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A novel Kalman filter based approach for multiscale reacting flow simulations

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ABSTRACT

A multi-scale approach for coupling a coarse-grained (CG) deterministic solution for a reacting flow with a fine-grained (FG) stochastic solution is proposed. The model includes a CG solution for the mass density and momentum and a FG solution for the temperature. A model for the turbulent transport in the FG solution is implemented using the linear-eddy model (LEM), which combines a deterministic implementation for reaction, diffusion and large-scale transport with a stochastic implementation for fine-scale transport. A common variable is obtained from these solutions based on a CG density field defined from continuity on the coarse scales and the spatial filtering of the density derived from the state equation in the FG solution. Kalman filtering is used to combine these two solutions. The resulting CG density is both smooth and steered by heat release from the FG solution. The algorithm is demonstrated on a 1D model combining continuity and the Burgers' equation for the CG solution and the temperature equation with heat release for the FG solution. The results establish the feasibility of Kalman filtering in coupling deterministic CG solutions and stochastic FG solutions in reacting flow applications.

1. Introduction

A principal challenge in modeling turbulent combustion flows is their complex, multiscale nature [1–3]. Traditional paradigms in turbulent combustion modeling have sought to bridge the gap of large scales, which are partially determined by the device geometry and thin micron-scale reaction layers in combustion through various approaches (e.g. fast chemistry, thin flamelets relative to turbulence scales). These approaches may be limited by their inherent assumptions related to the combustion regime (e.g. flamelet vs. distributed reaction) and combustion mode (e.g. premixed vs. non-premixed). However, it is common, and perhaps even prevalent, for the combustion process in modern combustion device to feature spatial and/or temporal variations in combustion modes and regimes.

With the emergence of large-eddy simulation (LES) as a viable modeling approach in combustion, the important role of large scales may be captured; however, there remain important challenges to capture unresolved sub-filter scales where important physics resides. Closure for these finer scales is the primary scope of the state-of-the-art turbulent combustion models today, and this closure has been approached through different strategies. One promising class of strategies seeks to directly simulate the sub-filter scale physics through low-dimensional or low-order models. Such strategies include for example, the tracking of notional particles and the solution of their joint scalar or scalar-velocity probability density functions (PDFs) [4]. Alternatively, the LEMLES [5] and the ODTLES [6] approaches involve the coupling of LES with 1D fine-grained (FG) stochastic models using the linear-eddy model (LEM) [7] and the one-dimensional turbulence (ODT) model [8]. These models potentially offer the ability to capture different combustion regimes and modes.

A number of issues arise with the coupling of LES with low-dimensional stochastic models. The first issue is related to the layout of grid structures of LES and the layout of low-dimensional stochastic models. Recently, Cao and Echekki [9] and Park and Echekki [10] used a fixed lattice of ODT domains embedded on the LES grid. Alternatively, ODT domains may be embedded normal to a flame brush and are advected with the flow [11]. A second issue is to decide which equations or quantities to solve by both solutions. This decision also determines the degree of coupling and the redundancies between them. As proposed by Cao and Echekki [9] and Park and Echekki [10], a reasonable choice is to allow the LES to capture the flow (i.e. continuity and momentum), while ODT is tasked with the solution for the thermo-chemical scalars (e.g. composition, temperature). In the Cao and Echekki [9] and Park and Echekki [10] model, both LES and ODT solve for a momentum equation. The momentum equation in ODT features contributions from large-scale transport through the filtered velocity field and small-scale transport through a stochastic implementation of stirring events using the ODT model [8].

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Nomenclature

Da	Damkohler number for reaction rate
G	LES spatial filter
$\hat{l}$	eddy size length for stirring events
$f(\hat{l})$	eddy size distribution
$\mathbf{H}$	matrix relating observation to variable in the state vector
$\mathbf{K}$	Kalman gain matrix
L_T	turbulence integral scale, also the size of the largest eddy
$\mathbf{M}$	matrix for the discretization of the continuity equation
N_C	number of coarse grid in 1D solution
$\mathbf{P}\_$	*a priori* estimate covariance matrix
$\mathbf{P}$	a posteriori estimate covariance matrix
Pr	Prandtl number
$\mathbf{Q}$	error covariance matrix for density from the coarse-grained continuity equation
$\mathbf{R}$	error covariance matrix for the fine-grained solution based density
Re	reference Reynolds number of normalization
Re_t	turbulence Reynolds number
t	time
T	temperature
$\tilde{u}$	density-weighted filtered velocity
$\mathbf{v}$	vector of errors associated with the discretization of the continuity equation in fine-grained density solution
$\mathbf{w}$	error associated with the discretization of the coarse-grained continuity equation
x	1D domain coordinate
X	1D domain size

