Multi-timescale Modeling of Ignition and Flame Propagation of Diesel Surrogate Fuel Mixtures

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The ³rd order Weighted Essentially Non-Oscillatory (WENO) scheme and a recently developed Dynamic Adaptive Chemistry (DAC) method are integrated with the hybrid multi-timescale (HMTS) method and an adaptive unstructured grid system for computationally efficient and adaptive direct numerical simulation. The results show that compared to the ¹st order total variation diminishing (TVD) scheme, the ³rd order WENO scheme dramatically reduces the numerical dissipation while keeping good computational efficiency. In the dynamic adaptive chemistry method, the kinetic mechanism is dynamically reduced by the Path Flux Analysis (PFA) method on each computational grid. A hybrid multi-timescale method, which combines the implicit and explicit Euler schemes, is used to solve the chemical reactions based on the dynamically reduced mechanism. The algorithm is validated and applied for simulation of ignition and unsteady flame propagation of n-decane/1,2,4 trimethyl benzene (TMB) diesel fuel surrogate mixtures. The results show the present algorithm is not only computationally efficient but also robust and accurate. The DAC method increases the computation efficiency dramatically. Moreover, the unsteady flame propagation simulation shows that the ³rd order WENO scheme can significantly reduce the numerical dissipation and predict a more accurate flame speed compared to the ¹st order scheme.

1. Introduction

Due to the energy security, energy sustainability and global warming issues, increasing the fuel efficiency of internal combustion engines and reducing their emissions are of global importance. Recent years, there is increasing interest to develop internal combustion engines working at low temperature combustion regime, such as the homogeneous charge compression ignition (HCCI) and the reactivity controlled compression ignition (RCCI) engines [1, 2], to improve engine efficiency and emissions. Detailed kinetic modeling of these new kinds of engines is of great importance to optimize the ignition and combustion process. However, combustion process is a multi-scale physical and chemical process and involves a large range of time and length scales [3], especially when turbulent transport involved. As such, accurate modeling of ignition and combustion in a practical engine with a detailed chemical kinetics remains extremely challenging.

In turbulent combustion modeling, large numerical dissipation may introduce a unphysical numerical diffusion [4], which can diminish the small eddies in the turbulent flow when a coarse grid system is used. Therefore, a high order accuracy scheme is needed in numerical modeling to capture the sharp feature and avoid large numerical dissipation. The high-order accurate weighted essentially non-oscillatory (WENO) scheme [5-9] has the advantage of high order accuracy and
robust, sharp, and essentially non-oscillatory shock resolution [6]. However, most of the WENO schemes used in the literature are based on the structured, uniform grid system.

Another difficulty in combustion modeling is the large and stiff detailed chemical mechanisms. Recently, there have been many efforts in developing large detailed kinetic mechanism for diesel and jet fuels. However, a detailed kinetic mechanism can contain hundreds of species and thousands of species. For example, a detailed n-heptane mechanism can have 1034 species and 4236 reactions [10]. Even with the availability of high performance supercomputing capability at petascale and beyond, the numerical simulation with such a huge number of species and reactions is still too expensive. Therefore, the detailed mechanisms need to be reduced in order to realize direct numerical simulation (DNS). Many methods have been developed to do the chemical reductions. For example, recently, the Direct Relation Graph (DRG) [11, 12] method and multi-generation Path Flux Analysis (PFA) [13] method show great efficiency and accuracy in mechanism reductions.

However, there is a drawback for the global, pre-reduced mechanisms. In order to guarantee the accuracy of the reduced mechanisms in different conditions, they still contain a large set of species and reactions; even most of the species are not activated in a long time regime. Figure 1 shows the active species profile during the auto ignition process. In this figure, the homogeneous ignition of stoichiometric Aachen diesel surrogate fuel [14]/air mixture at 10 atmospheres and 1000K initial temperature is studied. The number of active species varies with time. After ignition, only a few species is active. But in order to be applicable to the whole process, the pre-reduced mechanism must contain all the species of which most of them are active in different time sequences. Therefore, the pre-reduced mechanisms suffer from the loss of computational efficiency to calculate all species at all time and space domains. In order to reduce mechanisms locally and obtain more compact reduced mechanisms, Gou et al. developed an error-controlled dynamic adaptive chemistry (EC-DAC) [15] method. It is based on the PFA method and does the chemical reduction dynamically at each grid point to obtain the sub-mechanism based on the local conditions. The threshold value of EC-DAC method is determined by a progress variable [16] to satisfy the required accuracy.

However, in the previous EC-DAC method, the VODE [17] solver is used to solve the chemical reactions. The CPU time cost by VODE solver, which contains Jacobian matrix decomposition, is proportional to the cube of the species number. Thus, the computing time will increase rapidly when the size of the mechanism getting larger. In order to increase the efficiency of computation of chemical reactions, a hybrid multi-time scale (HMTS) [18] method is developed by Gou et al. in 2010. HMTS solver combine implicit Euler method and explicit Euler method together and solved the species’ reaction based on their own characteristic time. HMTS method can dramatically reduce the computing time.

