

Simulations of Advanced Combustion Modes Using Detailed Chemistry Combined with Tabulation and Mechanism Reduction Techniques

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ABSTRACT

Multi-dimensional models represent today consolidated tools to simulate the combustion process in HCCI and Diesel engines. Various approaches are available for this purpose, it is however widely accepted that detailed chemistry represents a fundamental prerequisite to obtain satisfactory results when the engine runs with complex injection strategies or advanced combustion modes. Yet, integrating such mechanisms generally results in prohibitive computational cost.

This paper presents a comprehensive methodology for fast and efficient simulations of combustion in internal combustion engines using detailed chemistry. For this purpose, techniques to tabulate the species reaction rates and to reduce the chemical mechanisms on the fly have been coupled. In this way, the computational overheads related to the use of these mechanisms are significantly reduced since tabulated reaction rates are re-used for cells with similar compositions and, when it becomes necessary to perform direct integration, only the relevant set of species and reactions is taken into account.

The proposed approach named tabulation of dynamic adaptive chemistry (TDAC) has been implemented in the Lib-ICE code, which is a set of libraries and applications for IC engine modeling developed using the OpenFOAM® technology. In particular, a modified version of the in-situ adaptive tabulation (ISAT) algorithm has been developed for systems with variable temperature and pressure, and the directed relation graph (DRG) method has been used to reduce the mechanism at run-time. The validation has been carried out with HCCI and Diesel cases both using a simplified case to compare the results obtained with and without TDAC, and a detailed case that is validated with experimental data. For each tested condition, a detailed comparison between computed and experimental data is provided along with the achieved speed-up factors compared to the use of direct-integration.

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INTRODUCTION

In the current environmental context, many research projects in internal combustion engines focus on two primary topics: meeting the stringent emission standards and searching for alternative fuels. To reduce the emissions in conventional engines, various exhaust gas after-treatment strategies have been investigated but lately innovative combustion modes are also studied to further reduce the

emissions. These combustion modes include homogeneous charge compression ignition (HCCI) [1, 2], and other derived modes such as premixed compression ignition (PCI) [3], partially premixed combustion (PPC) [4] or radical controlled compression ignition (RCCI) [5]. Environmentally sustainable transportation is also a very important challenge. Biofuels are often mentioned as a possible solution to replace part of the fossil fuels but the combustion of new generation biofuels requires careful analysis and characterization.

To investigate both these topics, multi-dimensional models are widely applied, since they can predict the engine performance and pollutant emissions. Furthermore, they allow a very detailed investigation of the main thermal and chemical phenomena taking place in the engine cylinder during fuel-air mixing and combustion processes. Within this context, the use of kinetic mechanisms has become a fundamental prerequisite to simulate complex injection strategies or advanced combustion modes [6,7], but most of these studies use skeletal or reduced mechanisms to maintain a reasonable computational time. However, complex fuel kinetics in a large range of thermo-chemical conditions can be only taken into account through the comprehensiveness provided by detailed mechanisms. When complex chemical schemes are included in combustion models, the evolution of the chemical species in each computational cell is modeled by a system of nonlinear stiff ordinary differential equations (ODE). An efficient way to solve this system is to use the Jacobian of the chemical system to linearize it and then a semi-implicit solver. However, this is still computationally demanding when hundreds of species and thousands of reactions are involved, hence limiting the application of detailed kinetics for practical ICE simulations. For this reason, different approaches were proposed to reduce the computational effort and they can be divided in two groups: methods that reduce the impact of the number of cells, hence reducing the number of times the ODE system is solved, and methods that reduce the impact of the number of species in the kinetic mechanism, hence limiting the size of the ODE system. In the first group, since many cells may be in the same state, multi-grid methods group similar cells and solve them together [8]. Similarly, previously computed results may be adequate for the current cell, therefore the in-situ adaptive tabulation (ISAT) method [9] and the piecewise reusable implementation of solution mapping (PRISM) [10] store previously computed results dynamically and retrieve them according to specific regions of accuracy. In the second group, the reduction of the chemical schemes can be performed by skeletal reduction through elimination of species and reactions that have a small contribution to the overall activity of the system. These methods include sensitivity analysis [11], computational singular perturbation (CSP) [12], directed relation graph (DGR) [13], DRG with error propagation (DRGEP) [14], dynamic adaptive chemistry (DAC) [15], path flux analysis (PFA) [16] and element flux analysis (EFA) [17]. Other techniques could further reduce the resulting skeletal mechanism such as lumping [18], chemistry-guided reduction [19] or quasi steady-state assumptions (QSSA) [20]. Combining both dimension reduction and tabulation (or multi-grid) has been proposed as a preprocessing step with the intrinsic low-dimensional manifold (ILDm) [21], further developed in flame prolongation of ILDM (FPI) [22]. It has also been proposed as dynamic methods, for example: ISAT and rate-controlled constrained equilibrium [23] or adaptive multi-grid chemistry and DAC (AMC-EDAC) [24].

