Parallel Chemistry Acceleration Algorithm with Table Size Control Method for Gaseous Detonation Simulations

Wu Jintao, Dong Gang
National Key Laboratory of Transient Physics, Nanjing University of Science and Technology
Nanjing 210094, Jiangsu, China

1 Introduction

In the chemically reacting flow computations with the detailed reaction mechanism, the characteristic timescales among chemical species are extremely different between each other [1]. This leads to the serious stiffness of chemical source term and further causes the expensive computational costs when the term is directly integrated. In order to solve this problem, different types of storage/retrieval algorithms based on tabulation method are proposed. Among them, an ISAT (in *situ* adaptive tabulation) technique [2] constructs a data table for the implementation of various table operations including query, insertion and retrieval. As a result, the time-consuming processes of direct integrations (DI) in the reaction mapping are replaced by the time-saving processes of table operations. Subsequently, the ISAT technique is then widely applied in different computations of chemically reacting flows and is further developed into a parallel version [3]. However, the acceleration performance of ISAT technique (either in serial or parallel version) strongly depends on the specific physical problems. In the computations of steady combustion problems with low Mach number flows, the speedup ratio of ISAT is excellent. As for the computations of transient flows with high Mach number, the speedup ratio of ISAT is not so good, because a large number of data in table(s) may not be successfully retrieved due to the rapid change of thermodynamic states within each time-step. Furthermore, reduction on the retrieval possibility of data nodes in table(s) means that a lot of new data nodes have to be inserted into the table and thus give rise to the excessive growth of table size, which may further reach the upper limit of computer memory. Therefore, Dong et al. developed a dynamic storage/deletion method [4, 5] based on the reduced ISAT technique to maintain the table size in serial computations of two-dimensional gaseous detonation simulation. Based on this method, several parallel chemistry acceleration algorithms are proposed in our recent work [6] and all of them are examined to be accurate and efficient in detonation computations. In this paper, one of the parallel algorithms named TP/DEP is selected and combined with an innovative table size control method in the applications of gaseous detonation simulations. The effects of table size on both the computational efficiency and accuracy are studied.

2 Numerical Methods

Correspondence to: Dong Gang, dgvehicle@yahoo.com

The time-dependent, compressible, reactive Euler equations with detailed mechanism are employed to the simulations of two-dimensional $2H_2+O_2$ gaseous detonation propagation. A splitting algorithm is used to decouple the solutions of convection term and chemical source term. A 9th-order WENO (weighted essentially non-oscillatory) scheme [7, 8] is adopted to solve the inviscid fluxes and the parallel chemistry acceleration algorithm with the table size control method is proposed to approximate the chemical reactions. In present study, a detailed H_2/O_2 chemical reaction mechanism [9] is used to represent the combustion process.

The selected parallel chemistry acceleration algorithm is combined between two different parallel strategies [6] namely TP (Transposed Processing) and DEP (Data Exchange Processing), as shown in Fig. 1. For the TP strategy shown in Fig. 1(a), each data table (T_1-T_n) handles the data collected from the data blocks of the same position of different sub-zones (S_1-S_n), in order to keep the load balance among the table operations. In this strategy, the data blocks are reorganized into the transposed sub-zones which have the similar distributions of thermodynamic states that tables are mapped in. Note that the TP strategy is different from the PLP (Purely Local Processing) strategy proposed by Lu et al. [3], in which the data table is built on each parallel sub-zone locally, the table operations (chemical computations) can only be executed in its own table and there is no data passing among the tables that belong to different sub-zones. Furthermore, a DEP strategy that further improves the load balance among the table operations is proposed, as illustrated in Fig. 1(b). In this strategy, we first record the accumulated CPU times (wall-clock times) cost by table operations for each table before current time-step. Then, a half of data in the table with maximum wall-clock time (T_{max} in Fig. 1b) is exchanged with that in the table with minimum wall-clock time (T_{min} in Fig. 1b) through the data exchange among both tables. Similarly, such exchange process is executed between the table with second-maximum wall-clock time and the table with second-minimum wall-clock time simultaneously, and so on. Once all table operations are completed within current time-step, the exchanged data are transmitted back to their own tables. Lastly, the accumulated wall-clock times for all tables are recorded again and the new data exchanges are executed again within the next time-step. The purpose of this strategy is to keep the equal data size for different tables, besides the improvement of load balance among table operations. In summary, the procedure of TP/DEP algorithm with table size control method can be briefly described as follows, the details of the algorithm can be found in ref. [6].

