

Technical Paper

**High performance parallel computing for
Computational Fluid Dynamics (CFD) – Second Report**

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Aerodynamic characteristics of spherical objects assuming flying objects in an explosion were calculated by Computational Fluid Dynamics (CFD) using a parallel computer that is equipped with InfiniBand as a high-speed communication system and that can use a maximum 32 CPUs. CFD++ is general purpose CFD software to solve three-dimensional Navier-Stokes equations that represent characteristic of fluid viscosity and compressibility by using finite volume method. InfiniBand is effective in the calculations of aerodynamic characteristics by CFD. The calculation time could be shortened by a maximum of about five times compared with conventional communication systems. And also “CFD++” was used in analyzing the propagation of air blasts and was found that the TVD scheme was effective in forecasting the propagation of air blasts in comparison with experimental values.

Key Words: *CFD, parallel computer, TOP500, National Institute for Advanced Industrial Science and Technology, supercomputer, personal computer, scalability, CFD++, Linux, CPU, InfiniBand*

1. Introduction

Consideration for safety of storage of gunpowder and similar has recently become a worldwide problem for businesses handling them. Because of their properties, strict and safe management of gunpowder and similar is obligated by law and they are in many cases stored in one place. Forecasting the impact range by the air blast of an explosion and flying objects of shattered particles in the case of an explosion of them by accident is important in the design of storage sheds for gunpowder and nearby safety environments. A variety of data on gunpowder explosion is collected through explosion tests. However, in Japan, due to areas required for test sites, the amount of gunpowder that can be handled is limited to about several tens of kilograms and tests for explosions of gunpowder of 100 kg to several tens of tons cannot be made. For this reason, forecasts of explosion condition by large amounts of gunpowder based on test data on small amounts of gunpowder are needed.

Numerical simulation by a computer is used recently in such forecasts of explosion condition. However, the number of meshes becomes very large, ranging from several millions to several tens of millions depending on the test scale due to the

necessity of splitting spatial meshes, aside from the problem of numerical modeling of physical phenomena. Calculation time of several tens to several hundreds of hours is therefore needed for a computer, which is normally available, to calculate. In reality, calculations of explosion condition are mostly difficult. In general, calculations of such a large number of meshes are made and calculation time is shortened by splitting calculation domains and by allocating divided calculation domains to computers connected in parallel. The First Report on this research program reported that parallel computing technology was effective in aerodynamic calculations in computational fluid dynamics (CFD) and that a significant reduction in calculation time was achieved¹⁾. In this Second Report of the research program, the effectiveness of the parallel computing performance of the newly used high-speed communication system “InfiniBand” and results of application of CFD to analysis of propagation of air blasts during explosions achieved in joint research between the Research Core for Explosion Safety of the National Institute for Advanced Industrial Science and Technology are reported.

2. Parallel Computer

A full view of the parallel computer used in this research (“KHPC”) is shown in **Fig. 1** and the configuration of the KHPC is presented in **Table 1**. The KHPC is the prototype computer reported in the First Report plus 16 CPUs (8 nodes) capable of performing parallel calculations of a larger model. A simple increase in the number of CPUs in the use of the Gigabit Ethernet as a network system would greatly impact the communication speed and would cause a communication delay (latency), significantly increasing the overall calculation time. InfiniBand (manufactured by Silverstorm) with low latency and capable of transmitting a large volume of data at high speed was therefore added as a high-speed communication system.

As mentioned in the First Report, the throughputs of super-computers are increasing in logarithmic proportion to generations between the second half of the 1970s and the present. The world’s fastest computer measured by the benchmark software HPL (High-performance Linpack Benchmark) specified by TOP500 is Blue Gene (280TFLOPS, 131,072 CPUs) manufactured by IBM and used in the Lawrence Livermore National Research Institute of the U. S. Department of Energy. (Source: TOP500 ranking as of June 2007) The throughput of the KHPC measured by the same benchmark software was found to be equal to Supercomputer CM-5 (manufactured by Thinking Machines, 1,024 CPUs) about ten years ago.



Fig. 1 Full view of parallel computer KHPC

Table 1 Configuration of parallel computer KHPC

CPU	AMD Opteron 2.2GHz (64bit)
CPUs	32 (16 nodes)
Hard disk	For data storage, 1.5 Tbytes (RAID 5)
Network	Gigabit Ethernet, Infiniband
OS*1	Linux (64-bit version)

*1: "Operating system"

3. CFD Software

The CFD code used in this research program is “CFD++” (CFD Plus Plus) reported in the First Report. “CFD++” is general-purpose CFD software sold on the market developed by Metacomp of the United States mainly targeting the aerospace industry.

