \tag{17}$$

for any φ where $\Phi=\rho\delta(\xi-\xi^*)$. Since the term on rhs of Eq. (16) can be neglected, we note that these reference variables comply with the conditions imposed in deterministic MMC (Ref. 10) on the reference variables. Hence, the "filtered" CMC closure for these equations[35,36]

$$\frac{\partial Q\tilde{\Phi}}{\partial t}+\nabla\cdot(\tilde{\mathbf{U}}_\xi Q\tilde{\Phi})+\frac{\partial}{\partial\xi^{(i)}}\left(Q\overline{S}_\xi^{(i)}\tilde{\Phi}+Q\frac{\partial\overline{N}_\xi^{(ij)}\tilde{\Phi}}{\partial\xi^{(j)}}-\overline{N}_\xi^{(ij)}\tilde{\Phi}\frac{\partial Q}{\partial\xi^{(j)}}\right)=\tilde{W}_\xi\tilde{\Phi}, \tag{18}$$

neglecting correlations of the $\mathbf{U}$-Y conditional fluctuations creates variables $\mathbf{Y}=\mathbf{Q}(\xi,\mathbf{x},t)$ that are compliant with the FDF Eq. (5) assuming that the rhs of this equation is consistently neglected. In this work, however, we use the stochastic form of the MMC approach and do not need to employ this property directly. We imply that Eq. (18) is applicable to any of the scalars $Q^{(\alpha)}$, $\alpha=1,2,\ldots,n_s$ and $\mathbf{Y}=\mathbf{Q}(\xi,\mathbf{x},t)$ means that $Y^{(\alpha)}=Q^{(\alpha)}(\xi,\mathbf{x},t)$ for any α.

In stochastic MMC, the reference variables are used to enforce the desired properties on the mixing operator. The best known reference variable in nonpremixed combustion is, of course, the mixture fraction. Accurate simulation of the reference mixture fraction improves simulation of the scalars. Thus, the best possible simulation of mixture fraction is achieved by DNS, while LES represent the second best option with Eulerian subgrid fluctuations being filtered out. In general, these subgrid fluctuations can be emulated by a stochastic process[26] but it seems that under sparse conditions when Lagrangian grid scales are much larger than Eulerian, these additional Eulerian subgrid stochastic emulations do not have any significant effect on results.[7,8] Eulerian simulation of one additional scalar variable does not impose any significant computational cost on LES. It must be stressed that MMC does not reproduce a joint FDF distribution of scalars $\mathbf{Y}$ and reference variables ξ—the reference variables are only used to improve simulation of the joint FDF of the scalars $\mathbf{Y}$. The reference mixture fraction, say $\xi^{(1)}$, and the simulated mixture fraction, say $Y^{(1)}$, are represented by dif-

ferent variables. In sparse-Lagrangian formulation, a large saving of computational cost is achieved by evaluating reacting scalars $\mathbf{Y}$ only at relatively few Lagrangian particles. It must be noted that the chemical source terms depend only on the simulated scalars $\mathbf{Y}$ and do not depend on any of the reference variables ξ.

We now turn our attention to Lagrangian properties of the reference variables. These properties are analyzed from the perspective of moving particles: conventional fluid particles or diffusing particles that slightly deviate from the fluid particles due to random walk simulating molecular (or subgrid) diffusion. The Lagrangian properties of the reference variables are closely linked with the equation for expectation of a selected scalar Y conditioned on the reference variables.[37] The equation for conditional filtered average $\bar{Y}_\xi$ is now written in the form[35,36]

$$\frac{\partial \bar{Y}_\xi \bar{\Phi}}{\partial t} + \nabla \cdot (\overline{(\mathbf{U}Y)}_\xi \bar{\Phi}) + \frac{\partial \overline{(YS^{(i)} + YJ^{(i)})}_\xi \bar{\Phi}}{\partial \xi^{(i)}} = \bar{W}_\xi \bar{\Phi} + \overline{\rho^{-1} \nabla \cdot (\rho D \nabla Y)}_\xi \bar{\Phi}. \quad (19)$$