The goal of this paper is to develop a high order numerical scheme by using dynamic adaptive chemistry (DAC) method based on HMTS method and extending the 3rd order WENO scheme to an adaptive non-uniform grid system to achieve great computational efficiency and accuracy for combustion modeling with detailed chemical kinetics. The Aachen diesel fuel surrogate [14], which consists of 80% n-decane and 20% 1,2,4-trimethylbenzene by weight (77% n-decane and 23% 1,2,4 trimethylbenzene by volume) and contains 118 species and 527 species, is used to validate the integrated WENO-DAC- HMTS approach. The hydrogen mechanism [19] with 10 species and 23 reactions is used to test and validate the effect of WENO scheme on numerical dissipation. Numerical simulations of homogeneous ignition and unsteady flame propagation of diesel surrogate mixtures are carried out to demonstrate the accurate and robust of the proposed algorithm.
Fig. 1. Number of active species profile during homogeneous ignition process with stoichiometric Aachen surrogate fuel/air mixture at 10 atmospheres.

2. Numerical Methods

The development of an integrated WENO scheme and DAC method with HMTS solvers to simulate unsteady reactive flow with an adaptive unstructured grid system is based on our previous code, the adaptive simulation of unsteady reactive flow (ASURF) code [20, 21] developed at Princeton. The original scheme in ASURF, the 1st order total variation diminishing (TVD) scheme [22], is replaced by the 3rd order WENO scheme to improve the numerical accuracy and the DAC method is implemented at each grid point to reduce mechanisms locally.

2.1. WENO scheme

In order to minimize numerical dissipation while keeping good computational efficiency, the 3rd order WENO scheme [9] is applied to discretize the convective terms based on an unstructured, non-uniform grid system. Since the grids are not uniform, the WENO reconstruction fluxes and weight functions used here is derived from the original form of WENO scheme introduced by Shu [9]. In the 3rd order WENO scheme, a function $v(x)$ at the $i$th cell center point $x_{i+\frac{1}{2}}$ can be reconstructed as:
\[ v_{i+\frac{1}{2}}^{(0)} = \omega_0 v_{i+\frac{1}{2}}^{(0)} + \omega_1 v_{i+\frac{1}{2}}^{(1)} \]  

where \( v_{i+\frac{1}{2}}^{(0)} \) and \( v_{i+\frac{1}{2}}^{(1)} \) are two implementations of \( v(x) \) and \( \omega_0 , \omega_1 \) are there weights. The expressions of \( v_{i+\frac{1}{2}}^{(0)} \) and \( v_{i+\frac{1}{2}}^{(1)} \) are:

\[ v_{i+\frac{1}{2}}^{(0)} = \frac{\Delta x_{i+1}}{\Delta x_i + \Delta x_{i+1}} v_i + \frac{\Delta x_i}{\Delta x_i + \Delta x_{i+1}} v_{i+1} \]  

(2.a)

\[ v_{i+\frac{1}{2}}^{(1)} = -\frac{\Delta x_i}{\Delta x_{i-1} + \Delta x_i} v_{i-1} + \frac{2\Delta x_i + \Delta x_{i-1}}{\Delta x_{i-1} + \Delta x_i} v_i \]  

(2.b)

where \( \Delta x_j \) is the \( j \)th grid size and \( v_j \) is the value of function \( v(x) \) at \( j \)th grid point.

The weights \( \omega_0 \) and \( \omega_1 \) depend on the smoothness of the implementations \( v_{i+\frac{1}{2}}^{(0)} \) and \( v_{i+\frac{1}{2}}^{(1)} \).

\[ \omega_r = \frac{\alpha_r}{\sum_{s=0}^{n} \alpha_s} , \quad \alpha_r = \frac{d_r}{(\varepsilon + \beta_r)^2} , \quad r = 0,1 \]  

(3)

where \( \varepsilon \) is a small, positive real number to avoid the denominator being zero. Here we choose \( 10^{-6} \). \( d_r \) is the coefficient and \( \beta_r \) is the measurement of smoothness. They are functions of grid size:

\[ d_0 = \frac{\Delta x_{i-1} + \Delta x_j}{\Delta x_{i-1} + \Delta x_i + \Delta x_{i+1}} \]  

(4.a)

\[ d_1 = \frac{\Delta x_{i+1}}{\Delta x_{i-1} + \Delta x_i + \Delta x_{i+1}} \]  

(4.b)

\[ \beta_0 = \left( \frac{2\Delta x_i}{\Delta x_i + \Delta x_{i+1}} (v_{i+1} - v_i) \right)^2 \]  