The TVD scheme disperses three-dimensional Navier-Stokes equations containing viscosity and compressibility based on the finite volume method^{2, 3, 4, 5, 6, 7}. Several types of turbulent models can be selected including the k-ε model. For this reason, the model can be used in a wide range of Mach and Re numbers from subsonic to supersonic speeds. In this research program also, aerodynamic calculations of flying objects and simulation of explosion phenomena were performed by the same software package. The Intel 32-bit version and AMD 64-bit version are now available for parallel processing and with fast communication systems such as InfiniBand and Myrinet.

4. Parallel Calculation Performance of High-speed Communication System “InfiniBand”

The parallel calculation performance of the newly used high-speed communication system “InfiniBand” was studied using “CFD++.”

Fig. 2 shows the calculation model that was used as a benchmark test model for the parallel calculation performance. The calculation model is the same model as that used in studying the effectiveness of the high-speed communication system Myrinet in the First Report. The calculations were made assuming the conditions under which flying objects would fly on the ground (pressure 101.325 Pa, temperature 288.15 K, air density 1.225 kg/m³) at Mach 3.0.

The relationship among the communication system, number of CPUs, and calculation time is plotted in **Fig. 3**. The calculation time with Gigabit Ethernet, which is normally used, can be shortened up to 16 CPUs. However, the calculation time conversely lengthens if the number of CPUs is increased to 32 CPUs. As long as the number of CPUs with Gigabit Ethernet is small, the problem scale per CPU is large and the impact of network communication on the overall processing time (communication speed and latency [communication delay] speed) is small. However, as the number of CPUs increases and the problem scale per CPU decreases, the impact by network communication on the overall processing time gradually increases, lengthening the calculation time. Compared with this, the communication speed of InfiniBand is fast and its latency speed is low so that the impact of network communication on the overall processing time decreases and the calculation speed increases as more CPUs are installed. This explains that the high-speed communication system InfiniBand is very effective in reducing the calculation time.

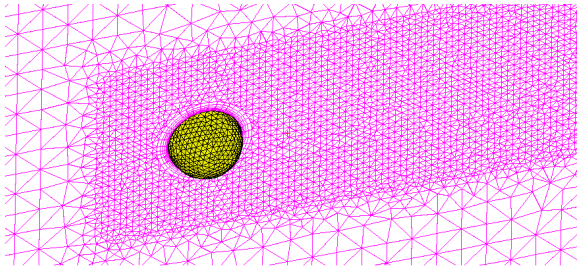


Fig. 2 Aerodynamic calculation model for flying objects

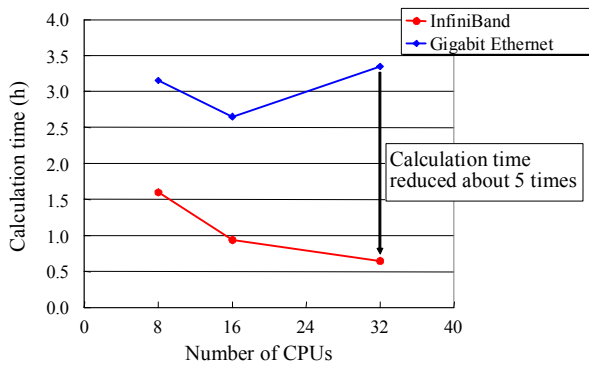


Fig. 3 Relationship among the communication system, number of CPUs, and calculation time

5. Analysis of Air Blast Propagation

This research program studies two problems in the safety of explosions. One problem is that of the aerodynamic characteristics of flying objects studied in the First Report, “How far would flying objects in an explosion fly?” The other problem is that of air blast propagation, “What impact would an air blast have around it in an explosion?” This chapter studies the following two matters using CFD++ and describes the results of the studies.

- (1) Status of air blast propagation
- (2) Comparison of numerical calculation data and bibliographic numeric data

5.1 Calculation Conditions

The entire diagram of a calculation model space is illustrated in Fig. 4. The space in the neighborhood of an explosion source is shown in Fig. 5. A high-pressure air source equal to 7.5 kg of TNT gunpowder was installed 18 cm above the ground surface as an explosion source. Air blast observation points were installed at a height of 1 m from the explosion source at distances (scaled distances) of 1-, 2-, 3-, and 4-m radius from the explosion source to evaluate propagating air blasts, in order to calculate time variations of air blast pressure. Air blast pressure by the explosion of an explosive can be evaluated using scaled distance R_s based on the relationship between distance and mass that provides the same air blast

pressure called Hopkinson’s Law (cubic root law)⁸⁾. Scaled distance R_s can be calculated by the following formula:

$$R_s = \frac{R}{M^{(1/3)}}$$

Where R_s is a scaled distance, R , the distance from the explosion center, and M , the dosage equivalent to TNT gunpowder. The relationship between a real distance and scaled distance under the conditions used in this research program is shown in Table 2.

