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A bluff body jet mixer simulation with a new developed OpenFOAM based sparse-Lagrangian Multiple Mapping Conditioning model

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Abstract

Turbulence provides effective mixing of entrained fluids to a molecular scale. This has wide-ranging consequences in engineering applications, particularly in turbulent combustion, where there is a diffusive-reactive balance at these smallest, unresolved scales. Probability Density Function methods that were introduced in the 1980s have been shown to give a successful statistic prediction of turbulent mixing and reaction. However, two major issues prevent this advanced method from being widely adopted for engineering applications: the high computational cost which is related to the large number of Pope Particles involved in conventional PDF simulations; and the ongoing need for a robust code that can handle all the modelling problems in engineering applications such as complex geometry and so on. To address the abovementioned problems, a C++ implementation of the efficient sparse-Lagrangian Multiple Mapping Conditioning model based on the popular Computational Fluid Dynamics toolkit OpenFOAM is introduced here. The results for a bluff body jet mixer demonstrate the new open source combustion platform, laying a foundation for connecting the cutting edge turbulence research with real engineering simulations.

Introduction

In non-premixed combustion, fuel and oxidizer enter into the combustion chamber separately. Subjected to fluid motion, a mixing layer is formed between fuel and oxidizer streams and burning happens at the interdiffusion stoichiometry surface at a molecular level. The molecular diffusion process controls the the reaction rate. Under the compelling need of increasing efficiency and eliminating emission, modern combustors are often designed to work under turbulent condition to achieve a rapid mixing. At the same time in order to ensure a proper flame stabilization, complex flow patterns like swirl and recirculation are adopted as well. To model combustion in such configuration both the large scale unsteady turbulent flow structure and the small scale molecular mixing need to be taken into account. This has posed a great challenge for combustion modelling. Apart from the physics, the combustion code, to be of practical use, should be flexible enough to handle varied and mixed combustion regimes, large spatial scales and complex geometries. To fulfill these requirements for practical combustion modelling, a high quality sparse-Lagrangian MMC model and its implementation are discussed here.

With a phenomenal and sustained increase in the computing power, the velocity fields of many practical flows can now be modelled with large eddy simulation (LES) which directly solves for the large scale unsteady turbulent motions, while modelling the more universal dissipative range [12]. However the molecular mixing which determines the chemical reactions happens at the sub-filter scale; the chemical source term in the LES reactive scalar transport equation remains unclosed. Alternatively a probabilistical description of this molecular scale interaction based on the transport probability density function has been very successful [13]. Combining the merits of both methods, a joint composition filtered density function (FDF) [11] has been proposed to adopt this PDF model in LES context. In the FDF equations the convection and reaction terms are in closed form while a sub model is used to model the molecular mixing process. Several different mixing models have been developed over years [5, 3, 15] and the LES-FDF model has been successfully validated against a number of well documented laboratory flames across a range of combustion regimes [10, 14]. However, it normally comes with a considerable computational cost.

The FDF is dominantly solved by a particle approach using Pope particles (notional particles carrying properties and modelled with the aid of mixing [8]) and the common intensive LES-FDF simulations use a large number of such Pope particles per Eulerian LES grid cell to ensure localness in the mixing model. For a laboratory scale flame simulation, the previous intensive FDF simulations require only 1 or 2 million LES grid cells but as many as 15 or even 50 million Pope particles [14]. Application of intensive FDF methods to large scale practical combustors is not feasible with the current computing power.

The recently developed sparse-Lagrangian FDF methods [1] use far fewer Pope particles for the FDF than there are grid cells for the LES. The use of so few Pope particles, even for difficult flames with significant local extinction and reigntion [6], is made possible by the use of a mixing model based on Multiple Mapping Conditioning (MMC) [9]. The MMC model is an advanced modeling concept which is compatible with all the criteria of a quality mixing model [15]. Through the use of a reference variable to control the particle mixing MMC can preserve the localization in composition space even when mixing particles are in different LES grid cells. All sparse simulations to date have used the mixture fraction as the reference variable. Since the computational cost is directly related to the number of particle, sparse-Lagrangian simulations of laboratory flames have a demonstrated computational cost saving of up to three orders of magnitude relative to the comparable intensive simulations [6].

