Technical Paper

High performance parallel computing for Computational Fluid Dynamics (CFD)

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The supersonic aerodynamic coefficient of a sphere that represents a broken piece of structure under explosion was obtained by using Computational Fluid Dynamics (CFD).The computer that was used in this study was self-made cluster type parallel machine and available maximum number of CPU was 128. The CFD software named CFD++ was used in this study. 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. Using the parallel computer, computational time was reduced dramatically. The importance of network performance was mentioned in this study. Since Ethernet required more time for communication between CPUs, that performance was limited under the condition of small number of CPUs. However, using high-speed network system (Myrinet), we could get more performance even large number of CPUs. The use of 64bit CPUs was also effective to reduce computational time, in addition to provide advantage for building a large-scale computational model through an expansion of memory space.

Key Words: *CFD, parallel computer, TOP 500, National Institute of Advanced Industrial Science and Technology (AIST), supercomputer, personal computer, scalability, CFD++, LINUX, CPU*

1. Introduction

Consideration of safety in storing and keeping of explosives is becoming a global issue recently in businesses that handle explosives. Because of their characteristics, strict safety administration is obliged for handling explosives, and they are often stored in one place. Forecasts of impact areas by blasts and the dispersion of flying objects in case of an accidental explosion are important for the design of storage sheds and settings of the ambient safety environment. Various data on explosives explosions are collected through explosion tests. In Japan, the amount of explosives that can be tested is limited to only about several tens of kilograms due to limited test grounds, and it is not possible to test cases where several hundreds of kilograms to several tens of tons of explosives that are actually stored are exploded. Forecasts of blasting states using a large amount of explosives are therefore necessary using data of experiments that use small amounts of explosives.

In these forecasts, numerical simulations using computers are made. In particular, computational fluid dynamics (CFD) is a technology that can be used in forecasting the dispersion of flying objects, in studying the impact of air blasts and for other purposes. In addition to problems faced in turning physical phenomena into numerical models, another problem with CFD is that the number of meshes expands to several million to several tens of millions depending on the experiment task when spatial meshes have to be divided. Computational time is several tens of hours to several hundred hours using computers that are normally available for computations, and this is not practical in many cases.

In this study, through joint research with the Research Center for Explosion Safety of the National Institute for Advanced Industrial Science and Technology, CFD analysis was conducted using a parallel computer that connected plural CPUs, to make simulations feasible through a drastic reduction in this computation time. An increase that could be achieved in the processing speed is reported.

2. Background

The need for high-performance computers in numerical simulations that require mesh and time division as in CFD are not new, and at one time, a development competition between Japan and the United States for a supercomputer evolved into an economic problem. At the time when high calculation speeds of one processor were pursued, American supercomputer manufacturers including Cray Research were leading, and Fujitsu and NEC of Japan caught up with them. Large host computer manufacturers competed with each other to develop new CPUs, and machines costing several hundred million yen were installed in the research organizations of universities and the state, large automobile manufacturers and other purchasers. These hardware units were housed in workshops with air conditioning facilities, becoming status symbols showing their technical level.

On the other hand, information service companies rented supercomputers purchased by themselves by the hour and were selling CPUs in the form of rental per hour. Komatsu used a supercomputer in this style temporarily.

Since then, the performance of CPUs made by so-called UNIX-based workstation (EWS) manufacturers such as DEC and SGI has enhanced, and many users seem to have changed to simulations on a level that better suits the development lead time using available EMS rather than conducting large-scale simulations using a supercomputer. Excluding some research organizations and large automobile manufacturers, the supercomputer has clearly become "not cost competitive" in terms of cost of installation, maintenance and management.

The development competition for supercomputers waned thereafter, while the performance of CPUs for personal computers manufactured by Intel and AMD has improved significantly. The application of these CPUs has expanded from word processing and spreadsheets for business use to image processing and Internet utilization, resulting in high-volume production by finding outlets in the homes of citizens as a market. The cost per CPU has been drastically reduced through high-volume production. At present, the basic performances of CPUs for personal computers, of memories and of hard disks have reached a level suitable for use in simulations including CFD. In fact, recently, Windows personal computers are replacing UNIX EWSs. **Figure 1** traces the development history of high-performance computers called supercomputers. One Intel CPU has performance better than that of a supercomputer made 15 years ago.

In the area of software, operating systems (OSs) have been unified to UNIX in EWSs from OSs of host computer manufacturers. At present, Linux can build an environment almost equal to that of UNIX, also for personal computers. Linux is an open system and is modified every day, paving the way to use state-of-the-art technology in parallel calculations also.