(5.a)

\[ \beta_1 = \left( \frac{2\Delta x_i}{\Delta x_{i-1} + \Delta x_i} (v_{i-1} - v_i) \right)^2 \]  

(5.b)

If the grids are uniform, the reconstruction decays to the normal 3rd order WENO scheme [6], which people always use:

\[ v_{i+\frac{1}{2}}^{(0)} = \frac{1}{2} v_i + \frac{1}{2} v_{i+1}, \quad v_{i+\frac{1}{2}}^{(1)} = -\frac{1}{2} v_{i-1} + \frac{3}{2} v_i \]  

(6)

\[ d_0 = \frac{2}{3}, \quad d_1 = \frac{1}{3} \]  

(7)

\[ \beta_0 = \left( v_{i+1} - v_i \right)^2, \quad \beta_1 = \left( v_{i-1} - v_i \right)^2 \]  

(8)

2.2. Dynamic Adaptive Chemistry

In this paper, both HMMS and VODE solvers are used to solve the stiff ODEs of detailed chemistry and their computation efficiencies are compared. In order to obtain the adaptive submechanism based on the local, the PFA method is applied to each grid point. The Aachen surrogate fuel [14] with 118 species and 527 reactions is used here to validate the present algorithm.
The PFA method can identify and keep important species and reaction pathways based on the production and consumption fluxes, and remove trivial species and reactions. For simplicity, all the studies in this paper only contain the first generation flux although the method can include multi-generation path flux analysis. For species $A$, the overall production and consumption fluxes, $P_A$ and $C_A$, can be expressed as:

$$P_A = \sum_{i=1,I} \max(v_{A,i}, \omega_i, 0), \quad C_A = \sum_{i=1,I} \max(-v_{A,i}, \omega_i, 0)$$

where $v_{A,i}$ is the stoichiometric coefficient of species $A$ in the $i$th reaction, $\omega_i$ is the net reaction rate, $I$ is the number of reaction order.

While the production and consumption fluxes between species $A$ and species $B$, $P_{AB}$, $C_{AB}$, are:

$$P_{AB} = \sum_{i=1,I} \max(v_{A,i} \delta_B^i, \omega_i, 0), \quad C_{AB} = \sum_{i=1,I} \max(-v_{A,i} \omega_i \delta_B^i, 0)$$

where $\delta_B^i$ is unity if species $B$ is involved in $i$th reaction and 0 otherwise.

Then we use the maximal production or consumption flux to normalize $P_{AB}$ and $C_{AB}$ and obtain the flux ratios for production and consumption of species $A$ via species $B$:

$$r_{\text{pro-1st}}^{AB} = \frac{P_{AB}}{\max(P_A, C_A)}, \quad r_{\text{con-1st}}^{AB} = \frac{C_{AB}}{\max(P_A, C_A)}$$

The PFA calculation starts from a preselect list of important species and flags all the species related to the preselect species. If their flux ratios $r_{\text{pro-1st}}^{AB}$ or $r_{\text{con-1st}}^{AB}$ great than the threshold value, they will be add to the select list. Then, the program will start from the select list and do the iteration again and again, until there is no new species added into the select list. Finally, the local reduced mechanism can be constructed by the species contained in the select list. A 0.005 threshold value is used in this paper.

In the dynamic adaptive chemistry (DAC) process, the PFA reduction is applied at each grid point every 10 or 100 time steps. This process is very efficient because only reaction rates need to be calculated. The time consuming of PFA is proportional to the total number of species.

3. Results and discussion

In order to validate the algorithm and test its performance, a simple hydrogen mechanism with 10 species and 23 reactions and a detailed Aachen diesel fuel surrogate (a mixture of 80% n-decane and 20% 1,2,4-trimethylbenzene by weight and 77% n-decane and 23% 1,2,4-trimethylbenzene by volume) mechanism with 118 species and 527 species are used in the simulations. The premixed hydrogen flame propagation process with stoichiometric H$_2$/air mixture is calculated by both the 3rd order WENO scheme and the 1st order total variation diminishing (TVD) scheme to show the dramatic decrease of numerical dissipation in the higher order scheme. The homogeneous ignition of Aachen diesel surrogate at different initial temperatures and equivalent ratios are modeled by the VODE and HMTS solver with and without dynamic adaptive chemistry. The results demonstrate the great efficiency and accuracy of DAC method. Also, a study of an outwardly propagating premixed spherical flame of stoichiometric Aachen surrogate fuel/air mixture with and without DAC is carried out to validate the DAC method in unsteady flame propagation process.
Fig. 2. Dependence of flame propagation speed versus grid size with stoichiometric H2/air mixture at 1 atmosphere and 300K.