The sparse-Lagrangian method has been demonstrated against laboratory piloted jet diffusion flames [6, 1] but wider application is limited by its numerical implementation; the current in-house code can only easily account for relative simple flame configurations. To fully explore the potential of sparse-Lagrangian MMC, a general implementation is required that is capable of simulating complex geometries and different regimes (e.g. premixed, spray, etc.). The emerging OpenFOAM toolkit is a well maintained and easily extendible open-source platform for computational fluid dynamics which takes advantage of objective oriented programming in C++. It is a popular and robust CFD code that is compatible with widely adopted commer-

cial pre- and post-processing software. OpenFOAM is readily shared among a growing network of researchers.

In this paper the model formulation of the sparse-Lagrangian MMC modelling are given. The MMC mixing model are presented in the context of its OpenFOAM implementation together with the design of the new Pope particle class. To demonstrate the new code, a simulation on a turbulent bluff body jet mixer [4] is perform and qualitative results are shown. Conclusion is drawn in the end.

Sparse-Lagrangian MMC model formulations

The sparse-Lagrangian MMC model involves a hybrid LES-FDF scheme which consists of two separate solvers, the Eulerian LES solver and the stochastic Lagrangian particle FDF solver, and a coupling mechanism between the two. The Lagrangian FDF scheme requires velocity and reference variable input from the Eulerian LES scheme. At the mean time, a density feedback mechanism is used to ensure consistency of the hybrid scheme. For details of the density feedback in sparse method, readers are refered to the author's previous work [6].

The Eulerian LES flow solver

In LES the large scales are separated from the small via a low-pass filter operation. Apply the Favre filtering to the conservation equations for mass, momentum, and reference mixture fraction gives

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial}{\partial x_i}(\bar{\rho}\widetilde{u}) = 0 \tag{1}$$

$$\frac{\partial \bar{\rho}\widetilde{u}}{\partial t} + \frac{\partial \bar{\rho}\tilde{u}_i\tilde{u}_j}{\partial x_i} = -\frac{\partial \bar{P}}{\partial x_j} + \frac{\partial \tau_{ij}}{\partial x_i} - \frac{\partial \tau_{ij}^{sgs}}{\partial x_i} \tag{2}$$

$$\frac{\partial \bar{\rho}\widetilde{u}}{\partial t} + \frac{\partial \bar{\rho}\tilde{u}_i\tilde{f}}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\bar{\rho}D\frac{\partial \tilde{f}}{\partial x_i}\right) + \frac{\partial \tau_f^{sgs}}{\partial x_i} \tag{3}$$

with τ_{ij} being the resolved viscous stress

$$\tau_{ij} = 2\bar{\rho}\nu(\widetilde{S}_{ij} - \frac{1}{3}\tau_{kk}\delta_{ij}) \tag{4}$$

ν is the kinematic viscosity and D is the molecular diffusivity which is given by $D = \nu/\sigma$. $\sigma = 0.7$ is the Schmidt number.

The two unclosed terms in the filtered equations are sub-filter stress $\tau^{sgs} = \widetilde{u}\widetilde{u} - \widetilde{u}\widetilde{u}$ and sub-filter mass flux $\tau_f^{sgs} = \widetilde{u}\widetilde{f} - \widetilde{uf}$. Following other LES combustion publication they are closed by a simple eddy viscosity model

$$\tau_{ij}^{sgs} = -2\bar{\rho}\nu_t\tilde{S_{ij}} \tag{5}$$

with a Smagorinsky model for ν_t

$$\nu_t = C_\nu \triangle^2 |\bar{S}| \tag{6}$$

where $\bar{S} = \sqrt{2\tilde{S}_{ij}\tilde{S}_{ij}}$ is the magnitude of strain rate and Δ is the width of the filter. The coefficient C_ν is determined dynamically. The sub-filter mass fluxes τ_f^{sgs} in equation (3) is also determined according to an eddy diffusivity model

$$\tau_f^{sgs} = -\bar{\rho}D_t\frac{\partial \tilde{f}}{\partial x_i} \tag{7}$$

where $D_t = \nu_t/\sigma_t$ and $\sigma_t = 0.4$ is the turbulent Schmidt number.

