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CFD Parallel Computing Technology for Chemical Non-Equilibrium Flow Based on Large Scale Linear Algebraic Equations

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The purpose of this study is to understand the operation mode of computational fluid dynamics (CFD) parallel computing technology for non-equilibrium flow. To this end, this paper mainly studies the flow field of supersonic ramjet engine (Scramjet). Through simulation of various component equations, chemical non-equilibrium effects, turbulence equations and transport coefficients, etc., it also studies the CFD parallel calculation by simulating the flow field of the scramjet. Innovative insights were put forward for each aspect, and the three-dimensional massively parallel software platform AHL3D oriented to chemical non-equilibrium flow mainly used in the simulation of the flow field of the scramjet engine was developed. Finally, it realizes the multi-block parallel computing for docking grid, the misaligned splicing grid and the overset grid. This algorithm has better robustness, simple implementation, and also low computational complexity, high computational efficiency and high application value.

1. Introduction

Computational Fluid Dynamics (CFD) is an algorithm that combines computer programs to numerically simulate and calculate fluid flow dynamics. It has achieved excellent results in previous applications. In theory, tCFD calculation needs to be combined with other numerical equations, such as the Euler equation for the motion law of the fluid, and the NS equation, etc. Then, these equations are solved by the numerical calculation method of CFD, and the fluid motion characteristics can be studied to obtain the temporal and spatial flow law of the fluid.
In order to understand the CFD algorithm, combined with the flow field study of the scramjet engine, this paper is based on the simulation scene for parallel computing. This idea also appeared in previous studies, as one of the sub-subjects in the integrated design technology of the 863 hypersonic aircraft body/propulsion system. To be specific, the main goal of this research idea is to establish an integrated, universal, powerful CFD massively parallel software system for chemical non-equilibrium flow, which is mainly applied to the flow field simulation of a scramjet.

2. Literature review

In order to obtain performance data quickly and accurately in the design stage of the scramjet engine, a large number of engineering and numerical simulation analysis software have been developed at home and abroad. Among them, the National Aeronautics and Space Administration's software is the most representative. These softwares are powerful, comprehensive, and have a wide range of calculations. The following is a brief introduction to the domestic and international research on the flow field simulation software of the scramjet engine.
The GASP (General Aerothermodynamic Simulation Program) software was developed by AeroSoft Corporation of the United States since the early 1990s under the auspices of NASA's SBIR fund. The latest version 4.2.2 was released in April 2005. According to the AeroSoft website, the GASP software has become the standard for NASA outflow computing. GASP uses a finite volume method (Alpak et al., 2016). The Euler equation, the space-propagating PNS equation, the thin-layer approximate N-S equation, the all-N-S equation,

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and the incompressible N-S equation can be calculated. Ideal gases, chemically unbalanced flows, thermochemically unbalanced flows, balanced flows, and frozen flows can be simulated. One-dimensional, two-dimensional/axis-symmetric, three-dimensional steady or unsteady flow can be solved. In order to solve the computational problems of complex systems, GASP software supports multiple docking grids, overlapping grids and misaligned stitching grids (Garicano-Mena et al., 2018).

GASP implements parallel computing using MPI and supports automatic region decomposition and artificial region decomposition. The "burrowing" of overlapping grids and the search of interpolation templates can be operated in parallel. Semi-automatic load balancing is supported. Load balancing takes into account the difference in processor speed and does not take into account the difference in computational complexity of different regions due to the use of different equations and time-propulsion algorithms (Jo et al., 2018). Cockrell used the GASP software to calculate the X-43A (including inflow). In terms of integral force and moment, surface pressure, the results are consistent with the results of wind tunnel experiments. GASP software is also heavily used for engine performance studies.

The VULCAN (Viscous Upwind Algorithm for Complex Flow Analysis) software was developed by the Hyperpersonic Airbreathing Propulsion Branch of the NASA Langley Research Center in the United States. The latest version 5.0.3 was released in January 2006. VULCAN is considered by NASA to be a standard for simulating the in-flow characteristics of high-speed propulsion equipment. VULCAN uses the lattice finite volume method (Kone et al., 2017). The three-dimensional turbulent reaction flow equations (including Euler equation, space-propulsion PNS equation, thin-layer approximate N-S equation, and all-N-S equation) that are spatially elliptical and parabolic can be calculated. Ideal gas, chemically unbalanced flow, and frozen flow can be simulated. Two-dimensional/axisymmetric, three-dimensional steady or unsteady flow can be solved. In order to solve the computational problems of complex systems, VULCAN software supports multiple docking grids and misaligned stitching grids (Modirkhazeni and Trelles, 2018).