**Figure 2** shows the hydrogen flame propagation speed as a function of grid size. In this simulation, a 1D flat flame of premixed stoichiometric hydrogen/air mixture at 300 K and 1 atm is initiated by a hot spot of 1600 K with a length of 2 mm at the end of the left hand side boundary. The reflective and transmissive boundary conditions are imposed, respectively, on the left and right boundaries. Note that the speed here is not the flame speed but the flame propagation speed relative to the stationary coordinate. Due to the transmissive boundary condition on the right-hand side, the unburned gas moves to the right, leading a higher flame propagation speed than the flame speed. Moreover, it is seen that at a coarse grid, the numerical dissipation introduces additional numerical diffusion flux to the transport process, which leads to the larger numerical flame propagation speed compared to the real propagation speed. With decrease of the grid size, the numerical dissipation decreases and the predicted propagation speeds also decrease. Figure 2 clearly shows that the 3rd order WENO scheme gives smaller propagation speed, which implies less numerical dissipation. Thus, the high-order WENO scheme can reduce the numerical dissipation significantly. When grid size getting smaller, the propagation speeds calculated from the 1st order TVD scheme and the 3rd order WENO scheme approach to the physical flame propagation speed.

**Figure 3** shows the ignition delay time of Aachen surrogate/air mixture as a function of initial temperature at 10 atmospheres, 0.6, 1.0 and 1.6 equivalent ratios, with and without DAC. The
maximal error in the results is 0.5%. The excellent agreement between the results with DAC and without DAC validates that the accuracy of DAC method is good enough to provide local reduced mechanism within a large range of temperature and equivalent ratio.

![Graph showing ignition delay time comparison](image)

**Fig. 3.** Comparison of ignition delay time between modeling with and without DAC, with Aachen surrogate fuel/air mixture at P=10atm.

**Figure 4** and **Figure 5** show the homogeneous ignition process’s CPU time comparison of VODE solver with and without DAC and HMTS solver with and without DAC, respectively. They give the dependence of CPU time on different initial temperature at 10 atmospheres, 0.6, 1.0 and 1.6 equivalence ratios. The CPU time is normalized by the CPU time without DAC. It is seen that for VODE solver, DAC method can increase the computational efficiency by 40 to 60 percent in a broad temperature and equivalence ratio range. For HMTS solver, the DAC method can increase the computational efficiency by about 5 to 30 percent, especially when fuel is rich. However, this is just for homogeneous ignition process. For most of the situations that DNS applied, chemical reactions just happen in a very narrow time and spatial regime. In the other nonreactive regimes, there will be only a few of active species given by DAC. Thus, in a long time regime and large spatial area, the ode solvers just need to solve these a few active species. That will cause computational efficiency increase a lot. **Figure 6** shows the CPU time comparison between VODE and HMTS solvers with and without DAC at 10 atmospheres and stoichiometric condition. All the CPU time is normalized.
by the CPU time of VODE solver without PFA. It clearly demonstrates that HMTS solver is much more efficient than the VODE solver.

**Fig. 4.** CPU time comparison between VODE solver with and without DAC for Aachen surrogate fuel/air mixture ignition at 10 atmosphere.
Fig. 5. CPU time comparison between HMTS solver with and without DAC for Aachen surrogate fuel/air mixture ignition at 10 atmosphere.
Fig. 6. CPU time comparison between VODE solver and HMTS solver with and without DAC at 10 atmospheres and stoichiometric condition.

Figure 7 shows the premixed spherical flame trajectories with and without DAC. The mixture is Aachen surrogate fuel and air at stoichiometric condition and 300 K, 1 atmosphere. They are ignited at the center by a hot spot of 1600 K with a radius of 2 mm. The chemical reactions are solved by HMTS solver. It is seen that the flame trajectories are almost the same, the largest error is less than 2%, which can demonstrate the accuracy of DAC method in unsteady flame propagation process.
Fig.7. Flame position versus time with stoichiometric Aachen surrogate fuel/air mixture at 1 atmosphere and 300K.

4. Conclusion

The 3rd order WENO scheme based on an unstructured grid system and the dynamic adaptive chemistry (DAC) method combined with HMTS solver and VODE solver are developed and integrated into the adaptive simulation of unsteady reactive flow (ASURF) code. The results show that the 3rd order WENO scheme can significantly reduce the numerical simulation, and the DAC method can increase the computational efficiency a lot while keeping excellent accuracy. The simulation of homogeneous ignition of Aachen surrogate fuel/air mixture at 10 atmospheres, with different initial temperature and equivalent ratios show that the DAC method can improve VODE solver’s efficiency by 40 to 60 percent and increase HMTS solver’s efficiency by about 5 to 30 percent, with is much faster than the VODE solver. Moreover, the study of unsteady flame propagation demonstrates the DAC method with HMTS is not only computationally efficient but also accurate and robust even when transport is included. Therefore, the HMTS solver coupled with DAC method has a great potential to be used in the DNS area.
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Reference