The approach of parallel computation by plural CPUs, which could be accomplished in the past only by certain supercomputers, has become feasible thanks to the high performance of hardware for personal computers, low price and software environments such as Linux. The basic approach is simple. Several tens of personal computers to several hundred sold on the market are connected by a network. For this reason, a concept called "self-made parallel machines" has emerged. The concept calls for the assembly of an inexpensive high-performance supercomputer using personal computer components sold on the market and Linux, OS of open source licenses. Even though special computer knowledge and network knowledge is needed to some extent, the layperson wishing to do something with this computer can handle it.

In this study also, a self-made computer developed by the Research Center for Explosion Safety of the National Institute for Advanced Industrial Science and Technology for CFD simulations was used.

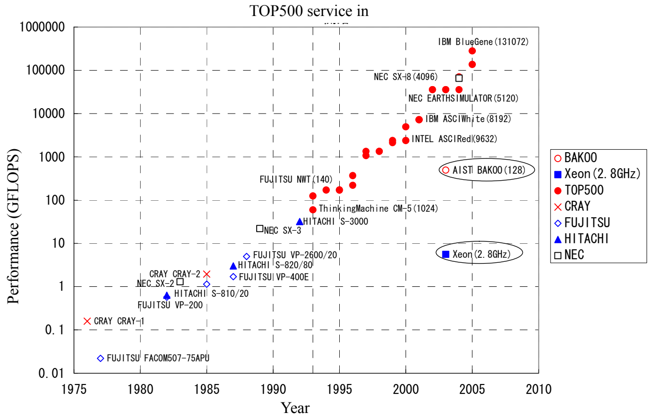


Fig. 1 Development history of high-speed computers

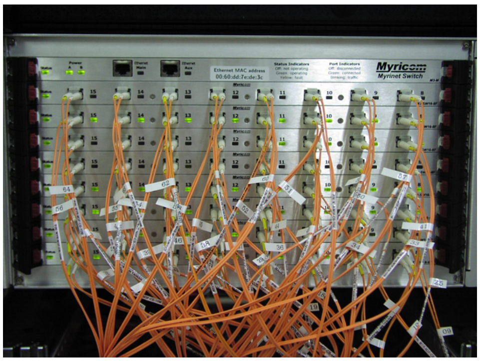
3. Parallel Computer in this Study

3.1 Parallel computer of the Research Center for Explosion Safety (BAKOO)

The parallel computer of the Research Center for Explosion Safety of the National Institute for Advanced Industrial Science and Technology (BAKOO) is shown in **Fig. 2**. The parallel computer has 128 CPUs comprising 64 nodes, each node packaging two Intel Xeon processors on one motherboard. The total memory capacity is 192 Gbytes. The network has a Myrinet card, a high-speed communication device, and a Myrinet switch.

The BAKOO configuration is summarized in **Table 1**. BAKOO is a perfect self-made computer for use in CFD. However, it ranks 351st in the world and 27th in Japan in the TOP500 ranking (rankings of top 500 supercomputer of the world by a Linpack benchmark based on the linear equation solution by LU resolution) for 2003. (See **Fig. 1**. The Earth Simulator SX6 of NEC [5120 CPUs, 35Tflops] ranked first for 2003)

Full view of BAKOO System



Myrinet hub

Fig. 2 BAKOO System

Table 1 BAKOO configuration

CPU	Intel Xeon 2.8GHz
Number of CPUs	128 (64 nodes)
Memories	192 Gbytes
Hard disk	30 Gbytes for each node 3.4Tbytes for data storage (RAID5)
Network	Myrinet (LANai9.2 and PCI-X interconnectivity)
Operating system	Linux

3.2 64-bit prototype computer (KHPC)

CPUs of personal computers are catching up with UNIX EWSs in installing 64-bit CPUs. CPUs of the 64-bit architecture eliminate memory limits of 2 Gbytes per process, dramatically increasing the amount of data that can be handled. An increase in the bus width enhances the data transfer speed.

A parallel computer using 64-bit processors (AMD: Opteron 2.2 GHz) was manufactured for use in a study of a next-generation self-made parallel computer (KHPC). An appearance and the inside of KHPC are shown in **Fig. 3**. KHPC is housed in a server casing and is installed in a 19" rack. The parts inside KHPC were purchased from electronic parts stores. The configuration of the KHPC computer is specified in **Table 2**. The KHPC has eight nodes, 16 CPUs and a memory capacity of 32 Gbytes.

