Acceleration of Detailed Chemistry Calculation in Multidimensional Engine Modeling Using DOLFA

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Abstract

A storage-retrieval scheme for accelerating detailed chemistry calculation in multidimensional CFD, DOLFA, has been developed and implemented in STAR–CD. This paper demonstrates its performance on predicting autoignition in engines operated in a homogeneous-charge compression-ignition (HCCI) mode either with premixed charge (nearly homogeneous to moderately non-homogeneous systems) or with liquid fuel direct-injection (highly non-homogeneous mixture). The strategies for effective use of DOLFA for multidimensional engine modeling, including judicious specification of the control parameters and dynamically reducing database size, are explored and discussed. With this approach, it is less computationally expensive to include detailed chemistry in multidimensional CFD of combustion in IC engines and other applications.

1. Introduction

Multidimensional modeling of turbulent combustors has been efficiently used to improve the design in efforts to reduce the fuel assumption and pollutant emissions. It is of great importance to include detailed chemical mechanisms for an accurate representation of real combustion processes. However, direct evaluation of chemical source terms using direct integration (DI) needs to solve nonlinear, stiff differential equations, which will lead to huge computational cost, particularly for a mechanism with hundreds of species and thousands of reactions.

Two of the most frequently used strategies to accommodate detailed chemistry in CFD are mechanism reduction and storage-retrieval schemes. Mechanism reduction can greatly reduce the number of degrees of freedom for the mechanism, but it usually requires varying assumptions that are only valid for specific conditions and systems. In a storage-retrieval storage scheme called In situ Adaptive Tabulation (ISAT) [1], the change in composition due to chemical reaction over a computational timestep is computed and tabulated as a function of initial composition on-the-fly (in situ). Its value is retrieved instead of doing a DI if a similar initial composition is encountered later. It also has explicit manipulation of retrieval/interpolation errors. ISAT originally was developed in the context of the Lagrangian Monte–Carlo algorithms for PDF-based turbulent combustion modeling. Applications to date have been mainly limited to homogeneous systems and to statistically stationary configurations (e.g., turbulent jet flames) where constant-pressure high–temperature chemistry dominates.
In such cases, high table retrieve rates can be reached and speedups approaching a factor of 1,000 have been realized, while factors of around 100 are more readily obtainable. Embouazzai, Haworth and Darabiha [2] implemented ISAT into simulation of HCCI engines. Speedups between a factor of five and ten were obtained compared to direct integration for nearly homogeneous and moderately non-homogeneous systems. However, in the highly non-homogeneous cases (a direct injection engine) that were explored, little advantage was found with ISAT compared to direct integration.

DOLFA (Database for On-Line Function Approximation) [3] was developed to address some of the shortcomings of ISAT. In ISAT, all information, no matter how long since it was generated, is kept in the table and is only removed when the table becomes full (exceeds the specified maximum size). In DOLFA, a point that has not been used recently can be deleted from the database. Another performance improvement in DOLFA is that it can guarantee that if there exists a table entry that is within the error tolerance for a new query point, this table entry will be found; that is not the case for ISAT. Veljkovic et al. [3] and Haworth et al. [4] compared the performance of DOLFA to ISAT in simulations of a HCCI engine using a n-heptane mechanism of 40 species and 165 reactions on a 1,024–cell mesh. For highly non–homogeneous (direct–injection and stratified–charge) cases, DOLFA CPU time is approximately 40% less than for ISAT. And by the end of run, the ISAT database reached approximately 500 MB compared to less than 10 MB for DOLFA.

DOLFA now has been implemented in STAR–CD. In this paper, its effectiveness on multidimensional engine modeling is demonstrated on a real engine configuration with a complex and fine mesh (compared to the 1,024 cell in–cylinder mesh in [4]). The engine is operated in a homogeneous-charge compression-ignition (HCCI) mode either with premixed charge (nearly homogeneous to moderately non-homogeneous systems) or with liquid fuel direct-injection (highly non-homogeneous mixture). The strategies for effective use of DOLFA for multidimensional engine modeling, including judicious specification of the control parameters and dynamically reducing database size, are explored and discussed.

2. DOLFA algorithms

In the STAR–CD code [5] used here, the governing equations for mass, momentum, energy and species mass fractions for the gas and droplets are solved numerically to obtain the gas and spray motions, the fuel evaporation, mixing and combustion. Here the turbulence is modeled using high-Reynolds-number k-ε models with associated wall functions.