These conditional equations can be derived by using techniques of Ref. 11 to obtain equations for fine-grained PDFs and then applying filtering instead of the ensemble averaging. If $D=0$ and $W=0$, Eq. (2) governs trajectories of fluid particles. We can introduce Lagrangian FDF $\bar{\Phi}_L = \bar{Y}_\xi \bar{\Phi} / Y_0$ where Y_0 is a normalization constant and Lagrangian conditional averages $\bar{\varphi}_{L\xi} = \overline{(Y\varphi)}_\xi / \bar{Y}_\xi$ for any φ and note that in this case the FDF Eq. (15) is still valid but Eulerian averages must be replaced by Lagrangian averages for the coefficients of this equation. This feature was first noted by Pope.[1] If, however, $D \neq 0$, an additional term—the last term of the Eq. (19)—appears in the FDF equation. The FDF equation can be written in alternative, dissipative form

$$\frac{\partial \bar{Y}_\xi \bar{\Phi}}{\partial t} + \nabla \cdot (\overline{(\mathbf{U}Y)}_\xi \bar{\Phi}) + \frac{\partial \overline{(YS^{(i)})}_\xi \bar{\Phi}}{\partial \xi^{(i)}} + \frac{\partial^2 \overline{(YN^{(ij)})}_\xi \bar{\Phi}}{\partial \xi^{(i)} \partial \xi^{(j)}} - \frac{\partial \overline{((D + D_\xi) \nabla Y \cdot \nabla \xi^{(i)})}_\xi \bar{\Phi}}{\partial \xi^{(i)}} = \bar{W}_\xi \bar{\Phi} + \nabla \cdot \rho D_\xi \nabla (Y \Phi \rho^{-1}) + \nabla \cdot \overline{\Phi (D - D_\xi) \nabla Y}. \quad (20)$$

Note that, even if $D=0$, this equation differs form the equation, which can be formally obtained from Eq. (16) by replacing Eulerian averages by Lagrangian averages, due to the last term on lhs of Eq. (20). The reference variables are used in Sec. VI to define the MMC-LES model.

VI. THE MMC-LES MODEL

Improvements in simulation of mixing are achieved in MMC by localizing mixing in the space of the reference variables. These improvements can be considered from the perspective of equation for filtered average $\overline{\langle Z \rangle}_\xi$ that is conditioned on given values of the reference variables. The equation for the value of Z averaged over subgrid fluctuations modeled variable takes the form

$$\rho \frac{\partial \langle Z \rangle}{\partial t} + \rho \mathbf{U} \cdot \nabla \langle Z \rangle - \nabla \cdot (\rho D \nabla \langle Z \rangle) = \rho W + \rho \left[\frac{d\langle Z \rangle}{dt} \right]_{\mathrm{mix}} \quad (21)$$

and is derived in Ref. 9. The last term in this equation is kept since this term is responsible for numerical diffusion induced by mixing. This equation results in the following equation for the conditional average:

$$\frac{\partial \overline{\langle Z \rangle}_\xi \bar{\Phi}}{\partial t} + \nabla \cdot (\overline{(\mathbf{U}\langle Z \rangle)}_\xi \bar{\Phi}) + \frac{\partial (\langle Z \rangle S^{(i)} + \langle Z \rangle J^{(i)})_\xi \bar{\Phi}}{\partial \xi^{(i)}} = \bar{W}_\xi \bar{\Phi} + \overline{\rho^{-1} \nabla \cdot (\rho D \nabla \langle Z \rangle)}_\xi \bar{\Phi} + \overline{\left(\left[\frac{d\langle Z \rangle}{dt} \right]_{\mathrm{mix}} \right)}_\xi \bar{\Phi}. \quad (22)$$

Comparing Eqs. (19) and (22) indicates that the last term in Eq. (22) is spurious. Generally, we would like to have

$$\left[\frac{d\langle Z \rangle}{dt} \right]_{\mathrm{mix}} \approx 0 \quad (23)$$

