Effective Use of Storage/Retrieval-Based Chemistry Acceleration in CFD

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Abstract

Database for On–Line Function Approximation (DOLFA) is a storage/retrieval chemistry–acceleration scheme that is based on Pope’s ISAT method [S.B. Pope Combust. Theory Modell. 1:41-63, 1997]. Recent developments in DOLFA are reviewed and the effective usage of DOLFA in multidimensional in-cylinder CFD is discussed. Highly nonhomogeneous systems with direct in-cylinder liquid fuel injection are considered, and results with and without a Lagrangian particle probability density function (PDF) method are presented. Numerical experiments show that all three approximations (linear, constant, and hybrid) yield global in–cylinder pressure, temperature, and species profiles that are in good agreement with those obtained using direct integration for an absolute error tolerance of $10^{-3}$. A smaller tolerance is required if one requires, for example, that the maximum cell-level mean temperature be within 50 K (say) of that obtained using direct integration. In addition to the error tolerance, scale factors also affect computational efficiency and accuracy. The benefits of DOLFA are greater in cases where the particle PDF method is used.

1. Introduction

Numerical simulation is becoming an increasingly important tool in the design of advanced internal combustion (IC) engines [1]. The accuracy of the simulations depends on many factors, including the level of thermochemistry that is adopted. Numerical prediction of phenomena such as autoignition and pollutant formation requires consideration of chemical mechanisms that involve tens-to-hundreds of chemical species and hundreds-to-thousands of chemical reactions. In such cases, the calculation of chemical source terms dominates the CPU time, especially when turbulence/chemistry interactions need to be considered and are accounted for using Lagrangian–particle–based Monte Carlo probability density function (PDF) methods [2–5]. In that case, the number of computational particles is typically 20 to 100 times the number of finite-volume cells.

One approach to reduce the computational overhead of large chemical mechanisms in CFD is storage/retrieval database schemes. Pope’s in situ adaptive tabulation (ISAT) method [6] is one of the most promising approaches that has appeared to date. In ISAT, the database is generated on-the-fly (in situ) during the CFD calculation, and retrieval/interpolation errors are controlled by user-specified error tolerances and other parameters. Numerical experiments have shown that ISAT can achieve speedups approaching a factor of 1000 compared to direct integration for statistically stationary systems (e.g., turbulent jet flames) where an asymptotic state corresponding to nearly 100% retrieves eventually is reached [7]. Smaller, although still significant (factors of 10 to 100) speedups have been demonstrated for homogeneous or nearly homogeneous transient systems (e.g., autoignition in HCCI engines) where spatial variations in thermochemical state are small [8]. It has proven more difficult to demonstrate significant and consistent advantages for highly nonhomogeneous time-dependent systems (e.g., direct–injection stratified–charge engines) while maintaining acceptable accuracy.

Database for on–line function approximation (DOLFA) [9] is an ISAT-based storage/retrieval algorithm that has been developed for highly transient combustion systems, such as those occurring in an IC
engine. By contrast to statistically stationary systems, database retrieve rates for transient systems are much lower, and the probability of reusing a previously tabulated entry decreases toward zero with increasing age of the entry. These characteristics have led to different choices in data organization compared to ISAT, and to the development of various strategies for database cleaning.

In the following section, the basic ISAT and DOLFA algorithms are reviewed with particular emphasis on recent developments in DOLFA. In Section 3, results for autoignition in direct-injection engines are presented with and without the particle PDF method. The influence of DOLFA input parameters on accuracy and efficiency is investigated, and recommendations are provided for the specification of key parameters.

2. DOLFA

ISAT and DOLFA are generic tabulation algorithms. In the context of computational combustion, they are used to store and retrieve solutions to the following system of ordinary differential equations (ODE’s):

\[
\frac{d\phi}{dt} = S(\phi).
\]

(1)