The filtered density function and Lagrangian solver

Filtered density function in LES is analogous to the probability density function. The joint composition filtered mass density function represents the sub-filter turbulent fluctuations in the composition scalar field probabilistically. For a n_s species composition field, It is defined as

$$F_L(\psi;x,t) = \int_{-\infty}^{+\infty} \rho(y,t)\zeta[\psi,\phi(y,t)]G(y-x)dy \tag{8}$$

and

$$\zeta[\psi,\phi(y,t)] = \delta[\psi-\phi(y,t)] = \prod_{\alpha=1}^{n_s}\delta[\psi_\alpha - \phi_\alpha(y,t)] \tag{9}$$

ψ is the random variable in the composition domain. The integration of the filtered mass density function F_L yields the filtered density

$$\int_{-\infty}^{+\infty} F_L(\psi;x,t)d\psi = \bar{\rho}(x,t) \tag{10}$$

Using these definitions, the transport equation for the joint composition FDF can be written as [2]

$$\frac{F_L}{\partial t} + \frac{\partial}{\partial x_i}(\tilde{u}_i F_L) + \frac{\partial}{\partial x_i}(\widetilde{u_i'|\psi}F_L) = -\frac{\partial}{\partial \psi}\left[\left(\frac{1}{\bar{\rho}}\overline{\nabla\cdot\rho D\nabla\phi|\psi} + W(\psi)\right)F_L\right] \tag{11}$$

The reaction source term,W, is in closed form and no modelling is required. whereas the sub-filter velocity fluctuation conditioned on the scalar, $\widetilde{u_i'|\psi}$ and the conditional scalar dissipation, $\overline{\nabla\cdot\rho D\nabla\phi|\psi}$ are both unclosed and require modeling.

The conditional velocity term is modelled by employing the gradient-diffusion hypothesis

$$\widetilde{u_j'|\phi}F_L = -\bar{\rho}D_T\frac{\partial F_L/\bar{\rho}}{\partial x_j} \tag{12}$$

.

The FDF transport equation is a high dimensional equation, and conventional Eulerian solution scheme are not tractable. The Lagrangian particle scheme developed by Pope [13] is the dominant solution scheme.In the particle approach, equation (11) is replaced by equivalent stochastic differential equations: [1]

$$dx_i^p = [\tilde{u}_i + \frac{1}{\bar{\rho}}\frac{\partial}{\partial x_i}(\bar{\rho}(D+D_t))]dt + \delta_{ij}\sqrt{2(D+D_t)}d\omega_j \tag{13}$$

$$d\phi_\alpha^p = (W_\alpha^p + S_\alpha^p)dt \tag{14}$$

Here, the superscript $p = 1,2,...N$ is a particle index and indicates a stochastic value evaluated on or assigned to the Pope particles and ω_j is the independent Weiner process.

In equation (14), S_α is the unclosed mixing operator which models the conditional sub-filter scalar dissipation term in equation (11). The mixing models which are commonly used for PDF modeling are the modified Curls models [3], the IEM [5]

Table 1: New Pope particle design

Classes	Popeparticle	Popecloud	sub-classes
Member functions	1.Move 2.React	1.Particle tracking 2.Particle number control 3.Density feedback	1.Mixing model (MMC mixing) 2.particle inflow BC

and the EMST model [15]. In the common practice of LES/FDF method within the filter grid a lot of particles are used for the mixing model to ensure localness in mixing.

Performing the LES/FDF under "sparse" condition reduces the computational cost significantly. However, under sparse condition particles are further apart and the FDF is more sensitive to the mixing model. A high quality mixing model is required to ensure localness in the mixing when particle are physically cells away. Unlike existing IEM or Curl's model which enforce localness in the mixing through particle number density(number of particle per LES cell for intensive methods, or number of particle per region for sparse methods), localness in MMC mixing is ensured by conditioning on reference variable. In non-premixed combustion the primary choice of this reference variable is the resolved mixture fraction from LES scheme. Apart from localness, MMC satisfies all the requirements for a good mixing model that truly represent the micro-mixing terms [15]. In contrast with the Curl's mixing model which selects mixing particle randomly, the MMC-Curl's model selects mixing particle pairs specifically. The details of the MMC-Curls mixing model is discussed with its OpenFOAM implementation in the next section.