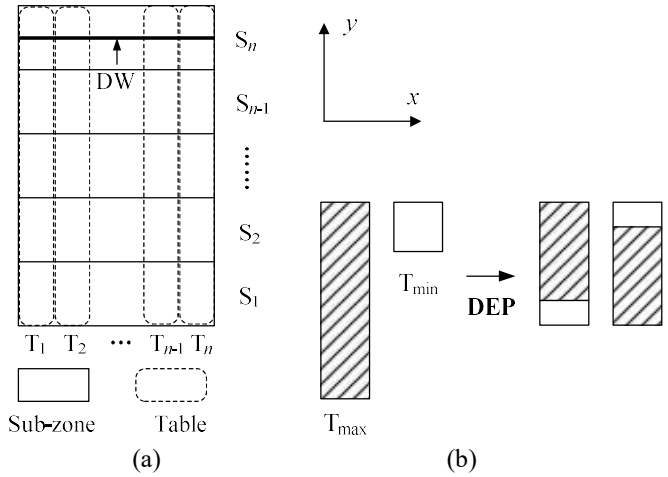

Figure 1. Parallel strategies (T- table, S – sub-zone). (a) TP strategy, (b) DEP strategy

(1) The empty tables are initially constituted in computer memory with the same number as the sub-zones of computational domain.

(2) The TP strategy is adopted to set up one-to-one mapping between an empty table and the transposed data resulted from data blocks of sub-zones, see Fig. 1(a).

(3) For each table, the stiffness ODE solver is used to solve the chemical reactions of the first node within one time-step and then stores the results (chemically thermodynamic states) in the table.

(4) A query process is executed for the inserted nodes. Once the queried data fall into the error range of a node, the data in this node can be retrieved from the table and used in computations of the next time-step.

(5) If the query process fails, a direct integration (DI) method by using the stiffness ODE solver is used to obtain the new data. Meanwhile, a node whose data are closest to the new data is searched. If the difference between the searched node and the new node is less than an error tolerance ε_{tol}, the error range of data on the searched node is then enlarged, else the new data are inserted into the table as another node.

(6) Repeating the steps (4) and (5) within one time-step of simulations. Once the time-step is completed, the DEP strategy is employed to carry out data exchanges between the different tables (see Fig. 1b) for the use of the next time-step.

(7) The ISAT table size (number of nodes in a table) control method for the parallel computation is employed to avoid the over-growth of data tables. The method is composed by two controlling factors, namely single table size (M_{sin}) control and total table size (M_{tot}) control. For the M_{sin} control, a nodal deletion operation [6] for the single table is activated when the size of this table reaches M_{sin}; while for the M_{tot} control, the nodal deletion operation is performed for every table only if the total size of all tables reaches M_{tot}.

In above procedure, a data structure named balanced binary tree (BBT) is adopted to construct the data table. The typical table operations in present study include the processes of query, retrieval, insertion, enlargement and deletion of nodes in the table, in which the processes of query and insertion are processed by a global traversal method, while the deletion process is carried out by a non-recursive traversal method.

3 Results and Discussions

Gaseous detonation is one of the typically transient compressible reacting flows. In order to identify the performance of the parallel TP/DEP algorithm with ISAT table size control method, we carried out the 2D numerical simulations of $2H_2+O_2$ gaseous detonation wave propagation. Figure 2 gives the schematic of the computational configuration. The computational domain is a rectangle with $L_x \times L_y$ = 3mm×9mm, and is covered by square grids with size of $\Delta x=\Delta y$=0.01 mm. Such mesh size corresponds about 24 grids in half reaction zone length of $2H_2+O_2$ detonation and is sufficient to describe the structures of detonation wave. The zero gradient condition is used for the top and bottom boundaries of the domain in y direction, while the left and right boundaries along x direction are the adiabatic slip rigid wall condition. In addition, we adopt a moving computational domain along the direction of detonation wave propagation. Such motion of the domain ensures enough long distance for the propagation of detonation wave in y direction. Initially, a ZND detonation of $2H_2+O_2$ premixed gases is set within the region of y = 0-3 mm (see the gray part of the computational domain in Fig.2), and the $2H_2+O_2$ premixed gases with initial temperature T_0=300K and initial pressure p_0=1atm are placed in the rest part of the domain. Moreover, a small disturbance area with high pressure of $38p_0$ is placed on the location just above the ZND region to form a cellular detonation rapidly. Considering the non-physics of disturbance, only the results during the quasi-steady propagation (time-step=18,000-28,000), in which the disturbance goes completely out of the domain, are processed and

analyzed. Our previous work [6] has proved that the computational efficiency of the parallel algorithm is not influenced by the non-physical process, thus, we can only discuss the quasi-steady propagation of detonation wave in present study. For the purpose of parallel computations, the entire domain is divided into 15 sub-zones with the same size along y direction, as shown in Fig. 1(a).