Here \( \phi = [\phi_1, \phi_2, \ldots, \phi_D] \) and \( S = [S_1, S_2, \ldots, S_D] \) are the dependent–variable and source–term vectors, respectively. In combustion, \( \phi \) typically corresponds to a set of species mass fractions and \( S \) corresponds to the time–rates–of–change of species mass fractions due to chemical reactions. In a more generic sense, \( \phi \) represents a point in the \( D \)-dimensional composition space. For a given initial condition \( \phi_0^0 \) at \( t = t_0 \), Eq. (1) has a unique solution \( \phi(t) \) at \( t = t_0 + \delta t \) for a fixed \( \delta t \). We denote \( \phi(t) \) by \( R(\phi_0) \), the reaction mapping: the time integration of Eq. (1) for \( \delta t \) maps the initial condition \( \phi_0^0 \) to the end–of–timestep value \( \phi(t) = R(\phi_0^0) \). The quantity \( A(\phi) \) is the mapping gradient matrix:

\[
A_{ij}(\phi) = \frac{\partial R_i(\phi)}{\partial \phi_j}.
\]

(2)

The basic idea of the storage/retrieval algorithm of ISAT or DOLFA is to approximate \( R(\phi) \) by interpolation from exact solutions (those obtained via direct integration of Eq. (1)) that are tabulated on–the–fly in the course of the CFD simulation. Initially, the database or table is empty. When the first query is made, the reaction mapping of the query point \( \phi^q \) is calculated by direct integration (DI), and \( \phi^0 \) and \( R(\phi^0) \) are added to the table. For later queries, the database is searched to find an entry \( \phi^0 \) that is “close” to \( \phi^q \). The region of accuracy (ROA) about each tabulation point is the region inside which the local error is smaller than a user-specified error tolerance \( \varepsilon_{tol} \), i.e.,

\[
\varepsilon \equiv || R(\phi) - R^\varepsilon(\phi) || \leq \varepsilon_{tol} ,
\]

(3)

where \( R \) is a scaling matrix, \( \phi \) is any point inside the ROA, and \( R(\phi) \) and \( R^\varepsilon(\phi) \) are, respectively, the exact and approximated reaction mappings. For a linear approximation,

\[
R^\varepsilon(\phi) = R(\phi^0) + A(\phi^0) \cdot (\phi - \phi^0) ,
\]

(4)

while for a constant approximation,

\[
R^\varepsilon(\phi) = R(\phi^0) .
\]

(5)

The ROA is not known a priori, and is approximated by an ellipsoid of accuracy (EOA) that is defined using \( A \) [6]. For query composition \( \phi^q \) and database entry \( \phi^0 \) that is “close” to \( \phi^q \):

- If \( \phi^q \) is within the EOA of \( \phi^0 \), \( R(\phi^q) \) is approximated by \( R^\varepsilon(\phi^q) \), i.e., a retrieval.
  
  During this stage the local error may be randomly checked against the exact value of \( R(\phi^q) \) calculated by DI. If \( \varepsilon > \varepsilon_{tol} \), the existing EOA is shrunk, and a new table entry is created to store \( \phi^q \) and \( R(\phi^q) \).

- If \( \phi^q \) is outside of the EOA of \( \phi^0 \), both \( R(\phi^q) \) and \( R^\varepsilon(\phi^q) \) are calculated (the former by DI), and the local error is evaluated. If \( \varepsilon \leq \varepsilon_{tol} \), the EOA is grown. Otherwise, \( \phi^q \) and \( R(\phi^q) \) are stored as a new table entry, i.e., an addition.

Differences between DOLFA and ISAT are highlighted in the remainder of this section. First, binary space partition (BSP) trees are employed in DOLFA (as in ISAT) to organize convex regions (polytopes) formed by dividing planes in the composition space. In DOLFA, a list is maintained for each region that includes all tabulation points whose EOAs reside in or intersect with
that region. This guarantees that if \( \phi^0_i \) lies in the EOA for an existing table entry, that table entry will be found. This improves the retrieve rate compared to an approach where a single table entry is associated with each region.

Second, a hybrid approximation method has been implemented in DOLFA in addition to the constant and linear approximations. With the hybrid approximation, the reaction mapping of a query point is estimated using a linear approximation whenever the retrieval condition is satisfied. The EOAs of the tabulated points, however, are determined based on an approximation that reduces matrix-multiplication operations. Consequently, the hybrid approximation method has higher computational efficiency than its linear counterpart, while it is more accurate than the constant approximation method.