Pope particle and MMC mixing implementation in OpenFOAM

OpenFOAM is an object-oriented software toolkit designed to facilitate research in physical modelling by separating the handling of physics from the numerical discretization [7]. OpenFOAM supports complex unstructured meshes which is the foundation for applying sparse-Lagrangian MMC to complex geometries. More importantly, the use of advanced features of C++ and object-oriented programming ensures that new code development in OpenFOAM can be easily managed. Inheritance, polymorphism and encapsulation allow simple and secure high-level reuse and extension of existing code. All these features are best demonstrated in the implementation of Pope particle for sparse-Lagrangian modelling.

In OpenFOAM there is already a Lagrangian particle tracking (LPT) scheme which utilizes two base classes, the particle class and the cloud class. The particle class records the position and location of a particle within the mesh, while a cloud class is a list of particles with the capability of adding, deleting and tracking particles. The base cloud class also supports parallelization. So no modification to the parallelization code is required when new particle classes are derived from them.

For the sparse-Lagrangian MMC solver Pope particle and Pope cloud classes are derived from those two base classes. The class design and member functions are shown in Table 1.

The Pope particle class is derived from the base particle class. The base class carries only particle location while in addition the Pope particle class carries particle values for fluid velocity, species mass fraction, standardized enthalpy, equivalent enthalpy and mixture fraction. Pope particles are moved by the governing stochastic differential equation and subject to mixing and chemical reaction.

The Pope cloud class applies the tracking capabilities of the base cloud class to the Pope particles and controls the particle number density to balance the stochastic error. The Pope cloud class contains the sub-class handling mixing and boundary conditions.

MMC-Curl's mixing model is implemented in the mixing sub class. In MMC-Curl's mixing, all particles in the whole domain are formed into pairs (p and q) such that their normalized square distance in extended physical and reference mixture fraction, space [6]

$$d^2_{(p,q)} = \frac{1}{1+\lambda^2} \times \left[\sum_{j=1}^{3} \left(\frac{x_j^{(p)} - x_j^{(p)}}{L_x} \right)^2 + \left(\frac{f^{\tilde{(p)}} - f^{\tilde{(p)}}}{L_f} \right)^2 \right] \tag{15}$$

is minimized (approximate minimization is performed by a divide-conquer method similar to the k-d tree algorithm [1]). L_x and L_f, are characteristic physical space and reference space scales. These two parameters directly control the behavior of the model and are thoroughly studied and reported in Ref. [6]

Once selected, the pair of mixing particles, p and q, mix linearly and discretely over a finite time step Δ_t such that

$$\begin{aligned} \phi^p_\alpha(t+\Delta t) &= \phi^p_\alpha(t) + \mu\left(\bar{\phi}^{p,q}_\alpha(t) - \phi^p_\alpha(t)\right) \\ \phi^q_\alpha(t+\Delta t) &= \phi^q_\alpha(t) + \mu\left(\bar{\phi}^{p,q}_\alpha(t) - \phi^q_\alpha(t)\right) \end{aligned} \tag{16}$$

where $\bar{\phi}^{p,q}_\alpha$ a is the two-particle mean, which may be weighted if variable mass particles are used, and $\mu = 1 - exp(-\Delta t/\tau^{p,q}_L)$ the extent of mixing controlled by a mixing time scale, $\tau^{p,q}_L$. The mixing timescale is determined locally and instantaneously for each mixing pair and is related to the dissipation time. [6]

Simulation of mixing in bluff body flow

Currently the implementation of MMC mixing has already finished. Here the new implementation is used to simulate a turbulent isothermal mixing in bluff body. The geometry of the simulation case is the same as the Sydney bluff burner [4]. The Sydney burner consists of a cylindrical bluff-body with diameter $D = 50mm$, which is located in a coaxial flow. On the centerline, a nozzle of diameter $d = 3.6mm$ ejects fuel into the domain and creates a inner recirculation zone. The flow field features strong turbulence and intense mixing. The computational domain has a diameter of $3D$ and a length of $4D$. In the calculation equally spaced LES grid has 256 cells in the axial direction, 160 cells in the radial direction and 32 cells azimuthally and 1 Pope particle per 10 Eulerian cell. The velocity inflow boundary for the jet is $108m/s$ while the coflow is $35m/s$.