Our focus is on the calculation of chemical source terms in the species equations. In a time-splitting method, the following differential equation for cell-level composition needs to be solved:

$$\frac{d\phi}{dt} = S_{\bar{\phi}},$$

where $S_{\bar{\phi}}$ is the chemical reaction source term. For a fixed timestep $\delta t$, the solution $\phi(t + \delta t)$ is a unique function of the initial condition $\phi_0$, denoted by $R(\phi_0)$, which is called reaction mapping [1].

In DOLFA, similar to ISAT, starting from an empty information base, a table is built up as the reactive flow calculation is performed. A table entry usually consists of: an initial composition $\phi^0$, the reaction mapping $R(\phi^0)$, the gradient of the mapping $\nabla R(\phi^0)$, and the specification of an ellipsoid of accuracy (EOA). A linear approximation to the mapping for a query composition
that is close to a tabulation point \( \phi^0 \) is:

\[
R'(\phi^q) = R(\phi^0) + A(\phi^q - \phi^0) .
\]  

(2)

The local error for this interpolation is defined as:

\[
\varepsilon = \| D(\phi^q) - R'(\phi^q) \| ,
\]

(3)

where \( D \) is a scaling matrix for an appropriate scaling of the different components of \( R \) and \( R(\phi^q) \) is the exact mapping for \( \phi^q \). DOLFA approximates the region of accuracy for each tabulation point \( \phi^0 \) by a hyper–ellipsoid, called the ellipsoid of accuracy (EOA), which is defined with the following relation:

\[
(\phi^q - \phi^0)^T A^T A (\phi^q - \phi^0) \leq 1 .
\]

(4)

Given the query composition \( \phi^q \), an element \( \phi^0 \) that is close to \( \phi^q \) in the current table is located first. Then one of the three actions is taken:

- If \( \phi^q \) is within the EOA of \( \phi^0 \), a table look–up and interpolation operation (based on Eq. 2) is performed (a retrieve).

- If \( \phi^q \) is outside the EOA of \( \phi^0 \), a DI is performed to determine the mapping \( R(\phi^q) \), and the local error is measured. If \( \varepsilon \leq \varepsilon_{\text{tol}} \), the EOA is grown (a grow).

- Otherwise if \( \varepsilon > \varepsilon_{\text{tol}} \), a new table entry is created (an add).

In DOLFA, the time when each point was last used for a successful retrieve is monitored. A point that has not been used recently can be deleted from the database, in a “periodical clean–up”. There are two user–specified parameters associated with periodical clean–up: \textit{CleanPoint} and \textit{CleanDelete}. The database cleaning is performed every \textit{CleanPoint} queries. Then points that have not been accessed in the last \textit{CleanDelete} queries are deleted. The cost of this clean–up operation is linear in the number of points stored in the database. Following this process, a new rebalanced table is rebuilt based on the remaining data points. This approach enables more efficient database searches and reduces the database size. DOLFA guarantees that if there exists a table entry that is within the error tolerance for a new query point, this table entry will be found. This is accomplished by maintaining a list of database points whose EOAs intersect a region. Then for the given query composition, these EOAs are checked to determine if any of them includes the query point. An efficient algorithm has been developed to determine whether a EOA intersects a region. This algorithm is used for designing a new EOA or changing an existing EOA by performing a grow operation.

A key to effective use of DOLFA is judicious specification of the control parameters. These include scale factors, error tolerance, and a reduced set of composition variables. A positive scale factor can be assigned to each component of composition space \( \phi \) and to each component of the reaction mapping \( R(\phi) \). Thus, each component of \( R(\phi) \) has the same weight for calculating the error using Eq. (3). Otherwise, the component that has the larger value may dominate the error evaluation. The error tolerance \( \varepsilon_{\text{tol}} \) needs to be specified for the accuracy of the interpolation. Small \( \varepsilon_{\text{tol}} \) usually yields more accurate results (closer to those from direct integration), but fewer retrieves, larger tables and longer computational time. In the standard ISAT algorithm, the end–of–timestep species mass fractions are tabulated as functions of the beginning–of–timestep pressure, temperature and all of the species mass fractions. This results in a high memory requirement and long computational time, particularly when \( A \) needs to be computed and stored. In our calculation, the methodology developed in [2] is adopted. Instead of retaining the full set of composition
variables, only a reduced set of independent composition variables that does not change with the chemical mechanism is used. The subset of independent variables is selected based on a trial-and-error approach. Here five independent chemical species are retained: fuel, $O_2$, $CO_2$, $H_2O$ and CO. Each species appears/disappears at a different stage of the autoignition process: from fuel breakdown, through the cool flame, to the high-temperature combustion. Thus there are seven independent variables (density, temperature and five species) regardless of the size of the chemical mechanism. Table size then dramatically drops.