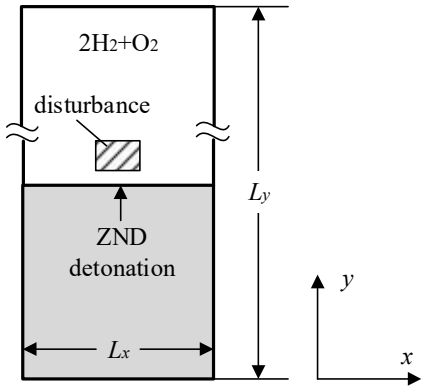

Figure 2. Computational setup

Our previous work [10] has discussed the relationship between the total table size and the single table size, besides their influences on the computational efficiency of the parallel chemistry acceleration algorithm. In present study, we presented five computational cases with different values of M_{tot}, as shown in Table 1, in which the emphasis is placed on the effect of the total table size to the speedup performance of our algorithm. The single table size is fixed to $M_{sin}=9.0\times10^6$. The error tolerance ε_{tol} is set to 1.0×10^{-3} for all of these cases in Table 1.

Table 1: Different computational cases with $M_{sin}=9.0\times10^6$

Case	1	2	3	4	5
M_{tot} ($\times10^6$)	27.0	45.0	63.0	81.0	99.0
R_s	3.243	4.292	5.515	3.934	4.756
σ_f	1.765	0.724	0.516	0.743	0.617
p	2.732	2.538	2.297	3.466	3.479

Figure 3 shows the speedup ratios R_s of all cases in Table 1 at time-step=28,000. Here R_s is defined as a ratio of wall-clock time cost by DI computation to the wall-clock time cost by present algorithm. Basically, larger M_{tot} provides larger memory space for the tables and is more beneficial for higher R_s. However, if M_{tot} continuously increases, a part of tables can reach the M_{sin} but another part cannot. This means that deletion events in all tables are occurred asynchronously and large amount of times will be wasted on waiting for each other. Thus, there is a stage of decrease on R_s after $M_{tot}=63.0\times10^6$. It is interesting that further increasing M_{tot} can give rise to the re-growth of R_s. In fact, the very large M_{tot} becomes useless in controlling the table size and thus the M_{sin} starts to play a leading role. Since the single table size we set in present study is large enough, almost all tables have less than one time of deletion event during the entire computation. Such small number of deletion events is not enough to destroy the load balance among table operations and thus increases the speedup ratio again. At the last time-step, the maximum speedup ratio of 5.515 is obtained for case 3 with $M_{tot}=63.0\times10^6$, as shown in Table 1.

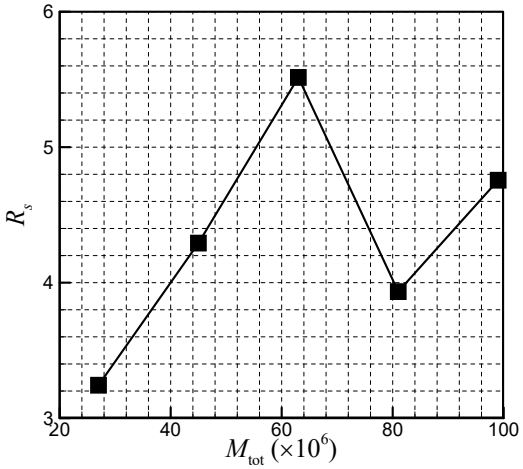

Figure 3. Speedup ratios of all cases by the parallel TP/DEP algorithm with ISAT table size control method

To further investigate the effect of M_{tot} on the speedup performance of the algorithm, we define a standard deviation of the nodal deletion frequency of the tables, σ_f, and a time utilization rate, p, to character the load balance and synchronization among table operations, respectively. The smaller σ_f and p mean the better load balance and synchronization that feature the better speedup performance. Table 1 lists both parameters for all cases at the last time-step. It can be found that minimum σ_f and p correspond the maximum R_s for case 3. Figure 4 presents the correlations between R_s and σ_f, and between the R_s and p, respectively, for all cases by the power fit method. It can be seen from Fig. 4(a) that a good correlation with correlated coefficient R^2=0.8464 between R_s and σ_f can be obtained, which suggests the load balance denoted by σ_f has important effect on the computational efficiency. However, Fig. 4(b) shows a poor correlation between R_s and p with R^2=0.0930 which implies synchronization plays an unimportant role. Note that the deletion frequencies of the tables are relatively small for all cases of present study, thus the synchronization among the deletion events is not obvious. When the frequent deletion events occurs during the computations, the effect of synchronization on the speedup still needs to be investigated.