The calculation space has its origin in the center of the explosion, covering a range of 0 to 18 m in the x and z directions and -0.18 to 17.82 m (the height from the ground surface to the top side of the boundary is 18 m) in the y direction. Two planes, the xy plane and the yz plane, are provided as spatially symmetrical planes. The boundary condition for the ground surface is slip and that for other surfaces is flow-out.

The space is a cuboid and the space inside the cuboid is divided by hexagonal meshes. Deformation of the hexagonal meshes becomes prominent near the outer periphery of a cylindrical space. However, the outer periphery is a domain that is adequately outside the points of measurement of air blast pressure, which are the target of evaluation, and impacts by mesh distortion are small. The space near the explosion source is divided so that it represents an equally spaced orthogonal grid of 6.5 cm on one side. As a result, the total number of cell used in the calculations is about 10 million meshes.

Basically, pressure P and temperature T are used in CFD++ as independent variables. For this reason, assuming an isochoric explosion, $P = 2.8$ GPa and $T = 5982$ K are set for the high-pressure air source and $P = 100$ kPa and $T = 290.8$ K are set for the peripheral atmosphere.

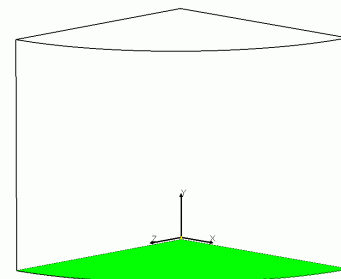


Fig. 4 Entire calculation space

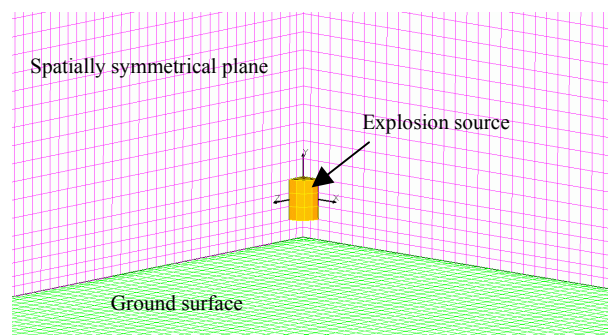


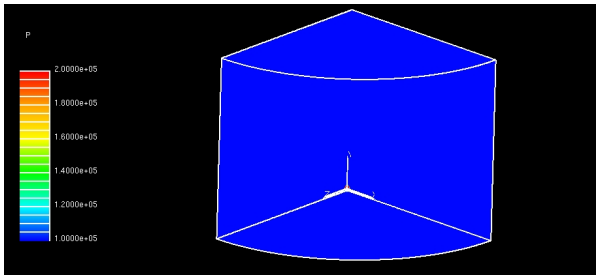
Fig. 5 Near the explosion source in the calculation space

Table 2 Relationship between real distance and scaled distance

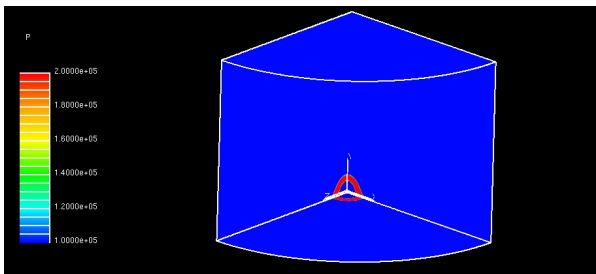
Real distance m	Scaled distance m/kg ^(1/3)
1.95	1.00
3.91	2.00
5.86	3.00
7.82	4.00
10.00	5.12
15.00	7.67
18.00	9.21

5.2 Calculation Results

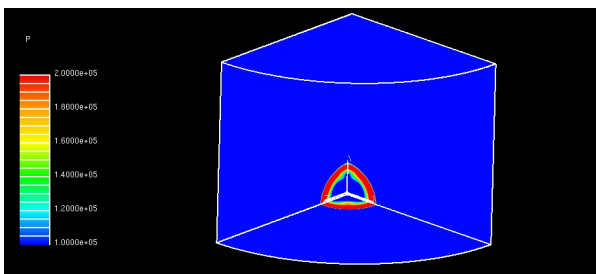
As a simulation result, the propagating behavior of an air blast visualized by a pressure value is shown in **Fig. 6**. An air blast spreading hemispherically from the explosion source soon collides with the ground surface and propagates in the space maintaining relatively high pressure even though the pressure decreases with distance. Trailing the air blast that spreads into the air, reflection waves from the ground surface also spread into the air.