but satisfying this condition is not practical or realistic with a limited number of particles. Numerical diffusion can be eliminated by introducing a very large number of particles and approaching the DNS limit. This computationally expensive option is not of prime interest in this paper dealing with sparse-Lagrangian simulations. There is another possibility of satisfying condition (23)—reducing or completely eliminating mixing. In terms of the characteristic mixing time, this option means $\tau \to \infty$. No mixing means no numerical diffusion introduced by mixing and Eqs. (19) and (22) coincide. If the velocity and reference fields are fully resolved, then Lagrangian particles without mixing would exactly reproduce the first moment average (conditional or unconditional) of the corresponding scalar (assuming that the exact value of the chemical source term is specified). In fact, $\langle Z \rangle = Y$ in this case—see Ref. 9. In practice, the average $\langle Z \rangle$ may be difficult or impossible to evaluate due to stochastic scattering and an insufficient number of particles, but this average is an objective characteristic that exists irrespective of the practical accuracy of its evaluation. These mixing-free simulations, however, do not reproduce the joint scalar FDF well since all variances in these simulations are absolutely inaccurate and the values of $z = Z - \langle Z \rangle$ are far too large to correspond to any physical case. Introducing mixing to reduce the scalar variances to an appropriate level also introduces its side effect of numerical diffusion. If τ is relatively large, then τ determines the dissipation rate of the simulated scalars. If τ becomes small (we also assume that a sufficiently large number of particles is introduced in this case to avoid excessive numerical diffusion), then the scalars deviate very little from their averages $Z \to \langle Z \rangle = Y$ and the dissipation of Z is essentially the same as the dissipation of Y. In this case mixing time determines only the level of fluctuations $\langle z^2 \rangle \approx \chi \tau$ but not the dissipation rate χ. As discussed in previous publications,[38,26,6] the time τ is selected in MMC to match the expected level of conditional fluctuations but not to match the overall dissipation rate since this rate is enforced by using reference variables.

In general, condition (23) can be replaced by a much weaker requirement

$$\overline{\left[\frac{d\langle Z\rangle}{dt}\right]_{\mathrm{mix}}} \approx 0. \tag{24}$$

As discussed Secs. I–V, this requirement is satisfied provided mean characteristics of the scalars do not change significantly on the distances comparable with the mixing distance. This requirement is normally observed in conventional simulations but this does not remove the spurious term from Eq. (22): condition (24) removes only the direct effect of mixing on the averages while numerical diffusion still strongly affects joint characteristics of the scalars. The MMC approach recognizes that achieving Eq. (23) is difficult and costly while condition (24) is insufficient for quality modeling and introduces the following condition:

$$\overline{\left(\left[\frac{d\langle Z\rangle}{dt}\right]_{\mathrm{mix}}\right)_{\xi}} \approx 0 \tag{25}$$

enforcing localization of the mixing operator in ξ-space. The physical and modeling equations for conditional expectations then coincide. Condition (25) effectively makes mixing compliant with properties of reference variables. Enforcing these properties improves simulation of mixing.

In MMC models, we distinguish major and minor fluctuations.[10] Major fluctuations are driven by the fluctuations of the reference variables in $\bar{Y}_{\xi}(\xi,\mathbf{x},t)$ while minor fluctuations represent fluctuations of Y with respect to the conditional averages $\bar{Y}_{\xi}$. If the conditional averages $\bar{Y}_{\xi}$ are accurately evaluated and the reference variables $\xi^{(i)}$ are simulated well then this automatically ensures correct modeling of the major fluctuations (here we are concerned with direct influence of mixing on major fluctuations and do not consider secondary influence of minor fluctuations on major fluctuation through chemical source terms and other nonlinear mechanisms present in turbulent reacting flows). The MMC approach, however, does not guarantee that the minor fluctuations, which are controlled by surrogate mixing, are correctly simulated. The parameters of mixing have to be selected to make minor fluctuations simulated as adequately as permitted by surrogate mixing. Improvements in MMC simulations of mixing are related to the fact that the influence of surrogate mixing operator is limited in MMC to minor fluctuations, while in conventional mixing models surrogate mixing directly influences all fluctuations. MMC is not intended to reproduce joint distributions of the simulated scalars Y and reference variables $\xi^{(i)}$. Nevertheless, enforcing correct values of $\bar{Y}_{\xi}$ improves simulation of the joint PDF/FDF of the scalars Y.