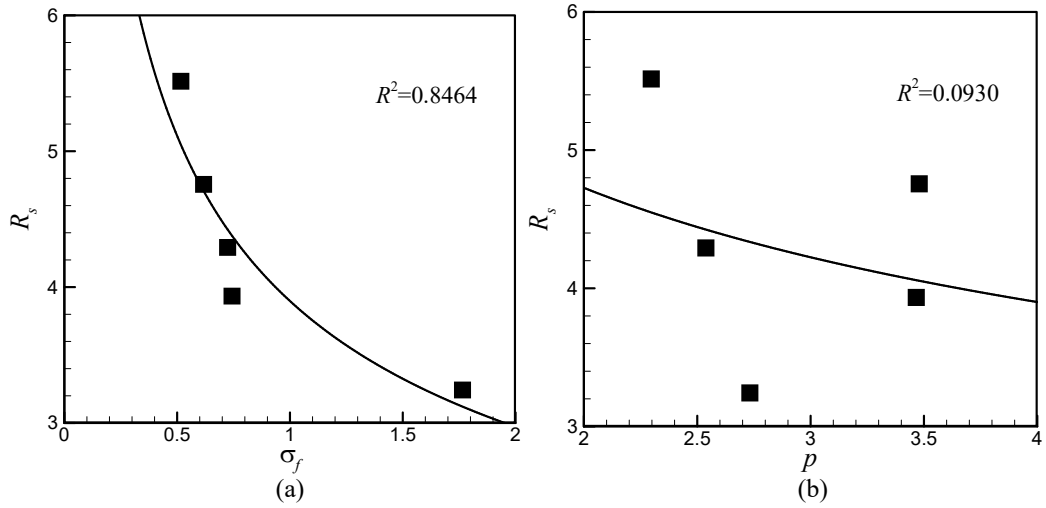

Figure 4. Correlations between (a) σ_f and R_s and (b) p and R_s

Lastly, we examine the computational accuracy of the algorithm, by examining the mean pressure and the mean H_2O_2 mass fraction along with the motion direction of detonation wave and the relative errors of propagating speed of detonation wave between the calculated value and the theoretical C-J one during the entire simulations, as shown in Fig. 5(a) and 5(b), respectively. It can be found that the pressure and H_2O_2 by the algorithm show good agreements with those by the DI method for all cases, while the relative errors of propagating speed of the detonation wave for all cases are less than 0.5%. The results indicate that the algorithm in present study can meet the requirement of computational accuracy.

4 Summary

For the purpose of chemistry acceleration in the parallel computations of transient, compressible and reacting flows, a TP/DEP algorithm enhanced with ISAT table size control method is proposed and applied in the numerical simulations of two-dimensional gaseous detonation wave propagation. The effect of total size control of all tables on the computational efficiency and accuracy was investigated. The results show that chemical speedup ratios of all case in present study are ranged between 3.2 and 5.2. The total size of ISAT tables has an obvious influence on the computational efficiency (chemical speedup ratio). The appropriate choice of the table size can keep the favorable load balance among table operations and thus accelerate the chemistry computations of gaseous detonation simulations, without the loss of computational accuracy. This work is supported by the Natural Scientific Foundation of China under grant No. 11872213.

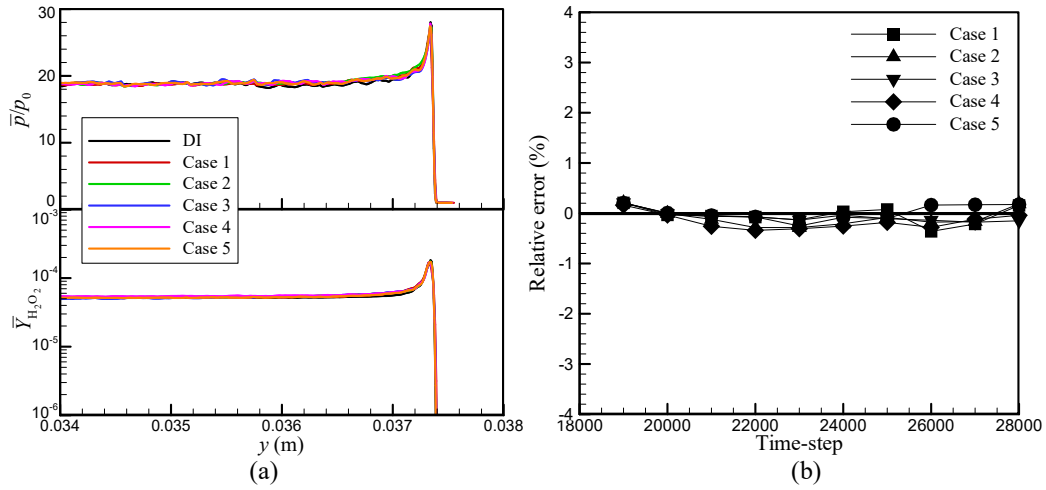

Figure 5. (a) Mean pressure and H_2O_2 mass fraction profiles and (b) the relative errors of mean propagating speed of detonation waves to theoretical C-J value for all cases by the TP/DEP algorithm with table size control method

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