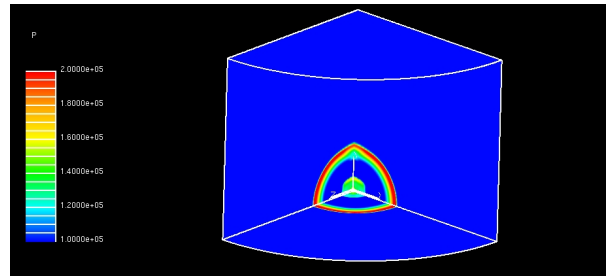
(1) Time t = 0.027 ms



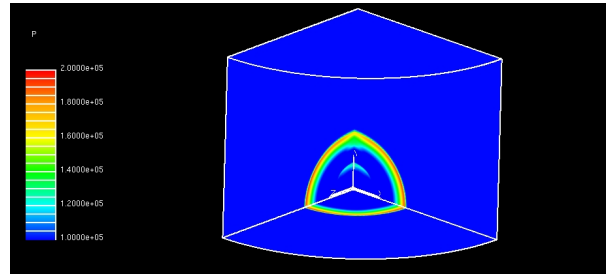
(2) Time t = 0.520 ms



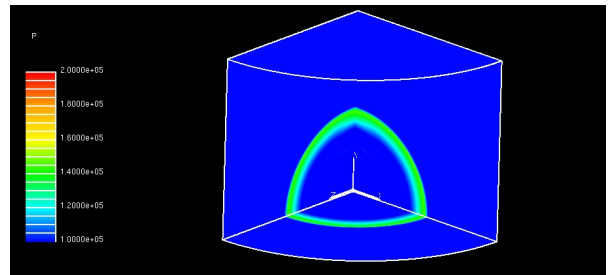
(3) Time t = 1.993 ms



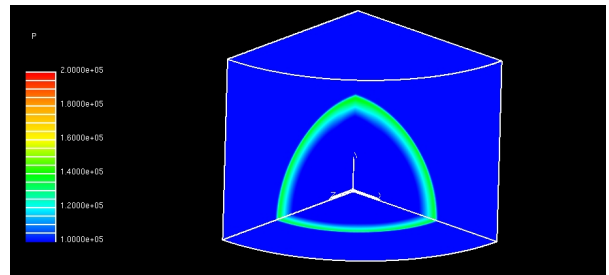
(4) Time t = 5.116 ms



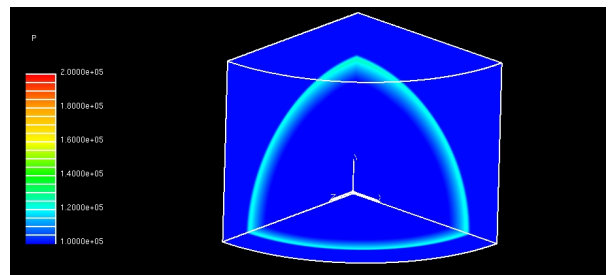
(5) Time t = 7.458 ms



(6) Time t = 13.314 ms



(7) Time t = 16.437 ms



(8) Time t = 26.978 ms

Fig. 6 History of air blast pressure propagation time

Fig. 7 shows the time history of air blast pressure at each point of observation. The axis of abscissas plots the propagation time of air blast pressure and the axis of ordinates plots air blast pressure, making detonation (TNT combustion time not included) the basis. The distances to the points of measurement are scaled distances normalized by the dosage. Propagation delay and lowering of peak pressure caused in accordance with the distance can be observed.