It should be stressed that, since in sparse-Lagrangian methods the concentrations of reacting species are evaluated at relatively few particles, it is difficult to determine the values of density at numerous Eulerian grid locations. The numerical problem of determining stable values of density exists even in intensive LES-FDF simulations[5] but for sparse simulations, this is a principal difficulty, which cannot be resolved by improving numerical accuracy and needs a modeling approach. Intensive simulations with sufficiently large number of particles per Eulerian cell can stably reproduce the filtered density in each cell[5] but sparse methods do not have this capability. Sparse methods are weak simulators and intended to reproduce only joint FDFs of reactive scalars but not complete turbulent fields of these scalars and, consequently, not the complete density field. The MMC-style solution of this problem is in using the conditional average of density $\bar{\rho}_{Y^{(1)}}=f_{\rho}(Y^{(1)},\mathbf{x},t)$ conditioned on a fixed value of the simulated mixture fraction which is denoted here by $Y^{(1)}$. The method used in the simulations should provide for smooth and stable function f_{ρ}. The determined function is then used to evaluate density ρ_{LES} at every Eulerian grid location according to $\rho_{\mathrm{LES}}=f_{\rho}(\xi^{(1)},\mathbf{x},t)$ where $\xi^{(1)}$ is the reference mixture fraction evaluated by Eulerian LES.

Enforcement of condition (25) is performed by redefining the distance between particles.[6] Let $\mathbf{x}_p(t)$ be the position of particle p in physical space at moment t. We also introduce the position of particle p in the reference space $\xi_p=\xi(\mathbf{x}_p(t),t)$ and particle p's position in the combined space $\mathbf{X}_p(t)=\{\mathbf{x}_p(t),\xi_p(t)\}$. The distance in combined space between particles p and q is defined by

$$d_{pq}^2 = g_{IJ}(X_q^I - X_p^I)(X_q^J - X_p^J), \tag{26}$$

where g_{IJ} is the metric tensor that determines the metrics of particle locality and the indices J and I run over all components of the vector $\mathbf{X}$. The metric tensor determines which particles are considered to be close to each other and are allowed to be mixed. It should be noted that improved localization in some directions, which are determined by the use of reference variables, inevitably worsens localization in the other directions if the number of particles used in simulations remains fixed. The components of the metric tensor are selected to minimize the effect of numerical diffusion as discussed in Sec. VII. In practice, it is probably sufficient to restrict g_{IJ} to a diagonal matrix. The elements of the metric tensor can be normalized in any way since only the relative values of these elements matter. The most simple choice is in selecting the same scaling for all physical coordinates and a different scaling for the mixture fraction-like reference variable—this scaling was used in Refs. 39, 8, 7, and 31. If physical directions are not equivalent, the definition of locality can be relaxed in more homogeneous directions and tighten in less homogeneous directions. From an MMC perspective, the whole DNS/LES programming block with Lagrangian particle tracking is used only to evaluate the combined reference variables $\mathbf{X}_p(t)$. These variables determine which particles are allowed to mix so that the mixing operation is localized in the combine reference space. This effectively acts as an enforcer of the "correct" values of conditional averages $\bar{Y}_X$ while the variations with respect to these averages are controlled by adjusting the mixing rate τ.

VII. WHY MMC-LES IS EFFICIENT

The MMC-LES approach has been implemented for two major flames: Sandia flames D and E.[7,8,31,39] The MMC-LES model used a single reference variable which was represented by the mixture fraction emulated by LES. The main purpose of these simulations was in demonstrating the possibility of high quality FDF simulations using a relatively small number of particles. While combustion in flame D does

deviate (but not very far) from the flamelet regime, flame E has significant extinctions and is a difficult case to model. Generally, it could be expected that a more difficult case needs more particles but it was found that 10 000 reacting particles are sufficient to have very good scatter plots of reactive species for both flames in a jet region stretching for 75 nozzle diameters. We refer to particles that are located within a jet region and have ongoing reactions as reacting particles—these particles impose the main computer cost. The rest of the particles, which are outside the jet region, do not have reactions switched on and do not impose any significant computational cost. Computations of realistic chemical kinetics with more than 30 species and more than 200 reactions were performed on a personal workstation. In both simulations, the LES density was evaluated with assistance of the flamelet model. Although it is obviously premature to discuss universality of MMC parameters, the same set of parameters was shown to fit well flames E and D. It is worthwhile to note that the high quality and efficiency of the MMC-LES model was understood and predicted even before the first MMC-LES simulations were performed. The reasons behind this high efficiency of MMC-LES approach are now considered.