VULCAN uses MPI to achieve parallel computing. VULCAN supports automatic load balancing. However, it only considers the difference in the total number of grids for different processors to be minimal, and does not seem to consider the overhead of communication. VULCAN supports parallel input and output operations. In addition, VULCAN has two communication modes. One is the standard communication mode, and the other is the cache communication mode (Scanlon et al., 2015). The former is generally used, but the latter is more advantageous when the amount of information is particularly large. VULCAN is widely used in the research of scramjet engines. Examples of applications published on its webpage include two-dimensional compression corners, nozzles, grooves, three-dimensional turbulent jets, jets and mixing of helium in the combustion chamber, and jets and combustion of three-dimensional combustion chambers.

The WIND software was developed by the National Project Application-oriented Research in CFD (NPARC). The NPARC Alliance consists of NASA's Glenn Research Center, the US Air Force Arnold Engineering Research Center, and Boeing. WIND uses the grid finite volume method. The Euler equation, the PNS equation, the thin layer approximation N-S equation, and the all N-S equation can be calculated. Ideal gas, hot complete gas, equilibrium air, frozen flow, and chemically unbalanced flow can be simulated. Two-dimensional, axisymmetric, three-dimensional steady or unsteady flow can be solved. In order to solve the computational problems of complex systems, WIND software supports multiple docking grids, misaligned stitching grids and overlapping grids, which can support both structured and unstructured grids.

WIND uses PVM to implement parallel computing. Its parallel mode uses master-slave mode. WIND has two task assignment modes. The first is that each computation block corresponds to one processor. This method is efficient, but the memory consumption is high. The second is that multiple computing blocks correspond to one processor. This method has low memory consumption. However, the burden of temporary documents has increased. The area decomposition of WIND takes into account differences in processor speeds and different computation block sizes. Slater used WIND to study the inlet passage and analyzed the flow characteristics from the low subsonic speed to the hypersonic inlet, and obtained the same results as the experiment.

MSD is a numerical calculation software developed by ONERA, France. It is widely used in the hypersonic advancement projects of ONERA and MBDA (Wagnild and Gallis, 2018). The MSD uses a finite volume method. Two-dimensional, axisymmetric and three-dimensional NS equations as well as PNS equations are solved. Multi-block docking grids, overlapping grids, adaptive grids, multiple grids, and motion grids are supported. MSD uses MPI to implement parallel computing. MSD supports static load balancing. Dufour used MSD to calculate the combustion of kerosene in the super-combustion combustion chamber, and obtained the distribution of wall pressure consistent with the experimental results. Davidenko used the MSD to calculate the hydrogen combustion in the pipeline. The effects of total temperature, wall state, chemical model and turbulent Prandt1 number on hydrogen combustion were analyzed in detail. In addition to the above several important CFD software, NASA also has CFL3d software. Some companies in the United States also have CRAFT, PAB3d software. There are NSMB software in Europe. These softwares can be used to calculate some or all of the flow field of a scramjet.

These foreign softwares are beyond the reach of China. GASP software is free for companies and universities in North America. However, users outside of North America need the US government's approval to get their PDF manual. WIND software is also freely available to US companies, government agencies, and universities, but cannot be used in research by non-US companies. Foreign research on CFD parallel computing for hypersonic vehicle propulsion systems is extremely confidential. Therefore, the development of a CFD parallel computing application development platform with independent intellectual property rights is of great significance to practical application topics. In contrast, the development of domestic parallel combustion calculation software for scramjet is still in its infancy. The function is weak, the scope of application is limited, and the software system has not yet been formed. At present, various units in China have recognized the gap and are catching up. Under the leadership and organization of the former Commission of Science, Technology and Industry for National Defense and the National "863" Program Aerospace Expert Committee, China has made some progress in the parallel computing of hypersonic CFD for chemical non-equilibrium flow.