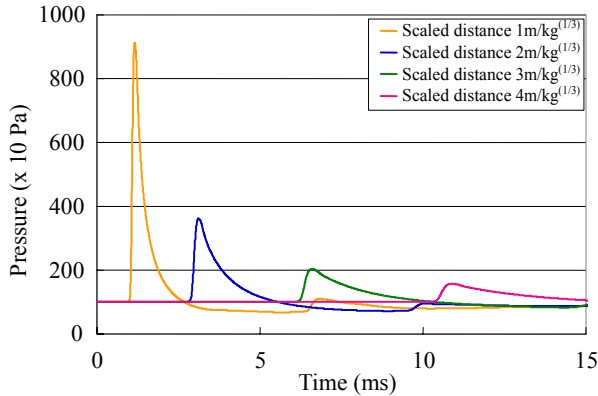


Fig. 7 Time history of air blast pressure at each point of observation of an air blast

5.3 Comparison of CFD with Bibliographical Values

Variation of peak pressure over the pressure propagation time is plotted in Fig. 8. The axis of abscissas plots the scaled distance normalized by the dosage. The axis of ordinates plots the peak pressure observed at each point of measurement. The diagram compares the results obtained in the research program with results based on W. E. Baker's paper⁹⁾. The simulation work in this research program is an explosion near the ground surface, and data of explosions in the air by Baker are converted into data equivalent to explosions on the ground surface.

A comparison of the CFD data with bibliographical values shows that the CFD values approach the results by Baker beginning near a scaled distance of $1 \text{ m/kg}^{(1/3)}$ and that the CFD values are almost identical above a scaled distance of $2 \text{ m/kg}^{(1/3)}$ even though the pressure peak values deviate greatly near an explosion source below $1 \text{ m/kg}^{(1/3)}$ in the scaled distance. The results obtained by Baker are based on an actual experiment, and impacts such as detonation gas are caused near the explosion source and are suspected of increasing the peak pressure. On the other hand, CFD provides only calculations of propagation of high-pressure gases and do not take actual impacts by detonation gas and other elements into consideration. For this reason, in the CFD calculations, peak pressure is considered to have lowered near the explosion source. At a scaled distance of $2 \text{ m/kg}^{(1/3)}$ and above, the bibliographical values and CFD results are almost identical, indicating that air blast pressure propagation by CFD is calculated accurately.

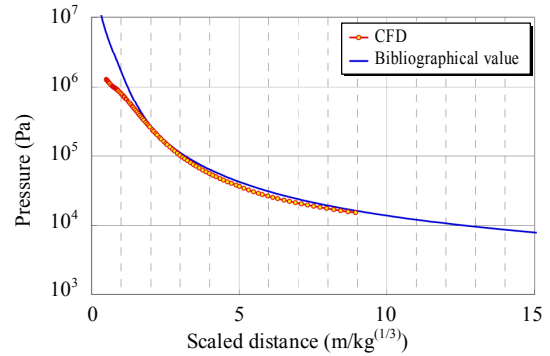


Fig. 8 Variation of peak pressure by pressure propagation distance

6. Conclusion

This research program has produced the following conclusions.

1) A combination of a parallel computer of our own making packaging usual personal computer components and CFD software sold on the market reduces calculation time by about 5 times more than Gigabit Ethernet that is commonly used, employing InfiniBand, a high-speed communication system operating at a communication speed.

2) Fluid calculations by the TVD scheme employed in CFD++ produce good results in analyses of air blast propagation even in comparison with bibliographical values, proving to be effective in analyses of air blast propagation.

7. Postscript

The prototyped parallel computer dramatically reduces calculation time and has reached a level assuring it to be fully viable as a design tool. The research program has used CFD as a benchmark, but the authors have found that the calculation time can also be reduced in explicit method FEM. The authors plan to expand the application of this technology to coupled calculations of CFD and rigid body analysis, and also to expand non-linear FEM in order to analyse complex physical phenomena.

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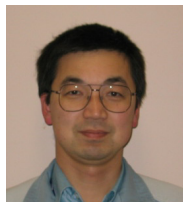
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 - linpack
HPL(High-Performance LINPACK Benchmark)
<http://www.netlib.org/benchmark/hpl/>
 - Silverstorm
<http://www.infinicon.com/>

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[A few words from the writer]

In the past, parallel processing was performed by supercomputers or similar computers and has not been familiar, everyday processing. The recently prototyped KHPC uses RAID, power supply, and a communication system for server use, but is almost a combination of components intended for general use. Recently, personal computers equipping two CPU cores into one processor have been sold and PLAYSTATION3 equips as many as nine CPU cores in one processor. Thus, parallel processing has become more familiar and is used in equipment around us. The processing speed of parallel computers as a design tool will increase further in the future as more CPUs are equipped and as the performance of communication systems is further enhanced. Tuned to this trend, the thinking of designers who effectively use these tools needs to evolve more rapidly to develop and provide better, less expensive products faster.