Third, multiple database cleaning strategies have been introduced into DOLFA. These include (1) local cleaning plus database-size-controlled global cleaning; (2) database-size-controlled global cleaning only; (3) user-controlled global cleaning only. Local cleaning refers to periodic cleaning of the database based on the usage statistics (“age”) of the tabulation points. Points that have not been accessed recently are removed from the database, and the BSP tree is rebalanced. In a global clean, the entire database is deleted completely, and a new BSP tree is built up from scratch. After local and global cleaning, the database only contains those points that either have been accessed frequently or have been added to the database recently. Therefore, high searching/retrieving efficiency can be expected in highly transient combustion simulations, where the accessed region of the composition space changes with time.

Two other improvements have been made on the application-code side. A stiff ODE solver that facilitates the calculation of \( A \) has been implemented [10]. And an option has been added to tabulate the change \( R_i - \phi^0_i \) rather than the end-of-timestep value \( R_i(\phi^0) \). This is especially important for species such as NO and NO\(_2\) that continue to evolve slowly after the bulk autoignition event is complete.

3. Results and Discussion

In this section, the impacts of the input parameters of DOLFA on accuracy and computational efficiency are explored. The CFD code is an unstructured, deforming-mesh, compressible finite-volume solver, in which a Lagrangian particle Monte Carlo method has been implemented to solve the modeled composition PDF transport equation using a consistent hybrid particle/finite-volume method [4]. A standard gradient transport approximation is used together with a two-equation \( k-\epsilon \) turbulence model to account for transport by turbulence velocity fluctuations, and a simple pair-exchange model is used for molecular mixing. Direct in-cylinder liquid fuel injection is modeled using stochastic Lagrangian models that are based on the KIVA spray formulation [11, 12].

A simple pancake-chamber engine is used for this study. The bore/stroke/clearance distance are 88.55/140/10 mm, respectively. The fuel injector is located in the center of the head, and injection is along the axial direction toward the piston. The fuel is n-heptane, and a reduced 29-species and 52-reaction mechanism is used to model the thermochemistry [13].

A coarse 3-D mesh of 2604 finite-volume cells is used. Computations begin at piston bottom-dead-center (180\(^\circ\)) with air at 450 K and 1 atm. Fuel injection starts at 190\(^\circ\) and ends at 205\(^\circ\), and the simulation is carried through autoignition to 30\(^\circ\) beyond piston top-dead-center (390\(^\circ\)). The total amount of fuel injected is 0.01 g. The walls of the engine are adiabatic.

Key DOLFA input parameters are the error tolerance and the scale factors. Temperature, pressure, fuel (n-heptane), O\(_2\), CO\(_2\), H\(_2\)O, and CO are chosen as the seven independent tabulation variables. The dependent variables, on the other hand, are all 29 species mass fractions. The scale factors for temperature and pressure are 1000 K and \( 10^7 \) Pa, respectively. The scale factors for all species other than those in the list of independent variables are set to 1.0. The maximum allowable database size (threshold for global cleaning) is 500 MB.

3.1. Tests without Monte Carlo-PDF method

This subsection presents results from numerical simulations with the particle Monte Carlo–PDF method turned off. In this case, a solution to Eq. (1) is required for each finite-volume cell on every computational timestep.

First, the constant approximation is used with the scale factors for all independent species set to 0.02. Four absolute error tolerances have been tested: \( \varepsilon_{tol,abs} = \)
$10^{-2}, 10^{-3}, 10^{-4},$ and $10^{-5}$. The relative error tolerance, $\varepsilon_{\text{tol,rel}}$, is set one order of magnitude smaller than $\varepsilon_{\text{tol,abs}}$ in all cases. The computational timestep size is $0.25^\circ$ before injection starts and $0.125^\circ$ thereafter. Figures 1–3 show the crank angle evolution of the global in-cylinder temperature, pressure, and species concentration of H$_2$O$_2$ in the engine. Also shown are the solutions obtained using DI. It can be observed that when $\varepsilon_{\text{tol,abs}} \leq 10^{-3}$, the solutions from DOLFA agree very well with their respective DI solution for all three quantities. The total CPU time for $\varepsilon_{\text{tol,abs}} = 10^{-3}$ is 57 minutes, while DI requires 138 minutes. While a factor of 2.42 speedup may appear to be disappointing, it should be noted that: (1) the system is highly nonhomogeneous; (2) the mesh is quite coarse; and (3) chemistry counts for only 27.7% of the total CPU time for this case.