The China Aerodynamics Research and Development Center has accumulated many years of experience in CFD parallel computing for chemical non-equilibrium flows. A parallel computing software based on the PVM environment was developed. One-dimensional, two-dimensional and simple three-dimensional calculations of the combustion chamber of a bimodal ramjet can be performed. However, because the research on this problem is relatively preliminary, and the physical model and calculation method of the problem are more complicated, the software still has much room for improvement in terms of function expansion and efficiency improvement. The 31st China Aerospace Science and Industry Corporation has cooperated with Northwestern Polytechnical University and China University of Science and Technology to conduct quasi-one-dimensional flow analysis of several dual-mode ramjet combustion chambers. Two-dimensional numerical simulation studies on the structure and performance of the flow field in the model supersonic combustion chamber were carried out. With the deepening of research on super-combustion ramjet propulsion technology, countries have successively entered the ground and flight test research phase.

A large number of experimental studies have found that the engine control system is important for the normal operation of the engine. The scramjet engine is generally integrated with the hypersonic vehicle, and the engine and the aircraft are highly coupled. The scramjet engine operates over a wide range of Mach numbers, which makes the control of scramjets difficult. In order to clarify the working mechanism of the scramjet engine and the coupling relationship between the engine and the aircraft, the engine control strategy can be accurately obtained. The control system provides fuel during engine operation. The fuel is distributed to optimize the thrust performance of the engine. At the same time, the safe operation of the engine work needs to be ensured. The model study of the scramjet engine has begun from the beginning of the study of supersonic combustion. These models include studies of various supersonic flow and physical effects in combustion and studies of integrated engine models. There are many physical effects inside the scramjet engine (Wicklein et al., 2016). These physical effects affect the main characteristics and performance of the engine. For many years, scholars at home and abroad have conducted extensive research in these areas. Many models of this aspect are given.

To sum up, with the rapid development of computer technology and CFD technology, great progress has been made in the research of the working process of scramjet through two-dimensional or three-dimensional numerical simulation. In recent years, a large number of papers have been published on the numerical simulation of the flow field of a scramjet engine. These research results involve various aspects of numerical simulation of flow field, such as chemical reaction model, turbulence model, numerical simulation method and so on. Therefore, based on the original physical model and calculation method of China Aerodynamics Research and Development Center, the program was rewritten by MPI, and a new program basic framework and basic data structure were established. A three-dimensional massively parallel software platform AHL3D for chemical non-equilibrium flow, which is mainly used in the simulation of flow field simulation of scramjet engines, was developed. Multi-block parallel computing of docking grid, misaligned splicing grid and overlapping grid is realized. This algorithm is robust. The calculation efficiency is high. This method has high application value.

3. Methods

3.1 Static load balancing strategy

It' mainly dominated by the static load balancing strategy method, because static load means that the tasks assigned to each processor are fixed in the parallel computing process, and dynamic refers to dynamically adjusting the tasks of all processers according to the load balance between processors. The two have their own advantages and disadvantages: the static load balancing is simple to implement, but difficult to achieve the true load balancing, while the dynamic load balancing effect is better but the implementation is complicated with large communication overhead. Since the calculation area of most CFD problems remains unchanged throughout the calculation process, the partitioning can be pre-completed, so most of the CFD problems use the static load balancing method.

3.2 Graph theory representation of static load balancing problem

P processors are denoted by the point set U= {u1, u2, ... un} on the plan view, and the possible connection lines F= {f1, f2, ... fn} of these points are used to indicate the communication line between the nodes. If it is a homogeneous network, the parameters of each node are the same. Assuming that the message transmission capability between the processors is independent of the direction, the weight of the nodes can be omitted, with no need to consider directionality of the edges, and the correlation of the processors can be represented by the undirected graph H = (U, F) (Figure1). A parallel application is described by the weighted graph$G = (V, E, p, \sigma)$, where nodes V= {V1, V2, ... Vn}, edges E = { e1,e2,...en } $\subseteq V * V$, node weights p: V→R, edges weight $\sigma: E \rightarrow R$ (Figure2).

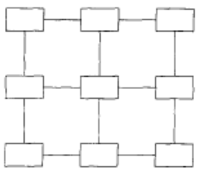

Figure 1: undirected graph representation of processor relationship

Figure 2: parallel application weighting diagram

3.3 Common static load balancing algorithm

Because this type of CFD calculation uses a structured grid, it can be partitioned along each calculated coordinate axis. The common CFD load balancing algorithm is an exploratory geometric partitioning method and greedy algorithm.

The exploratory geometric partitioning method is based on partitioning along the direction of each calculated coordinate axis. Without regard to the difference between processors, the basic idea of the algorithm is to calculate the computational overhead required for all possible processor decomposition methods, and the processor with the least overhead is the solution. The basic principle of this partitioning method considering the difference between processors is also to find the processor decomposition mode with the least computational overhead in all possible processor decomposition modes, and the calculation of the computational overhead should be adjusted according to the processor's dominant frequency. This heuristic CPU allocation method can achieve a better load balancing effect for a simple calculation area problem.

