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Linear eddy mixing based tabulation and artificial neural networks for large eddy simulations of turbulent flames

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ABSTRACT

A large eddy simulation (LES) sub-grid model is developed based on the artificial neural network (ANN) approach to calculate the species instantaneous reaction rates for multi-step, multi-species chemical kinetics mechanisms. The proposed methodology depends on training the ANNs off-line on a thermo-chemical database representative of the actual composition and turbulence (but not the actual geometrical problem) of interest, and later using them to replace the stiff ODE solver (direct integration (DI)) to calculate the reaction rates in the sub-grid. The thermo-chemical database is tabulated with respect to the thermodynamic state vector without any reduction in the number of state variables. The thermo-chemistry is evolved by stand-alone linear eddy mixing (LEM) model simulations under both premixed and non-premixed conditions, where the *unsteady* interaction of turbulence with chemical kinetics is included as a part of the training database. The proposed methodology is tested in LES and in stand-alone LEM studies of three distinct test cases with different reduced mechanisms and conditions. LES of premixed flame–turbulence–vortex interaction provides direct comparison of the proposed ANN method against DI and ANNs trained on thermo-chemical database created using another type of tabulation method. It is shown that the ANN trained on the LEM database can capture the correct flame physics with accuracy comparable to DI, which cannot be achieved by ANN trained on a laminar premix flame database. *A priori* evaluation of the ANN generality within and outside its training domain is carried out using stand-alone LEM simulations as well. Results in general are satisfactory, and it is shown that the ANN provides considerable amount of memory saving and speed-up with reasonable and reliable accuracy. The speed-up is strongly affected by the stiffness of the reduced mechanism used for the computations, whereas the memory saving is considerable regardless.

1. Introduction

Turbulent combustion is described as the continuous distortion of the local flame front by eddies distributed over a wide range of length and time scales [1]. The response of the flame front depends on the combined effect of molecular diffusion, turbulent transport and chemical reaction occurring across the flame, without any clear scale separation. From a computational point of view, direct numerical simulation (DNS) of high Reynolds number flows (typical of turbulent combustion) are not yet affordable, and thus, to render a practical solution to the turbulent combustion processes, the governing equations are solved either on a time (Reynolds averaged Navier Stokes (RANS)), or space averaged (large eddy simulation (LES)) sense [2]. For all of these methodologies, what is common, however, is the calculation of the chemical reaction rates: a set of coupled, non-linear ordinary differential equations (ODEs) has to be solved. It must be noted that the accurate prediction of the aforementioned features need radical species information [1,3,4]. However, as the number of the species increases, the size of the system of ODEs increases as well. Furthermore, since the radical species have time scales different by several orders of magnitude compared to the major species, the ODEs become stiff as well [5]. Thus, the process of calculating chemical source terms adds further computational burden to the flow simulation and needs to be handled carefully in a cost efficient manner.

Many approaches for efficient kinetics evaluation have been reported in the literature. The look-up table approach (LUT) [6], intrinsic low-dimensional manifolds (ILDM) [7], and, *in situ* adaptive tabulation (ISAT) [8], have all shown speed-up of the chemical kinetics calculations. LUT and ILDM depends on pre-computing and tabulating the reaction rate and/or the species information in the reduced state-space. One major drawback for both ILDM and LUT is that the information on the thermo-chemical state-space that is going to be accessed by the flow solver is not known *a priori*, and thus, huge tables have to be created. ISAT, on the other hand, constructs the look-up table during the actual flow simulation, and only the accessed region is stored. Thus, it yields a considerable

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amount of memory savings compared to ILDM and LUT. However, the ISAT table may also keep increasing beyond the memory limit of the PC parallel clusters, especially for LES applications [9].

The main purpose of the current study is to propose a tabulation strategy and an interpolation scheme, that may predict the thermo-chemical state-space *a priori* (unlike ILDM), and which can reduce locally memory needs (unlike ISAT) without any loss of accuracy and with speed-up. Here, the tabulation is achieved by using the stand-alone linear eddy mixing (LEM) [10–12] model calculations. LEM has previously demonstrated to account for the interaction between turbulent transport, molecular diffusion and chemical reaction at their respective time and length scales [13–15]. Once the thermo-chemistry is extracted through stand-alone LEM computations, an artificial neural network (ANN) architecture is trained on this data-set. ANN is basically an interpolation scheme that can be used to map arbitrary number of inputs to outputs [16,17]. Unlike LUT, ILDM, and ISAT, ANN does not require coupling the flow solver with a multi-dimensional thermo-chemical table, or a direct solver for the stiff kinetics equations.

ANN for the reactive flow computations has been used by different research groups in the past. Blasco et al. [18,19] performed one of the first attempts to incorporate ANN into chemical kinetics calculations, where the accuracy of the proposed model was tested in a plug flow reactor calculation. A speed-up of 2700 with ANN was obtained when compared to direct integration (DI). Choi and Chen [20] trained ANN for ignition delay time calculations and coupled it with a well-mixed reactor solver. A speed-up of 600 was obtained. Finally, an integration of ISAT with ANN for a partially stirred reactor computation was studied by Chen et al. [21], where ANN was trained based on an already existing ISAT table. Same approach was later re-visited by Kapoor et al. [22] and applied to unsteady scalar field evolution within LEM approach.

