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Research Paper

An investigation of in situ adaptive tabulation for premixed and nonpremixed combustion engine simulations with primary reference fuel mechanism

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HIGHLIGHTS

- Both premixed and non-premixed combustion process are used.
- Dynamic pruning strategy in ISAT is employed.
- Temperature inhomogeneity induced by different factors is investigated.
- The performance of ISAT with different memories is studied.
- Computational efficiency at different combustion stages is studied.

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ABSTRACT

The object of this work is to enhance the ISAT performance for transient combustion simulations for both premixed and non-premixed combustion process. In this work, dynamic pruning (DP) strategy for not-frequently-accessed tabulated points has been employed. For DP approach, the action considered when the table is full is to delete the most recently used leaf (at the tail of most recently used leaf) and replace it by the new entry in ISAT. The performances of ISAT with DP are presented firstly both in a homogenous charged compression ignition (HCCI) engine and a diesel engine. In present study, we investigate the sensitivity of ignition and composition inhomogeneity to heat loss/chemistry model for HCCI combustion. Composition inhomogeneity is governed by heat loss, turbulence diffusion and chemical reaction. Meanwhile, the effect of composition and temperature inhomogeneity on chemistry acceleration with ISAT-DP is studied in detail. It is shown that, ISAT-DP method can effectively reduce computational cost and achieve a large speedup factor of around 2 compared with original ISAT method. Memory size in ISAT has a tight influence on computational efficiency. And an overall speed up factor of around 4 for diesel engine is also achieved.

1. Introduction

In recent decades, to reduce pollutant emissions and improve fuel economy is required to meet stringent emission regulations and reduce fossil fuel consumption in internal combustion engines (ICE). Experiment methodology as a main tool plays a very important role on achieve these improvements from traditional ICE to current developing engine such as HCCI, PCCI [1,2] and RCCI [3]. However, whatever the engine types are, they all include complex physical-chemistry process in ICE, just the experiment method is not enough to exploit some important and complex combustion process, such as auto-ignition, emission formation process and even engine knock phenomenon. Thus computational methodology can be a valuable tool to reveal some fundamental knowledge to develop a new-generation high-efficient and low emission ICE.

In this context, multi-dimensional computational fluid dynamics of reactive flows has become an indispensable and effective tool for probing the multi-scale physicochemical processes involved such as liquid breakups, mixing, ignition and emission formation, parts of which are difficult to access in experiments [4]. Realistic chemical kinetics is an indispensable component of high-fidelity simulations for reliable prediction of near-limit flame phenomena and emissions in multi-dimensional engine simulations. It was found in [5] that small concentrations of very reactive chemical species such as nitric oxide (NO_x) have a very important impact

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on the onset of combustion, which may lead to irregular combustion phenomena and greatly affect the emissions. Therefore, the use of detailed chemistry is becoming a fundamental prerequisite for advanced engine simulations.

With detailed chemical kinetics being employed in IC engine simulations, the major computational challenge is the time-intensive nature of integrating chemical kinetics due to the large number of chemical species and wide range of chemical timescales involved, which may account for more than 90% of the overall simulation time [6,7]. Over the past, significant progress has been made to reduce the computational cost of detailed chemistry in engine combustion simulations [8–12]. These include:

- The development of skeletal or reduced mechanisms from large detailed mechanisms. A skeletal mechanism consists of a selected subset of species and reactions from the detailed mechanism, and is applicable to within certain accuracy, over a broad range (e.g., comparable to that of the detailed mechanism) of pressure, temperature and equivalence ratio conditions. Over the past decade, sufficiently accurate skeletal or reduced mechanisms have been developed for *n*-heptane [13] and isooctane [14], primary reference fuel [15,16] and biofuels [17]. These mechanisms generally consist of tens to hundreds of species.
- Cell agglomeration methods such as multi-zone models [18,19], in which Computational cells with similar compositions, e.g. temperature and species concentration, are agglomerated into a much smaller number of zones. Each zone thus becomes representative of a group of cells in the CFD domain. Chemistry calculations are performed for zones instead of computational cells, achieving significant computational saving since the number of zones is typically less than the number of computational cells by orders of magnitude. Goldin et al. [18] proposed a dynamic hash table to efficiently bin cells into high dimensional hyper-cubes in composition space. It achieved a maximum speed up factor of 6.5 for an axisymmetric partially-premixed IC engine. Liang et al. [20] used a dynamic multi-zone (DMZ) partitioning scheme to improve computational efficiency with detailed chemistry. For direct-injection compression-ignition engine cases with a computational mesh containing 15,000 cells, the DMZ scheme achieved a maximum speed up factor of 20.
- Dynamic adaptive chemistry [20–23]. For each CFD cell/particle, only a small subset of species and reactions in the full mechanism are retained to capture the dominant reaction pathways for each local thermochemical condition. It accelerates the time-integration of chemical kinetics by approximating the unimportant species to be chemically frozen and solving only the non-trivial ODEs governing the retained species together with mixture sensible enthalpy. DAC has been successfully demonstrated in multi-dimensional (unsteady) RANS simulations of turbulent combustion processes in internal combustion engines [8,9,24].
- Storage retrieval methods such a in situ adaptive tabulation (ISAT) [25,26] and database for online function approximation (DOLFA) [27]. In these methods, combustion chemistry computations are tabulated and are used to build inexpensive approximate solutions at a later stage of computation to reduce the overall cost. By tabulating solution to ordinary differential equations (ODEs) system governing chemical kinetics and reusing it, ISAT can substantially reduce the number of direct chemical kinetic integrations and significantly speedup the chemistry calculations. The computational efficiency of the ISAT algorithm is higher when the tabulated information can be re-used more frequently. For instance, speedup factors of 100–1000 can be achieved using ISAT for statistically stationary reactive flows [28].
- Dimension reduction methods. This method is based on the fact that chemical systems include reactions with a wide range of time scales. Consequently, reaction trajectories are attracted to lower-dimensional attracting manifolds in the composition space. Chemistry reaction calculation can be performed in a reduced space by identifying such low-dimensional manifolds, therefore the overall computational cost is reduced. In terms of this idea, two important milestones are the method of intrinsic low-dimensional manifolds (ILDM) [29] and computational singular perturbation (CSP) [30]. Based on the two methods, trajectory-generated low dimensional manifolds (TGLDM) [31], invariant constrained equilibrium-edge pre-image curve (ICE-PIC) [32] and level of importance (LOI) [33]. Another important method of rate controlled constrained equilibrium (RCCE) [34,35] is recently re-used.

In fact, in order to largely improve computational efficiency the above available methodologies can be used in combination to further reduce the computational cost significantly. The results by Zhou and Ren [9,24,36] show that the DAC method can efficiently speed up the calculation about 2 times in a realistic liquid spray and combustion process even using the already reduced chemistry mechanism by DRG method. Liang et al. [37] combined the DAC method and dynamic cell clustering (DCC) to simulate a realistic combustion process using realistic chemical kinetics in a diesel engine. They obtained a speed up factor of 11 in chemistry solution time and 6 in overall computational time with a 36 species mechanism. As a high-efficient and accurate method, the combined use of ISAT and DAC (TDAC) was proposed [38] for highly efficient IC engine simulations with detailed chemistry. A speed-up factor of hundreds to thousands was reported in subsequent simple IC engine simulations with accurate predictions of species concentration, heat release and emission profiles. This method has showed the greatest potential to improve the computational efficient in simply case. However, the TDAC method with extreme high speed up factor didn't consider the composition inhomogeneity, in recent study [39] the overall speed up factor of using TDAC in a heavy-duty diesel engine is only about 1.2 with 106 species and 420 reactions. Thus, the effect of compositions inhomogeneity on chemistry acceleration need be addressed. Actually, the performance of ISAT in this circumstance is a big challenge.

ISAT algorithm was originally developed for constant-pressure, statistically stationary systems (e.g. turbulent jet flames) with small or moderate sized chemical mechanisms. However, the engine application is transient (time-varying pressure) with complicated thermodynamic conditions. Transient characteristics and detailed chemical mechanisms significantly hinder the performance of ISAT, because: 1. The performance of ISAT deteriorates when the accessed composition space keeps on changing such that the pre-tabulated entries can rarely be re-used, e.g., when simulating the transient auto-ignition processes in compression ignition engines. Specific improvements such as a cleaning strategy for infrequently accessed tabulated points [40] have been proposed to improve the ISAT efficiency. 2. ISAT storage requirement and the retrieval time scale with n_s^2, which is significant for large mechanisms e.g., more than 50 species.

In previous study [41], it concluded that the computational efficiency becomes very low close to that with full mechanism due to temperature inhomogeneity at high temperature stage and post-combustion stage for ISAT. Therefore, the object of this work is to enhance the ISAT performance for transient combustion simulations for both premixed and non-premixed combustion process. In this work, dynamic pruning (DP) strategy for not-frequently-accessed tabulated points have been employed and investigated in homogenous charged compression ignition (HCCI) combustion