The basic idea of the greedy algorithm is to re-segment the grid blocks that are not conducive to automatic load distribution, so as to achieve load balancing. The process is: after reading the number of grid blocks and their size, determine the load size on each processor according to the number of processors; then, based on this value, re-segment the grid blocks larger than this value, and combine them into new grid blocks; finally, male automatic load distribution. This method can better distribute the load to each processor.

4. Results

4.1 Pipeline parallel technology

First of all, the parallel computing of complex computing area problems needs to be considered comprehensively in terms of processor allocation. From the perspective of pipeline parallelism, the processor allocation method of one-dimensional decomposition is more reasonable; but considering the parallel efficiency of other computing parts (rather than solving the linearization equation), based on previous studies, the processor allocation of 3D decomposition may be better, so the processor allocation method should be determined according to the characteristics of the actual problem. Secondly, since the computational area of complex computing area problem is composed of many physical blocks of different sizes and the communication relationship between blocks is very complicated, the main problems faced for the implementation of the pipeline parallel are: the number of physical blocks is large and the calculated coordinate system may be different; the data communication relationship between adjacent planes is very complicated; there may be multiple pipelines flowing simultaneously; the pipeline efficiency is low etc.

In view of the above problems, this paper carried out the correctness verification experiment of pipeline. In the experiment, Four typical calculating examples of the ball-head shock-induced combustion, the three-dimensional single-hole hydrogen lateral jet flow, a hydrogen fuel half-frame engine, and a hydrogen fuel slice were selected for parallel calculations of pipelines at different parallel scales. The first two examples gave the logarithmic density residuals of each output when the serial and CPU numbers were 32, as shown in Figure3 and4, and the latter two examples give the logarithmic density residuals with CPU number 64, respectively (Figure5 and 6), which indicates that the calculation results of different parallel scales are strictly consistent. In addition, since the three-dimensional single-hole hydrogen injection example adds the jet flow at 1000 steps, the logarithmic density residual is abruptly changed at 1000 steps.

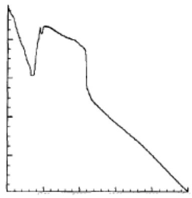

Figure 3: validation of pipeline correctness in ball head calculation

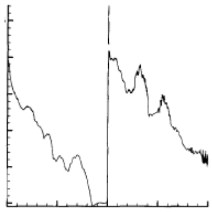

Figure 4: correctness verification of three dimensional single hole hydrogen injection calculation example

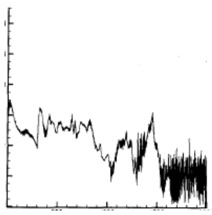

Figure 5: correctness verification of a half frame engine assembly line

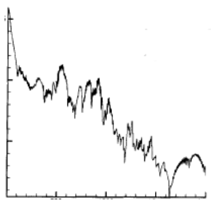

Figure 6: correctness verification of a chip engine assembly line

4.2 Correctness verification by interpolation method

Taking the two-dimensional cylindrical flow field simulation as an example, the theoretical values are given and compared, in order to verify the correctness of the inverse distance weighted interpolation method and the bilinear interpolation method based on the type function. It can be seen from the results that there exists the overlapping areas, indicating the effectiveness of both interpolation methods.

5. Conclusions

The methods proposed in this paper have been verified by practical calculation examples. The experimental results show that the overset grid preprocessing technique can still achieve better efficiency for large grid data volume, multi-level nested overlap and complex computing area problems. However, in the actual flow field calculation, we often encounter a type of overset grid problems with hollow graphics. Therefore, in the overlapping grid preprocessing method, we should consider not only the general problem of the main grid hole-cutting, but also some special cases that need to dig holes. So, it's necessary to automatically preprocess the problem of overset grid with the hollow graphics and adapt to the flow field calculation for the complex shape of the overset grid described above.

In the subsequent research, the importance should be attached to the load balancing problem caused by the communication and computational irregularities in the parallel computing of overset grid problem. The overset grid load balancing problem is one of the keys to improve the parallel computing efficiency of overlapping grids, and also be the main problem that needs to be solved during the pre-processing. In general, the algorithm has been verified in this paper, and the specific application method of the algorithm is known.

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