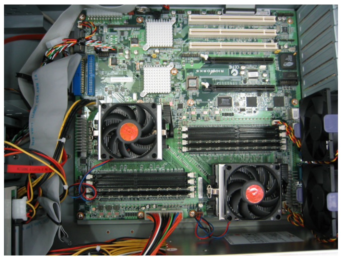


Fig. 3 Appearance and internal views of KHPC

Table 2 KHPC configuration

CPU	AMD Opteron 2.2GHz
Number of CPUs	16 (8 nodes)
Memories	32Gbyte
Hard disk	75Gbytes for each node 1.5Tbytes for data storage (RAID5)
Network	Gigabit Ethernet
Operating system	Linux

4. CFD Software

The CFD code used in this study is "CFD++ (CFD plus plus)." "CFD++" is general-purpose CFD software developed and sold by Metacomp of the United States mainly targeting the aviation and space industry.

Three-dimensional Navier-Stokes equations that represent the characteristics of fluid viscosity and compressibility are made discrete by the TVD scheme based on the finite volume method. [1)–7)] Several types of turbulent flows including Model k-ε can be selected. CFD++ can therefore be used widely in Mach and Re numbers from subsonic to supersonic speeds. The software package that was used in this study was also used in aerodynamic calculations of flying objects at high velocity and simulations of explosion phenomena. Parallel processing is also possible with the Intel 32-bit and AMD 64-bit versions.

Coupled calculations with rigid body motions with six degrees of freedom are embedded as a module, enabling calculation of a flying distance taking variations in air drag caused by changes in altitude into consideration by CFD while the solving motion equations of the flying objects. This study will be reported later.

5. Themes of Analysis

This study focuses on two problems in the safety of explosion. The first problem is how far flying objects in an explosion would fly, and the second problem, what impact an air blast by an explosion would have. The performance of the parallel computer that could be obtained in the computation process of the aerodynamic characteristics of the flying objects in an explosion by CFD is described.

5.1 Analysis model

A sphere of 14 mm in diameter was used in the calculations as the shape of the flying objects. Calculations for each Mach number were performed under conditions in which flying objects fly above the ground (pressure 101325 Pa, temperature 288.15 K, air density 1.225 kg/m^3).

Figure 4 shows the entire calculation model and external boundaries. The calculation model was performed by 3D CAD (Pro/Engineer) with external boundaries flying objects (sphere). An IGES file was fetched in ICEM/CFD, mesh-creating software, and meshes were created. Tetrahedrons (tetra meshes) were used as spatial meshes.

The behavior of the meshes near the flying object is illustrated in **Fig. 5**. The meshes are made fine nearer the object and trailing area, and made coarse nearer the boundary of the periphery. A pentahedron (prism meshes) is created for the surfaces of the flying object, taking the boundary layer into consideration.

Two nets were created to examine calculation performance by the model scale, one with about 1.23 million meshes and the other with about 6 million meshes. The meshes on a 1.23M-mesh surface of a symmetrical object are shown in **Fig. 6**. The calculation model is a half model, and symmetrical conditions were set on the symmetrical plane. The k-ε model was used as a turbulent flow model.

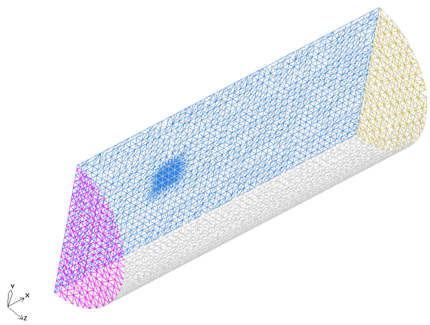


Fig. 4 Computational space and boundary conditions

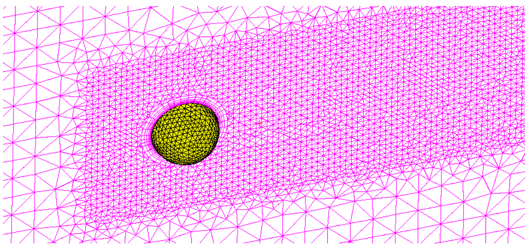


Fig. 5 Mesh of symmetrical surface

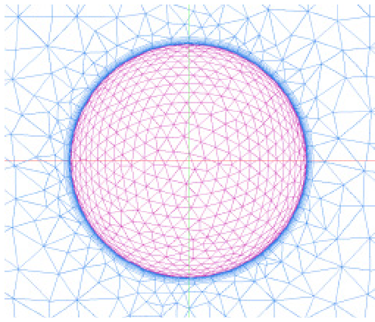


Fig. 6 Surface of 1.23M-mesh model

5.2 Calculation results

The calculation results of the air drag coefficient (Cd) to the Mach number are plotted in **Fig. 7**. CFD calculations solve the three-dimensional velocity components, pressure, temperature and turbulent flow characteristics (k, ε). The force applied to the model can be calculated as an integral of the surface pressure by post-processing of CFD++. The air drag coefficient (Cd) that used the diameter as a representative length was calculated using this force. As informative information, Cd by experiment is also shown.[8] The diagram shows that the calculations reproduce experiment values fairly accurately.

The spatial differential of the density in a flow direction calculated by CFD is shown in **Fig. 8**. CFD enables the visualization of various physical quantities. As shown in the diagram, the spatial differential in a flow direction can also be obtained. The spatial differential in a flow direction corresponds to a schlieren image in a wind tunnel test. The image clearly shows the behavior of a detached shock wave in front of the object and of the shock wave in the tail.

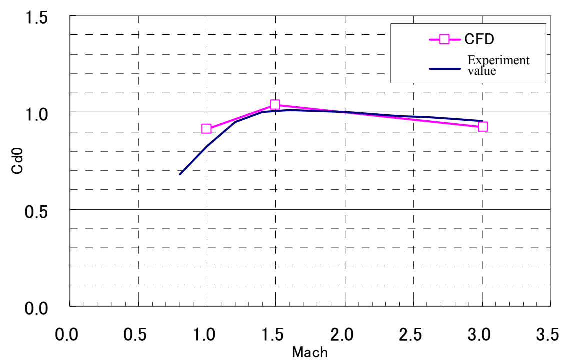


Fig. 7 Air drag coefficient (Cd) to each Mach

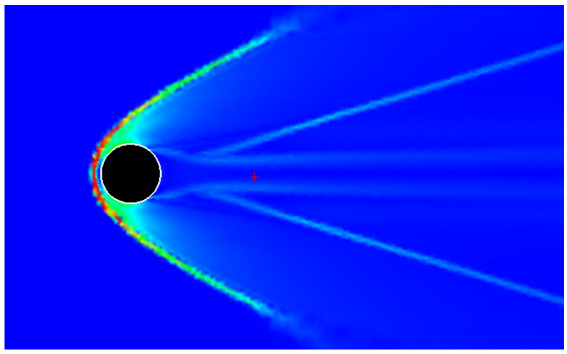


Fig. 8 Output corresponding to schlieren image

6. Higher Performance by Parallel Computation

6.1 Calculations by BAKOO of the National Institute for Advanced Industrial Science and Technology

Computation by BAKOO, a 32-bit machine, is described. BAKOO enables calculations by a maximum of 128 CPUs, and the performance of networks (Ethernet and Myrinet) can also be compared.

Calculations were made at Mach 3.0 of a half model of the sphere described earlier using two CPUs as a minimum configuration. The number of iteration cycles needed for the convergence of the calculations was fixed to 600 cycles.

An example of spatial division with four CPUs is shown in **Fig. 9**. Parallel computation requires spatial division in accordance with the number of CPUs. CFD++ comes with a domain division function. Using this function, a space was divided from 2 to 128. Each divided domain is allocated to one CPU, and calculations are executed while mutually communicating information at the boundaries.

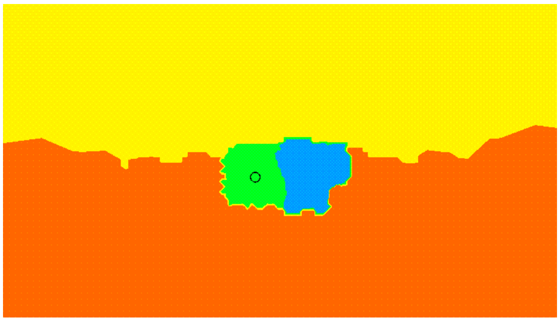


Fig. 9 An example of spatial division with four CPUs (symmetrical face)

The computation time needed for 1.23-Mega elements is shown in **Fig. 10**. The time needed for computation with two CPUs was 10.9 hours. The time with four CPUs on Ethernet was 6.1 hours and with four CPUs on Myrinet, 5.1 hours, or about half. However, with 16 CPUs, the time with Ethernet was 3.7 hours and with Myrinet, 1.6 hours, widening the gap. With 32 CPUs, the time with Ethernet was 4.5 hours, taking a longer time even though the number of CPUs was doubled. Myrinet accomplished calculations in 1.0 hour, reducing the computation time. Increases in the number of CPUs increase the domain divisions, thereby reducing the calculation volume per CPU. On the other hand, the overhead (other time needed for computation) of data communications between nodes determines the rate, and the CPUs idle when latency during communications is large. Networks with large latency (100 µs -) such as Ethernet nullify the effect of having more CPUs. This shows that a high-speed network device (- 10 µs) is needed in this case.

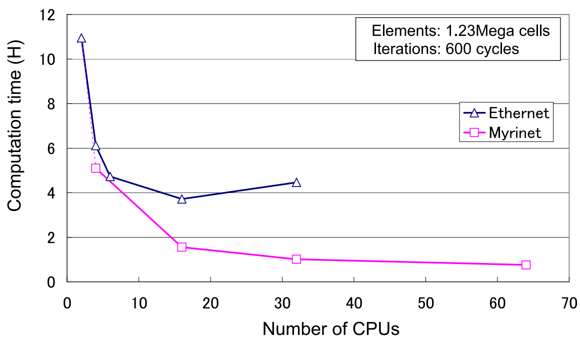


Fig. 10 Computation time of 1.23Mega elements

The computation time shows that it is not reduced simply in proportion to an increase in the number of CPUs even though Myrinet is used. In other words, the computation time does not necessarily decrease to half (1/2) even though the number of CPUs is twice increased. The relationship between increase in the number of CPUs and calculation time reduction is called “scalability.” Scalability exists if the computation speed increases twice (computation time 1/2) when the number of CPUs increases twice. However, normally, the overhead for communications and other factors does not allow scalability commensurate with increases in the number of CPUs.

Figure 11 plots the inverse numbers of the proportions of computation time for increases in the number of CPUs based on computation time for two CPUs (network not used). The dotted line in the diagram shows a case of a computation time in proportion to increases in the number of CPUs. This dotted line shows the ideal effect of the parallel computer. This diagram shows what effects an increase in the computation time illustrated in **Fig. 10** has on the number of CPUs. In Myrinet also, the effect of having more CPUs wanes beginning at about 32 CPUs. Similarly, the computation time of 6-Mega elements increases in proportion to increases in the number of CPUs up to about 32 CPUs. A large number of elements in the domain allocated to each CPU relatively reduces the proportion of communication time to computation time, thereby maintaining the effect of the increase in the number of CPUs. At 6-Mega elements, the computation speed for 32 CPUs is theoretically 32 times, but is actually about 18 times, resulting in drastically low efficiency.

This shows that, in terms of cost vs. performance, the rational number of CPUs is predetermined by the model scale (number of elements) of the analysis target when CFD++ is used, even though a high-speed communication device is used (Myrinet in this case).

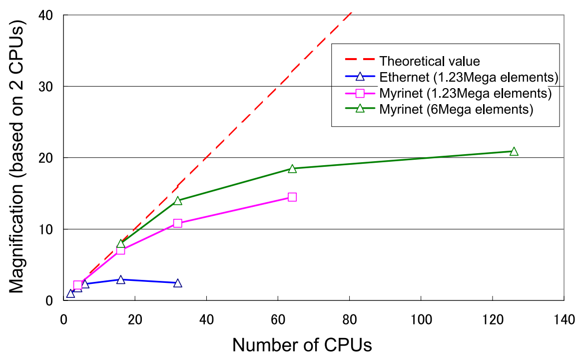


Fig. 11 Computational speed dependent on the number of CPUs (Magnification)

6.2 Calculations by prototype machine KHPC

A comparison of computation speeds by KHPC, a prototype 64-bit machine, and BAKOO is shown in **Fig. 12**. The computation speed of the prototype machine is faster on Ethernet when the number of elements is the same, 1.23 Mega, and with the same number of CPUs. The computation speed of the prototype machine is 1.5 times with two CPUs and about 1.4 times with four CPUs. BAKOO is about 27% faster in the CPU clock, but KHPC has higher calculation performance. The 64-bit bus width seems to contribute to not only memory space, but also calculation performance in these calculations. With 16 CPUs, however, BAKOO on Myrinet is faster. This means that the computation speed of KHPC with 32 CPUs lowers below that with 16 CPUs unless a high-speed communication device is provided. The calculation results for one CPU are also described as brief information. The computation time with one CPU was 15.5 hours, about twice that with two CPUs.

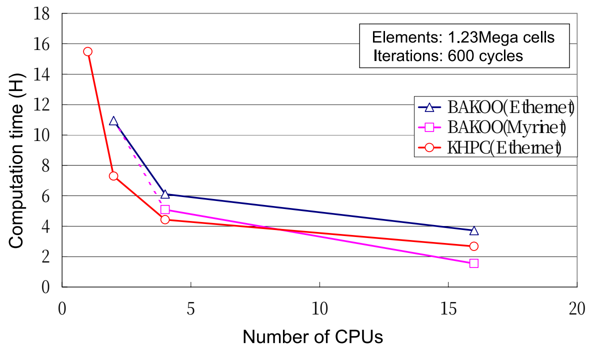


Fig. 12 Computational speeds of BAKOO and KHPC

7. Conclusion

The following conclusions were obtained through this study.

1) A self-made parallel computer assembled by using components for general-purpose personal computers reduces computation time more than 10 times using CFD software sold on the market.
2) The address space of the 64-bit CPU can be expanded by CFD, offering the advantages of handling a large-scale model and a high calculation speed.
3) More CPUs beyond a certain number conversely lowers the computation speed even though the number of CPUs is increased. A high-speed communication device to replace Ethernet is mandatory and is an important key technology for parallel computation.
4) A parallel computer with several thousand CPUs is a hot topic as "the world's fastest machine." However, the limits of scalability emerge early (with fewer CPUs), such as in the combination of general-purpose software and the analysis model used in this study. A system with a good cost vs. performance ratio needs be used suiting application work.

8. Concluding Remarks

The prototyped parallel computer is an ordinary personal computer except for the power source and other parts that require reliability, which were substituted by a server, a RAID5 1.5-Tbyte storage and rack mount. Partly because software (OS) and a monitor are not packaged, the price per node (2 CPUs) is about half that of a 2CPU Windows machine used in-house for analysis. Nevertheless, the machine may have maintenance servicing problems because it is a self-made computer. Even though the hardware cost is dramatically low, the software license cost relatively increases for parallel use. There are other several issues. However, the fact that computation can be performed in several tens of hours instead of several hundred hours will drastically change thinking toward simulations and simulation targets. This technology must be observed by machinery manufacturers such as Komatsu.

This study will be continued for both hardware and CFD analysis techniques. In addition to analysis by CFD, the effectiveness of parallel computation with FEM and other analyses will be verified.

References:

1) A.A. Amsden and F.H. Harlow, "The SMAC Method: A Numerical Technique for Calculating Incompressible Fluid Flows", Los Alamos Scientific Laboratory Report, LA-4370.
2) S.V. Patankar, "Numerical Heat Transfer and Fluid Flow", Hemisphere Pub, New York (1980).
3) S.V. Patanker and D.B. Spolding, "A Calculation Procedure for Heat, Mass and Momentum Transfer in Three-Dimensional Parabolic Flows", Int. J. Heat Mass Transfer, 15(1972) 1787.
4) Harten, A., "High resoluation schemes for hyperbolic conservation laws", J. Comp. Phys. 49(1983) 357-393.
5) Harten. A., "On a Class of High Resolution Total-Variation-Stable Finite-Difference Schemes", SIAM J. Numer. Anal., 21 (1984) 1-23.
6) S.R. Chakravarthy and S. Osher, "A New Class of High Accuracy TVD Schemes for Hyperbolic Conservation Laws", AIAA Paper 85-0363 (1985).
7) Robert L. McCoy "Modern Exterior Ballistics", Schiffer Publishing Ltd.

○myrinet
http://www.myricom.com
○Top500
http://www.top500.org
○metacomp
http://www.metacomptech.com
○linpack
As HPL (High-Performance LINPACK Benchmark)
http://www.netlib.org/benchmark/hpl/

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[A few words from the writer]

It is amazing that CFD computation that requires about a dozen hours can be completed in one hour. What is more amazing is that this can be accomplished by adding some functions to a personal computer that can be bought by anyone. The advances in CPU and network technologies let us enjoy the Internet at home through broadband technology. Applying these technologies, simulations by supercomputing, which were once something to gaze at in a shop window, are now becoming more readily available. We hear that parallel computers that are very low in price, but very high in performance using CPUs contained in a PlayStation (video game machine) are also sold. We are living in an interesting age. No matter how fast simulations can be made, they are meaningless unless design concepts and ideas are offered. We need to produce better products quickly at low price by skillfully using these tools.