A generalized technique, called TDAC (tabulation of dynamic adaptive chemistry), is presented in this work and applied to the simulation of combustion modes requiring the use of very detailed chemistry. To achieve a very high speed-up compared to direct-integration and significantly limit the operation of the ODE solver, TDAC combines on-the-fly mechanism reduction and tabulation techniques. In this way, only the relevant set of species and reactions is accounted for in each computational cell, and computed reaction rates can be re-used for cells having similar composition to the tabulated ones. A first version of TDAC, combining DAC and ISAT, was applied by the authors to simulate PCCI and HCCI combustion modes and satisfactory results were achieved [25,26]. The TDAC technique has been implemented by the authors into the Lib-ICE code, which is a set of libraries and solvers for ICE simulations based on the OpenFOAM® technology [27, 28, 29]. The object-oriented structure of the code allows to easily implement and test different tabulation and mechanism reduction methods, identifying the best combination for the different combustion modes that needs to be modeled. Two different cases were simulated to test the TDAC method: HCCI engine and diesel combustion at constant-volume conditions. For each of them the performance of the proposed technique was evaluated in terms of speed-up factor compared with direct-integration and agreement with experimental data of ignition delay, pressure trace and heat release rate profile.

COMPUTATIONAL METHODS

Including combustion in CFD simulations increases the total number of operations. The operations required for solving the chemical kinetics depend on the number of cells in the mesh and the size of the oxidation mechanism. The system of stiff nonlinear ODE is integrated in every cells and the size of the mechanism defines the level of complexity to integrate this system. Reduction of the computational effort for these separated aspects is achieved by the TDAC method, which is composed of two layers: a tabulation method and a mechanism reduction method. The tabulation method intends to reuse previously computed results, hence decreasing the effect of the number of cells, whereas the mechanism reduction method finds a skeletal mechanism at runtime, hence reducing the effect of the mechanism size (see [Figure 1](#)). In the following three sections, we present the ISAT algorithm used at the tabulation layer, then we describe the mechanism reduction layer, and finally the modification needed for the coupling between these layers are introduced.

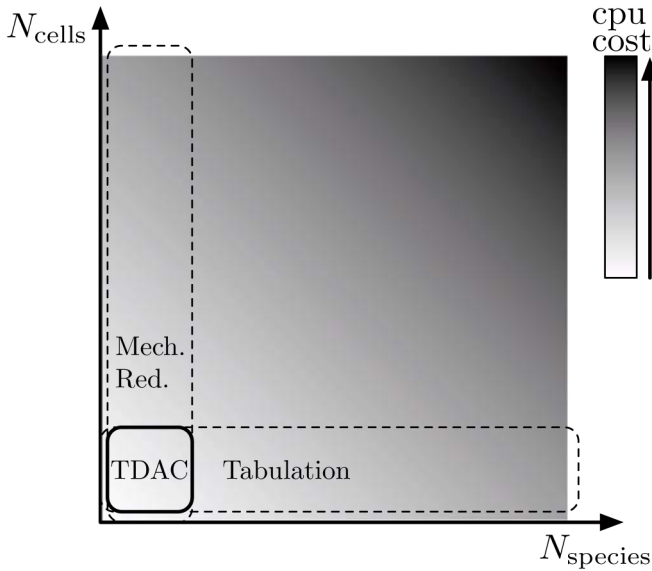


Figure 1. The TDAC method takes advantage of the synergy between the tabulation method and the mechanism reduction method. It reduces the computational cost associated with the number of cells in the mesh and the number of species in the kinetic mechanism.

IN SITU ADAPTIVE TABULATION

The ISAT algorithm is used when computationally demanding results, e.g. the integration of large and stiff ODE systems, can be stored for subsequent uses.