Figure 1 shows the instantaneous particle distribution in a cross plain. All particles are colored by their original position. the green particles are initially located in the middle of the domain while all blue particles are injected with the flow. It is clear that a strong outer circulation has brought the initially evenly distributed green particles to the centerline. At the same time cluster of green particles are engulfed by new injected blue particles near the bluff body. That is because at the nozzle exit, there is a steep velocity gradient and it creates a inner recirculation zone. The strong inner recirculation zone prolongs the residence time of the fuel and in consequences old particles are engulfed by fresh injected particles. This qualitative plot clearly shows that the new implementation has captured the unsteady recirculation structure of the bluff body flow.

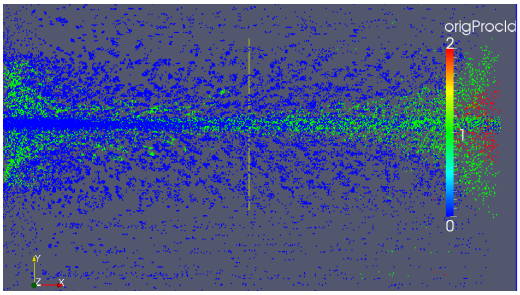

Figure 1: Recirculation in the bluff body jet mixer. Particles are colored based on their initial locations

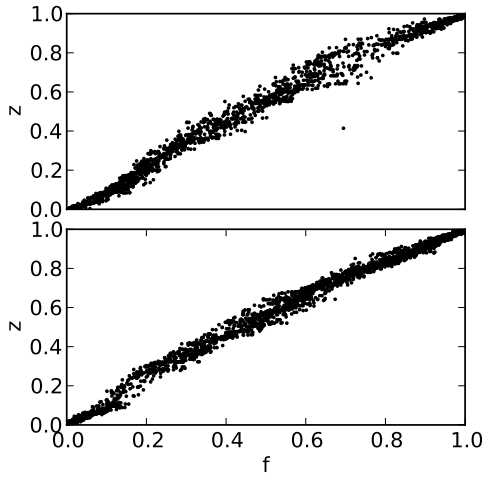

Figure 2: Instantaneous scatter plot of $Zv.sf$ at $x/D = 0.26$,top, and $x/D = 1.3$,bottom.

The correlation between the FDF and LES simulated mixture fraction fields is given by the scatter plots of instantaneous Z versus $\tilde{f}$ p at $x/D = 0.26$ and $x/D = 1.3$ in Figure 2 . All particles cluster around $z = \tilde{f}$ shows there is a clear correlation between the Z and $\tilde{f}$ fields. The scattering of z around $\tilde{f}$ is caused by the inherited stochastic nature of the Pope particle system. In MMC mixing this correlation can be improved at the cost of locality in physical space. Using the well resolved LES reference mixture fraction, $\tilde{f}$, to localize mixing provides a level of control of the fluctuations that is not possible with non-local mixing models.

Conclusions

Both large scale unsteady flow structure and molecular scale mixing are important in non-premixed combustion modelling. In sparse-Lagrangian MMC simulation the large scale unsteady flow structure is resolved by LES and the small scale molecular mixing is modelled by MMC mixing. Due to the high quality of the MMC mixing the sparse model can offer LES-FDF results of comparable accuracy to intensive methods but at a minimal cost. In order to explore the full potential of this promising method its implementation onto the open-source OpenFOAM platform is discussed. The model formulation of the sparse method and its related class design in OpenFOAM are presented in details. At the current stage, the code can account for turbulent mixing effects in a bluff body turbulent jet setup. The Sydney bluff-body flame is the target of the finished code in the future. The new open source platform built around sparse-Lagrangian MMC method is hoped to shorten the distance between the cutting edge theoretical development and its application in real engineering simulations.

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