3. Test cases

Parameters and operating conditions of the engine simulated here are summarized in Table 1. The computational mesh is shown in Figure 1. The mesh has approximately 22,000 cells in the exhaust port, 51,000 cells in the intake port, and 17,000 and 90,000 cells in the cylinder at the top dead center (TDC) and bottom dead center (BDC), respectively. Early calculations [6] indicated that it is necessary to compute through at least two full engine cycles to ensure a reasonably repeatable and representative combustion event. This is a result of the difficulties in setting the initial conditions (in-cylinder temperature, pressure and residual gas compositions) correctly. For all cases in this section, two full engine cycles are computed and all the results shown here are from 50° BTDC to 40° ATDC in the second cycle calculations, which covers the range where the chemistry is most active. A reduced n-heptane mechanism containing 29 species and 52 reactions [7] has been employed. The computational timestep corresponds to 0.2 crankangle degrees of rotation at 2000 r/min.

3.1. A premixed charge case

A mixture of n-heptane and air with an equivalence ratio of 0.3 is set as the inlet boundary condition at the intake port. The temperature and mixture composition are not perfectly homogeneous due to the incomplete mixing among fresh charge and residual products.

Three sets of DOLFA control parameters have been used for the present case, as given in Table 2. DOLFA results are compared with those obtained using direct-integration (DI) in Figures 2 and 3. The CPU time for each timestep is plotted as a function of crankangle in Figure 4. Apparently higher error tolerance ($\varepsilon=0.01$) consumes less CPU time but results in worse results than lower error tolerance ($\varepsilon=0.001$). With lower

<table>
<thead>
<tr>
<th>Configuration</th>
<th>Four-valve</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bore</td>
<td>90 mm</td>
</tr>
<tr>
<td>Stroke</td>
<td>116 mm</td>
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<tr>
<td>Connecting Rod Length</td>
<td>145 mm</td>
</tr>
<tr>
<td>Engine speed</td>
<td>2000 r/min</td>
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<tr>
<td>Compression ratio</td>
<td>14</td>
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<tr>
<td>Intake Temperature</td>
<td>380 K</td>
</tr>
<tr>
<td>Intake Pressure</td>
<td>1.01 bar</td>
</tr>
<tr>
<td>Fuel</td>
<td>n-heptane</td>
</tr>
<tr>
<td>Equivalence ratio</td>
<td>0.3</td>
</tr>
</tbody>
</table>
error tolerance, DOLFA– and DI– computed global in–cylinder pressures and H$_2$O$_2$ mass fractions are nearly indistinguishable. Even with the reduced set of DOLFA independent composition variables, minor species like H$_2$O also show excellent agreement (Figure 3). An interesting finding here is that when the scaling factor of density is increased from 15 to 150, the CPU time slightly decreases and the results are almost unchanged. This indicates that density does not play an important role in the error evaluation. A speedup of approximately thirty is obtained in the cases with the lower error tolerance. Figure 4 also clearly illustrates the relationship between DOLFA performance and the ignition process. Before the first–stage ignition, the significantly lower CPU time with DOLFA indicates high table reuse. During the ignition events where pressure, temperature and compositions vary rapidly and where it is expected that the dimensionality of the underlying intrinsic low–dimensional manifolds (ILDM) in composition space may not be adequately described using the seven independent variables that have been retained here, table reuse drops dramatically.

3.2. A liquid fuel direct injection case

Liquid fuel is directly injected into the cylinder at 180° BTDC such that the global equivalence ratio is approximately 0.3. The liquid droplets evaporate in the computational domain and mix with air in the cylinder. A highly non-
homogeneous mixture is formed before combustion occurs. This poses a challenging problem to storage-retrieval schemes. In the calculation, the maximum allowable database size is set as 300MB for DOLFA. As shown in Figure 5, the database is dynamically cleaned based on usage statistics when its size exceeds the maximum limit. Variable error tolerances are also used, with high value for the calculation before the main combustion event. Here with control parameters that yield acceptable accuracy compared to DI, a speedup of approximately three is obtained. The CPU time per timestep is shown in Figure 6. More tests are being performed to examine the optimal database cleanup frequency.

4. Concluding remarks

The effectiveness of DOLFA in multidimensional engine modeling has been demonstrated. Significant speedups have been realized for premixed charge cases, while smaller - but still significant - speedups have been found in highly non-homogeneous direct-injection systems. The guidelines for control parameter selection have been discussed. Further directions of this research include saving the database on the disk and restoring it for the subsequent runs, load balancing issues for parallel runs, and applications with probability density function (PDF) methods [8–10] where the turbulence-chemistry interactions can be captured and where most of the computational time is spent on detailed chemistry calculation.

References