First we stress that the numerical efficiency of Curl's mixing under sparse conditions[9] plays a role in MMC performance, although the issue of model quality is a modeling issue, which is not limited to pure numerics. Note that effective diffusion D_{eff} of Ref. 9, which is responsible for chaotic stirring of the particles, may have four components in a turbulent flow: molecular diffusion and Eulerian subgrid diffusion (which both are simulated by random walk), as well as numerical diffusion associated with mixing and turbulent diffusion induced by vortices whose size is compatible to the distance between particles. In conditions of having one or more particle per Eulerian cell, the last component is not needed.

The ability of the MMC approach to combine advantages of all of the major combustion models, which was noted in Introduction, plays its role in achieving high quality of MMC mixing and high efficiency of MMC-LES simulations. In general, as discussed in Ref. 26, MMC-LES does not have to be sparse but, in this case, the space for improvements determined by the high quality of MMC mixing would be limited due to reduced influence of particulars of the mixing model under these conditions.[6] Under sparse conditions, quality of the mixing model is the principal issue. MMC mixing is compliant with all major requirements that are desirable for good simulation of mixing.[1] MMC mixing is

- conservative (i.e., preserving the amount of scalars),
- localized (i.e., mixing is limited to the particles that are close to each other according to a selected definition of distance between particles),
- linear with respect to scalar values,
- independent for different scalars and
- preserving boundedness of the scalars.

As discussed in Sec. V, the MMC approach enforces desired conditional properties on mixing. The simulated scalars fluctuate jointly with reference variables (major fluctuations in MMC terminology) and also fluctuate with respect to averages conditioned on the reference variable (minor fluctuations). Thus, a good selection of reference variables and adequate emulation of these variables is beneficial for MMC modeling. In the original MMC model, the reference variables were simulated by a Markov stochastic process. The best emulation of any process is the process itself, hence using DNS or LES to generate reference variables is a logical step toward improving MMC simulations. However, using DNS/LES has some additional advantages. The MMC-DNS/LES simulations are performed for a given large-scale realization of the DNS/LES turbulent velocity field and this is a significant factor that reduces the number of Lagrangian particles needed for this simulation. Representing scalars for one realization needs fewer particles than that for the complete ensemble of realizations. In MMC terms, a complete localization of mixing in physical space under DNS conditions means localization in any possible physical reference space while partial localization in physical space involves at least some implicit localization in a selected reference space. An increase in computational cost induced by using DNS/LES (instead of Reynolds average models of turbulence) for evaluation of three velocity components, pressure, and mixture fraction is heavily compensated by savings of computational time due to evaluating hundreds of reacting species at relatively few particles.

As discussed in Ref. 7, the sparse-Lagrangian approach is designed to produce equivalent statistics but not the complete realizations of the turbulent fields. The small-scale details of the scalar fields are replaced by a surrogate mixing process. The MMC-LES approach is not intended to reproduce Eulerian subgrid quantities for every Eulerian cell—the task which imposes the heaviest computational cost on conventional simulations. MMC-LES simulations are performed at the level above Eulerian cells and this saves the largest fraction of the computational cost. Conventional FDF methods are more expensive while sparse MMC-LES is less expensive than direct LES of all reactive species neglecting the subgrid variance. Computational savings of MMC-LES are especially important for cases involving realistic chemical kinetics and dealing with hundreds of reactive species.

If the number of Lagrangian particles is small, this stimulates numerical diffusion due to mixing between particles when the distance between them is not as small as is needed to abate numerical diffusion. The definition of particle vicinity according to Eq. (26) creates a region around particle 1 where mixing with this particle is allowed. This region is shown in Fig. 2 for the case of using only one reference variable $\xi=\xi^{(1)}$ that represents the mixture fraction (another illustration of selecting particles for mixing in MMC-LES can be found in Ref. 7). Mixing is allowed with particles 2 and 3 that are located within the mixing volume V_m but is not allowed with particles 4 and 5 that are located outside this volume. A spherical mixing volume that is shown at the background would allow mixing with particles 2 and 4 but not with particles 3 and 5. Note that enforcing closer proximity in the mixture fraction space comes at the cost of localization in the physical space along the surfaces