A more stringent criterion compared to global values is to look at agreement between DI and DOLFA at the finite–volume cell level. Figure 4 shows the crank angle evolution of the maximum finite-volume cell temperature, $T_{\text{max}}$, for four cases. Difference between DI and DOLFA can be seen in all cases, and convergence of DOLFA toward DI with decreasing $\varepsilon_{\text{tol,abs}}$ is evident. It is emphasized that matching $T_{\text{max}}$ is an extremely severe test.

Next, the hybrid approximation method is considered. Again, DOLFA global quantities agree well with DI for $\varepsilon_{\text{tol,abs}} \leq 10^{-3}$ (not shown). The crank angle evolution of $T_{\text{max}}$ is shown in Fig. 5. In this case, the DOLFA result is nearly indistinguishable from DI for $\varepsilon_{\text{tol,abs}} = 10^{-5}$, illustrating on improvement in accuracy with respect to the constant approximation.

Finally, the linear approximation method is considered. The timestep size is now set to $0.25^\circ$ throughout the calculations for both DOLFA and DI. The influence of the scale factors on the accuracy is examined first. The absolute and relative error tolerances are fixed to $10^{-3}$ and $10^{-4}$, respectively, while the scale factors for the five independent species are assigned the following values: (1) 0.02 for all five species; (2) 0.01 for all five species; (3) 0.005 for all five species; (4) $Y_{i,\text{max}}$ (i.e., their respective maximum values over the entire combustion event); and (5) $Y_{i,\text{max}}/2$. Figure 6 presents the crank angle evolution of the maximum temperature for the above five cases. All cases predict the correct autoignition timing. The maximum temperatures after
factors are related to the autoignition, however, are overpredicted when the scale factors are set to 0.02. When 
\( \varepsilon_{\text{tol,abs}} > 10^{-3} \), autoignition timing is not predicted correctly, and there is a lag in crank angle with respect to the DI solution. When 
\( \varepsilon_{\text{tol,abs}} \leq 10^{-4} \), good agreement with DI is achieved.

The effect of the error tolerance for linear approximation is shown in Fig. 7. Three absolute error tolerances have been tested: 
\( \varepsilon_{\text{tol,abs}} = 10^{-2}, 10^{-3}, \) and 
\( 10^{-4} \). The relative error tolerances are one order of magnitude smaller than their respective 
\( \varepsilon_{\text{tol,abs}} \)'s. The scale factors of the independent species are set to 0.02. When 
\( \varepsilon_{\text{tol,abs}} > 10^{-3} \), autoignition timing is not predicted correctly, and there is a lag in crank angle with respect to the DI solution. When 
\( \varepsilon_{\text{tol,abs}} \leq 10^{-4} \), good agreement with DI is achieved.

3.2. Tests with Monte Carlo-PDF method

Next, the particle Monte Carlo-PDF method is enabled. In this case, a solution to Eq. (1) is required for each computational particle. Here 25 particles (nomi-

nally) are used per finite-volume cell, and chemistry dominates the computational time.

All three approximation methods have been tested for the following DOLFA input parameters: the scale factors for the independent species are set to 0.02, and the error tolerances are 
\( \varepsilon_{\text{tol,abs}} = 10^{-4} \) and 
\( \varepsilon_{\text{tol,rel}} = 10^{-6} \), respectively. The timestep size is 0.25°. The crank angle evolution of the maximum finite–volume cell mean temperature is shown in Fig. 8. Apparently, all three approximation methods result in very good solutions. Table 1 lists the cpu times used by DI and each approximation.
A maximum chemistry speedup of 3.37 is achieved for the hybrid approximation. Better speedups could be realized with relaxed error tolerance, and it appears that there is room to do that in this case.

4. Concluding remarks

Recent developments in DOLFA have been discussed, and applications to highly nonhomogeneous, nonstationary combustion in direct-injection IC engines have been presented, with and without a particle-PDF method. The new hybrid approximation appears to provide a good tradeoff between accuracy and computational efficiency. Further tests are underway on more representative mesh sizes to establish guidelines for database cleaning and to verify formal convergence rates. Work on parallel versions of DOLFA is in progress.

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References