A thermochemical state is defined by the composition

$$\psi = \{Y_1, Y_2, \dots, Y_{N_s}, T, p\}, \quad (1)$$

where Y_i are the species mass fractions, N_s is the number of species, T is the temperature and p is the pressure. The integration of the reaction equations for a fixed time step Δt maps the initial composition $\psi^0 = \psi(t_0)$ to the reacted value $\psi(t_0 + \Delta t)$ which is a unique function of ψ^0 called the reaction mapping, $\mathbf{R}(\psi^0)$.

During computation, given a query point, ψ^q , ISAT computes a linear approximation of the mapping from a previously stored point:

$$\mathbf{R}(\psi^q) \approx \mathbf{R}^l(\psi^q) = \mathbf{R}(\psi^0) + \delta \mathbf{R}^l, \quad (2)$$

where $\delta \mathbf{R}^l$ is the difference of reaction mapping due to the difference of composition between ψ^0 and ψ^q . $\delta \mathbf{R}^l$ is computed by

$$\delta \mathbf{R}^l = \mathbf{A}(\psi^0)(\psi^q - \psi^0), \quad (3)$$

where $\mathbf{A}$ is the mapping gradient matrix defined by

$$A_{ij}(\psi^0) \triangleq \frac{\partial R_i(\psi^0)}{\partial \psi_j}. \quad (4)$$

The matrix $\mathbf{A}$ is related to the first order sensitivity coefficients with respect to initial conditions defined by

$$C_{ij}(\psi^0, t) \triangleq \frac{\partial \psi_i(t)}{\partial \psi_j^0}, \quad (5)$$

with

$$\mathbf{A}(\psi^0) = \mathbf{C}(\psi^0, t_0 + \Delta t). \quad (6)$$

To compute $\mathbf{A}$, the following linear system of ODE is integrated implicitly from t_0 to $t_0 + \Delta t$:

$$\frac{d}{dt} \mathbf{C}(\psi^0, t) = \mathbf{J}(\psi(t)) \mathbf{C}(\psi^0, t), \quad (7)$$

where $\mathbf{J}$ is the Jacobian and the initial condition $\mathbf{C}(\psi^0, t_0) = \mathbf{I}$.

The linear approximation defined by equation (2) is only valid in the region

$$|\mathbf{R}(\psi^q) - \mathbf{R}^l(\psi^q)| = |\delta \mathbf{R} - \delta \mathbf{R}^l| \leq \varepsilon_{\text{ISAT}}, \quad (8)$$

where $\varepsilon_{\text{ISAT}}$ is a user-specified tolerance and $\delta \mathbf{R} = \mathbf{R}(\psi^q) - \mathbf{R}(\psi^0)$. The computation of this region is however prohibitive. It is therefore approximated by a conservative hyper-ellipsoid in the composition space called ellipsoid of accuracy (EOA):

$$\text{EOA} \triangleq \delta \psi^T \tilde{\mathbf{A}}^T \mathbf{B}^T \mathbf{B} \tilde{\mathbf{A}} \delta \psi \leq \varepsilon_{\text{ISAT}}^2, \quad (9)$$

where $\mathbf{B}$ is an optional scaling matrix, $\tilde{\mathbf{A}}$ is the modified $\mathbf{A}$ matrix and $\delta \psi = \psi^q - \psi^0$. $\mathbf{B}$ is used to manually modify the shape of the hyper-ellipsoid which can modify the retrieval tolerance for specific species (e.g. when the precision on a species of interest should be increased). $\tilde{\mathbf{A}}$ is obtained by limiting the smallest singular values to prevent them from generating very large principal axes (see [7, 30]).

During the simulation, the computed results are stored in a binary tree consisting of leafs and nodes: the leafs store ψ , $\mathbf{R}(\psi)$, $\mathbf{A}(\psi)$ and the EOA description; the nodes store the hyperplanes in the composition space that are used to scan the binary tree and to retrieve the closest stored composition. For each query, one of the following three operations is performed: retrieve if ψ^q is in the EOA and growth or

addition if ψ^q is not in the EOA. ISAT retrieves the reaction mapping of ψ^q using [equation \(2\)](#). For growths and additions, the direct integration of the reaction equations should be first performed. Then, ISAT checks the local error using [equation \(8\)](#). If the error is less than ϵ_{ISAT} , the current EOA is too conservative and it is grown to include ψ^q . Otherwise a new leaf is added to the binary tree to store $\mathbf{R}(\psi^q)$. Further details about ISAT can be found in [9].