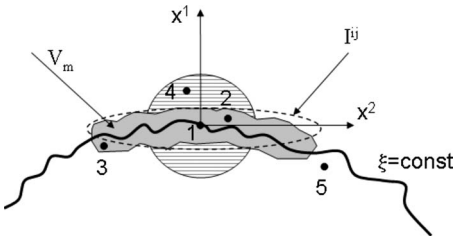

FIG. 2. Schematic of MMC mixing.

of constant mixture fraction. The ellipsoid of inertia I^{ij} of the mixing volume V_m is schematically shown in the figure. This ellipsoid illustrates the strength of numerical diffusion in different directions (weak across the surface of constant mixture fraction and strong along this surface—see Sec. III B in Ref. 9). We now demonstrate that only diffusional flux across the surface of constant ξ has a significant effect on the conditional expectation $\bar{Y}_\xi$. The equation for $\bar{Y}_\xi$ involves the term $\overline{(\nabla(D\nabla Y))}_\xi$—the last term in Eq. (19) representing the conditional average of diffusion of scalar Y. The following identities can be obtained by standard techniques for PDF derivations[11,40] for the case of constant density

$$\underbrace{\overline{(\nabla(D\nabla Y))}_\xi\bar{\Phi}}_{\mathrm{I}} = \underbrace{\frac{\partial\overline{(D\nabla Y\cdot\nabla\xi)}_\xi\bar{\Phi}}{\partial\xi}}_{\mathrm{II}} + \underbrace{\nabla\cdot(\overline{(D\nabla Y)}_\xi\bar{\Phi})}_{\mathrm{III}}, \tag{27}$$

$$\underbrace{\overline{\left(\nabla\cdot\frac{D\nabla\xi(\nabla\xi\cdot\nabla Y)}{(\nabla\xi)^2}\right)}_\xi\bar{\Phi}}_{\mathrm{I}} = \underbrace{\frac{\partial\overline{(D\nabla Y\cdot\nabla\xi)}_\xi\bar{\Phi}}{\partial\xi}}_{\mathrm{II}} + \underbrace{\nabla\cdot\left(\overline{\left(\frac{D\nabla\xi(\nabla\xi\cdot\nabla Y)}{(\nabla\xi)^2}\right)}_\xi\bar{\Phi}\right)}_{\mathrm{III}}. \tag{28}$$

These equations are identities and valid for any scalar Y. Terms I in both equations represent a conditional filtered average applied to the conventional molecular diffusion term in Eq. (27) and to a similar diffusion term in Eq. (28) that involves only component of the diffusion flux which is normal to the surface of ξ=const. Terms III are different in these equations but these terms are small in high-Reynolds flows. Terms II are identical in both equations and are linked to the last term on lhs of Eq. (20). Hence, to the leading order of our analysis, terms I are effectively the same. Thus, only one component of the diffusion fluxes of scalar Y—the component directed across the surfaces of ξ=const—has a significant effect on the term $(\nabla(D\nabla Y))_\xi$ in Eq. (19) and on the average $\bar{Y}_\xi$ conditioned on a fixed value of the mixture fraction ξ. Our strategy of minimizing numerical diffusion in the direction across the isoscalar surfaces enforces a reasonable value of the diffusion coefficient in this direction and this preserves the correct values of conditional averages $\bar{Y}_\xi$, which play an important role in MMC simulations of combustion.

In MMC-LES, the mixing volume V_m has two different characteristic scales and this creates more possibilities for selecting constant C_m in Eq. (13). In general, the mixture fraction-related scales of V_m can be expected to play a more prominent role in nonpremixed combustion due to strong dependence of the reaction process on the mixture fraction. As we increase the number of particles, two different convergence strategies discussed in Ref. 9 can be applied: convergence with localization and convergence with intensification.

In the first type of convergence, the increased number of particles is used to increase resolution and improve simulations so that the size of mixing volume V_m and time τ decrease as the distance between particles becomes smaller. This approach is most effective from the perspective of the efficiency criterion (quality per computational cost) and it converges to DNS when the number of particles tends to infinity. This convergence approach can preserve sparse conditions by having very few particles per Eulerian cell as the overall number of particles increases and the size of Eulerian cells decreases. It seems that simulations with well-localized Curl's mixing would allow to approach DNS at a reasonable computational cost. Whenever the true DNS regime is not reached, the stochastic variations $\langle z^2\rangle$ can play a positive role of simulating fluctuations that are still not resolved. Under these conditions, sparse-Lagrangian methods remain a FDF method up until all turbulent fluctuations are resolved and $\langle z^2\rangle$ becomes negligible.