Greek symbols

α	heat release factor
ε	error
Δt_s	time step for stirring events
Δx_c	grid size for coarse-grained solution
Δx_f	grid size for fine-grained solution
λ_r	eddy rate distribution
μ_t	eddy viscosity
ν_t	kinematic eddy viscosity
η	Kolmogorov scale
$\bar{\rho}$	filtered density

Subscripts

c	quantities associated with the coarse-grained solution
f	quantities associated with the fine-grained solution
$-$	Predictor step result

Superscripts

n	index for time iteration
s	index for integration sub-cycles in LEM solution
$\wedge$	quantities associated with Kalman filtering

A schematic of the coupling of ODTLES is shown in Fig. 1. The coupling involves a downscaling process in which information from the large-scale is passed to the ODT FG solution. In the present formulation, this information consists of the enforcement of the large-scale component of the ODT velocity field to be consistent with the LES-resolved velocity field. This enforcement involves two steps: (1) an interpolation of the LES velocity field onto the ODT grid, then (2) compounding of the large-scale velocity components, which consist of replacing the large-scale component of the velocity field in ODT by the interpolated LES solution.

There is a reverse process from the ODT FG solution to LES. Since ODT solves for thermo-chemical scales, it captures heat release, which in turn impacts the flow. This coupling is achieved through the density computed in ODT and filtered onto the LES grid. A potential drawback of this operation of filtering may result from the limited sample of ODT resolution used to evaluate the filtered density. Limited sample noise can be reduced by adding more ODT solutions within a LES cell; alternatively a smoothing process across a broad range of wave numbers can be carried out. This process is denoted as assimilation to relate the proposed procedure to strategies adopted in different disciplines (e.g. weather modeling) where combinations of measurements and simulations can improve the long-term predictions of models. The process of assimilation is the scope of the study proposed here.

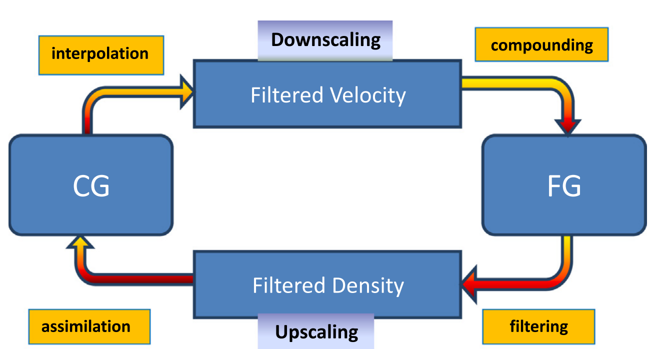

Fig. 1. Schematic showing the coupling between the coarse-grained (CG) and the fine-grained (FG) solutions.

This study attempts to address the coupling of a coarse-grained (denoted subsequently with the acronym CG) deterministic solution for the flow field and a fine-grained solution (denoted subsequently with the acronym FG) stochastic solutions for the thermo-chemistry. This coupling is relevant to the ODTLES approach, but it is demonstrated here using a simplified model. The coupling is established primarily through a redundancy in the computation of the CG density in both solutions. Kalman filtering [12,13] (subsequently denoted as KF) is used to combine these two densities, such that both mass conservation and an account for heat release are established. The implementation of the Kalman filter within the context of addressing the turbulent flow signal is not new. We cite for example the recent work by Cahuzac et al. [14,15] who attempted to isolate the fine- and large-scale or low- and high frequency contributions to the turbulence signal (e.g. contributions from low and high-frequency unsteadiness). A smoothing algorithm is proposed here as well; however, within the context of the proposed approach, the smoothing relies on two solutions of the same quantity, one based on the CG solution and the other based on the FG solution. The paper is organized as follows. In Section 2, the model formulation is presented. The results are presented and discussed in Section 3. Finally, these results are summarized and additional discussion of the implications of the proposed algorithm is presented in Section 4.

2. Model formulation

The hybrid model consists of the solution for continuity and momentum in 1D on the coarse-scales and for temperature in 1D