In a previous work, some modifications have been included to improve the efficiency of ISAT in engine cases [25]. For unsteady cases, the binary tree should be kept updated to properly predict the onset of the combustion. Therefore, we introduced two parameters to control the maximum number of retrievals and growths for any stored point. These parameters keep the binary tree updated without relying on ϵ_{ISAT} only, which significantly increases the performance during the main combustion.

In this paper, we have also introduced a cleaning and balancing procedure following the principles given in the DOLFA method [31]. This procedure first scans the binary tree after a given interval to remove points that are deemed too old. Then, it reshapes the binary tree so that the hyperplane of the root node goes through the mean composition and is perpendicular to the direction with maximum variance.

MECHANISM REDUCTION TECHNIQUES

The first version of TDAC only included the DAC method as the mechanism reduction layer [25]. The performances of other reduction techniques (DRG, DRGEP, PFA, and EFA) were subsequently assessed and compared to DAC within the TDAC framework [32]. The first three methods were initially developed for preprocessing the mechanism. We have therefore modified them to reduce the mechanism at runtime. In HCCI simulations, the DRG method was the most efficient and it is used in the following simulations. However, different reduction methods might have better performances in different cases because the interactions between the tabulation algorithm and the reduction methods are not trivial. This is beyond the scope of this paper and will not be detailed in the following sections.

The mechanism reduction methods reduce kinetic mechanisms based on a quantitative variable for the coupling between species. This coupling is characterized by the impact of removing one species on the production rate of another species. These methods abstract the couplings by constructing a graph with each node representing a species and each edge representing a strong coupling. If an edge goes from a species A to a species B, it indicates that the removal of B induces a significant error on the production rate of A. If A is kept in the mechanism, then B should also be kept. [Figure 2](#) shows a portion of an illustration graph constructed by the DRG

method. As an example, a graph generated by the DRG method for a real oxidation mechanism is shown in [Figure 3](#).

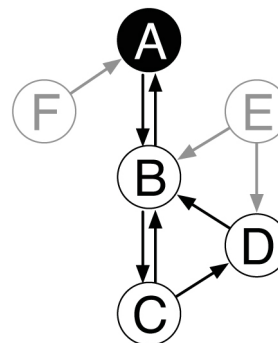


Figure 2. Given a starting species A, the species B, C and D are kept in the mechanism while E and F are removed.

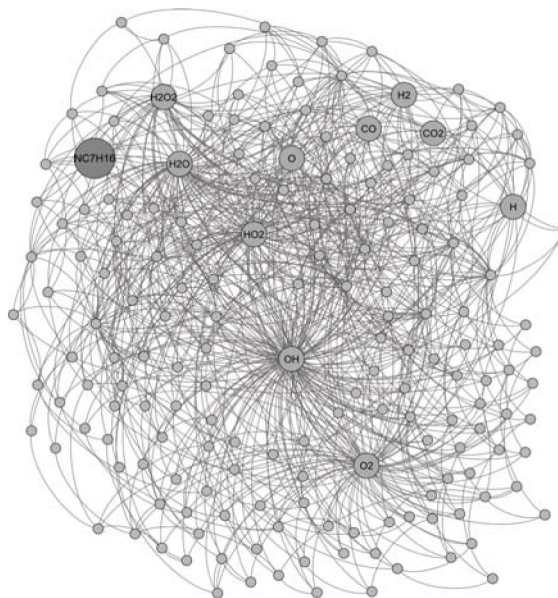


Figure 3. Network generated with Gephi [33]. It represents the active part computed with the directed relation graph method (adapted for runtime reduction) [13] of the n-heptane mechanism from Curran et al. [34] near top dead center.

The difference between many reduction methods relies on the way to compute the coupling. DRG only characterizes direct coupling, the strength of the path between two species is therefore characterized by its weakest link [14].

The reduction algorithm is executed before every call to the ODE solver. It first computes the strength of the direct links between species. Then, the algorithm computes the strength of the paths connecting all the species to a user-defined search initiating set of species. In the following simulations, fuel, CO, and HO₂ are used as the search initiating set. In the final step, the reduction scheme removes from the mechanism the species with a value of path strength