In the second type of convergence, the size of mixing volume V_m and time τ remain the same as the number of particles increases. The increasing number of particles in the mixing volume ensures that particles are fully stochastically independent from each other and, once independence is reached, additional particles do not change particle distributions that are controlled by the distribution of a single particle. An excessively large number of particles present in these simulations can be considered a waste of computational resources, although convergence to this limit has a methodological significance and allows for accurate evaluation of scalar averages. This limit does not approach DNS and represents a LES-type model where the scales smaller than the mixing scale are simulated and not resolved.

VIII. DISCUSSION AND CONCLUSIONS

Sparse-Lagrangian methods give an option of high quality simulations at relatively low computational cost due to a relatively small number of particles (as compared to the number of Eulerian grid cells) used in these simulations. The MMC version of the model involves conditioning on a reference variable (or variables) simulated by LES or DNS. The present article outlines the major principles of MMC-LES/DNS modeling and analyzes equations for the relevant scalar FDF. MMC conditioning is performed by localizing the mixing operation in the space of the reference variable. The best choice of the reference variable for nonpremixed combustion is represented by the mixture fraction. The reference mixture

fraction is obtained from Eulerian LES (or DNS). This LES-generated mixture fraction should not be confused with the mixture fraction that is evaluated with (or obtained from) reactive scalars. Conditioning on the reference variable(s) mitigates the influence of numerical diffusion and improves agreement between surrogate and physical mixing. The high quality of MMC mixing allows us to use a reduced number of particles in practical simulations.

The number of particles used in sparse-Lagrangian simulations is an important parameter, which affects quality of the simulations. Since increasing the number of particles creates possibilities for approaching DNS (as discussed in Refs. 6 and 9), the quality of simulations improves and the simulations become less dependent on particular features of the mixing model used in simulations when the number of particles is increased; although achieving a complete resolution of all small-scale details of the scalar fields would probably never be needed in practical simulations using MMC-LES. Comparison of different mixing models should be performed under conditions of using similar numbers of particles. It seems that the number of reacting particles (i.e., particles in the reacting region of the flow) per similar domains can represent a good criterion for comparison of the model efficiencies.

At these early stages of using sparse-Lagrangian MMC-LES models, it is difficult to give a general recommendation about the number of particles required for quality simulations. The answer depends on the complexity of the flow and the reaction mechanism, quality requirements imposed on the simulations and the ability to select optimal parameters for the mixing model. Generally, one can expect more complex combustion cases that are closer to extinction to need more particles [although we did not observe this trend in MMC-LES simulations of flame E (Ref. 31)].

If a small number of particles is used in MMC-LES simulations, then the spectrum of resolved scales becomes narrow and a large fraction of scalar fluctuations is controlled by the mixing operation. In this case, selecting adequate values of the model parameters (practically τ and g_{44}/g_{11}) is of principal importance. However, under conditions with a very large number of particles the fraction of Lagrangian subgrid fluctuations is small and the method becomes less sensitive toward selection of these parameters while the role of numerical efficiency and good spatial localization of mixing increases. A common choice of the MMC parameters was possible for flames D and E (Ref. 31) but, at present, the available experience with using MMC-LES is insufficient to discuss the universality of these parameters. One can recall that multiple attempts to find universal values of parameters related to various types of models of turbulence proved to be futile in most cases and universal values of the MMC model parameters may never be found for highly sparse simulations. This, of course, does not prevent from finding practical values of model parameters for a selected class of the combustion problems.

We can expect rapid development of sparse-Lagrangian MMC-LES models in the near future. These models are relatively simple and should work well when a sufficient number of particles is used in simulations. The main challenge that MMC model developers will have to face in the near future is determining optimal values or models for MMC parameters that would allow us to perform high quality simulations with a minimal number of particles. Knowledge of these optimal values for a given class of combustion problems would bring dramatic savings of computational cost required to solve these problems.

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