In more recent studies, ANN has been used within the LES computations of reactive flows. The work by Kempf et al. [23] investigated the structure of the SANDIA Flame D [24] by LES, where ANN was used to store a steady flamelet library to provide species mass fractions, density and viscosity. They reported that the ANN reduces the storage size of the chemistry library by three orders of magnitude having almost same efficiency with a linear interpolation scheme. Ihme and co-workers [25] used ANN to store a flamelet library and applied it to a bluff body stabilized flame. A general strategy to optimize ANNs (O-ANN) for the given number of layers and neurons per layers was also proposed. The ANN performance with respect to accuracy, data retrieval time and storage requirements was compared with the structured tabulation methods, and it was shown that ANN yielded comparable accuracy with considerably lower storage and computational time.

Previous work by Kempf et al. [23] and Ihme et al. [25] used ANN to store flamelet libraries in connection with the presumed PDF approach, where the thermo-chemistry is not computed directly within the LES, but rather obtained from the ANN. In this approach, flamelet itself already provides a considerable amount of speed-up compared to directly simulating the scalar field, and the merit of using ANN mostly lies in the memory savings. An alternative approach is to use ANN to directly represent the multi-step kinetics within the LES approach, and this has been recently investigated by Sen and Menon [26]. Here, a series of simulations of the *unsteady* evolution of flame–vortex interactions (FVI) were used to extract the thermo-chemical information for ANN training table construction. These simulations of FVI showed that, although the computations are started for a single large scale vortex, actually a large number of scales are present over the entire simulation period. Hence, each test case with an initial single vortex of a given size provided additional data over a much wider range of scales. The ANN was later used to replace the DI based on a 14-species, 11-steps reduced chemical kinetics mechanism within the LES sub-grid calculations of premixed, syngas/air flames. A speed-up factor of around 11 with considerable amount of memory savings was reported.

The current paper is extending the approach developed earlier [26]. In both the earlier and the present studies, the ANN is used to predict the instantaneous (unfiltered) reaction rates as a function of the thermodynamic state vector ($\dot{\omega}_i = f(Y_k, T)$), without any reduction in the number of parameters. The key difference between these two studies lies in the fact that the thermo-chemical states for ANN training here are extracted from stand-alone LEM simulations, rather than the DNS of FVI as done previously. The major advantage in this strategy is that LEM allows explicitly incorporating (albeit indirectly) the effect of the turbulent small-scale eddies on the reaction kinetics. This is in contrast to our previous approach [26] where only the effect of deterministic vortices on the reaction kinetics was considered. Regardless, both methods attempt to capture *unsteady* flame–turbulence–vortex interaction effects during the ANN database development, and are considered new strategies for ANN training.

The rest of the paper is organized as follows: the mathematical formulation of the LEM and ANN is reviewed in the next section, which is followed in Section 3 by the description of the test cases used to evaluate the accuracy of the proposed ANN methodology. ANN is used to replace a stiff ODE solver within the LES and stand-alone LEM computations. Results are presented in Section 4 for the mean and instantaneous species profiles, while conclusions are drawn in the final section.

2. Mathematical formulation

2.1. ANN training

ANN is a highly interconnected computing system made up of a number of processing elements (PEs) connected through uni-communication channels. The ANN code used in the study is based on a back-propagation learning with gradient descent rule (GDR) [16]. Since, the details of this basic algorithm is extensively discussed elsewhere [26], only the key concepts and new changes carried out are reported here.

The training algorithm basically consists of two parts: (i) forward propagating the input and (ii) backward propagating the error. For the given ANN architecture, the output of a single neuron i at iteration number k is calculated as: $y_i[k] = g(\sum_{m=0}^{M} W_{im}[k] y_m[k] - b_i[k])$. Here, $W_{im}[k]$ is the weight coefficient between PEs i and m, $y_m[k]$ is the output of the neuron m, $b_i[k]$ is the internal threshold for the PE i, and M is the number of PEs connected to the PE i. Also, $g()$ is the hyperbolic-tangent activation function given as: $g(z) = (e^z - e^{-z})/(e^z + e^{-z})$. Once the output is calculated for all PEs, the error for the current weight distribution is the difference between the desired (d_i) and the calculated ($y_i[k]$) value at the output layer:

$$E[k] = \frac{1}{2} \sum_{i=1}^{I} [d_i - y_i[k]]^2 \tag{1}$$

with I denoting number of PEs at the output layer.

It is well known that the standard GDR rule [16] has couple of drawbacks: (i) the non-linear activation function leads to a error surface with multiple local minima, where the GDR can be trapped, and (ii) the model coefficients need to be calibrated for each new case for optimum convergence. To overcome these problems, a new learning algorithm based on the extended delta-bar-delta (EDBD) model has been proposed [26]. This new algorithm uses the following rule to update the weights: