ANNUAL REPORT OF R&D ACTIVITIES
IN
CENTER FOR PROMOTION OF
COMPUTATIONAL SCIENCE AND ENGINEERING
FROM APRIL 1, 2004 TO MARCH 31, 2005

September 2005

Center for Promotion of Computational Science and Engineering

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Japan Atomic Energy Research Institute
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Annual Report of R&D Activities in Center for Promotion of Computational Science and Engineering from April 1, 2004 to March 31, 2005

Center for Promotion of Computational Science and Engineering

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This report provides an overview of research and development activities in Center for Promotion of Computational Science and Engineering (CCSE), JAERI, in the fiscal year 2004 (April 1, 2004 – March 31, 2005). The activities have been performed by Research Group for Computational Science in Atomic Energy, Research Group for Computational Material Science in Atomic Energy, R&D Group for Computer Science, R&D Group for Numerical Experiments, and Quantum Bioinformatics Group in CCSE. The ITBL (Information Technology Based Laboratory) project is performed mainly by the R&D Group for Computer Science and the Research Group for Computational Science in Atomic Energy. According to the mid-term evaluation for the ITBL project conducted by the MEXT, the achievement of the ITBL infrastructure software developed by JAERI has been remarked as outstanding at the 13th Information Science and Technology Committee in the Subdivision on R&D Planning and Evaluation of the Council for Science and Technology on April 26th, 2004.

Keywords: R&D Activities, CCSE, ITBL Project, Computational Science Research in Atomic Energy, Computational Material Science, Quantum Bioinformatics
日本の原子力研究所
計算科学技術推進センター

（2005年8月12日受理）

本報告書は、日本原子力研究所 計算科学技術推進センター（CCSE）における平成16年度の研究開発活動について報告するものである。これらの研究開発はCCSEの原子力エネルギー計算科学研究グループ、原子力物性計算科学研究グループ、原子力計算機科学技術開発グループ、数値実験技術開発グループおよび量子生命情報解析グループによって行なわれたものである。また、ITBL計画主として原子力エネルギー計算科学研究グループ、原子力計算機科学技術開発グループによって遂行されており、その開発について中間評価を受け、第13回科学技術・学術審議会 研究計画・評価分科会 情報化科学技術委員会（平成16年4月26日）において、原研担当の基盤技術について高い評価を得た。
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Acronyms

ADVENTURE  ADVanced Engineering analysis Tool for Ultra large Real world
AESJ          Atomic Energy Society of Japan
API            Application Programming Interface
BAAQ          Bioinformatics: Ask Any Questions
BCC            Body Centered Cubic
BEC            Bose-Einstein condensate
CAE            Computer Aided Engineering
CCJJ          Capacitively-Coupled Josephson Junctions
CCSE          Center for Promotion of Computational Science and Engineering
CMD            Computational Material Design
CTRTx         CT Radiotherapy
EAM            Embedded Atom Method
ES             Earth Simulator
FCC            Face Centered Cubic
FEM            Finite Element Method
FLOPS         Floating Operations Per Second
FS             Free Surface
GB             Grain Boundary
GIF            Graphic Interchange Format
GUI            Graphical User Interface
HPC           High Performance Computer
IMRT          Intensity Modulated Radiation Therapy
IT             Information Technology
ITBL         IT Based Laboratory
JAERI       Japan Atomic Energy Research Institute
JAXA         Japan Aerospace Exploration Agency
JST          Japan Science and Technology Agency
LBM          Lattice Boltzmann Method
MpCC         Mesh-based parallel Code Coupling Interface
MPI          Message Passing Interface
NAREGI     National Research Grid Initiative
NDB          Nucleic Acid Database
NIED        National Institute for Earth Science and Disaster Prevention
NIMS         National Institute for Materials Science
<table>
<thead>
<tr>
<th>Acronym</th>
<th>Description</th>
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<tr>
<td>PATRAS</td>
<td>PParallel TRacking And Steering</td>
</tr>
<tr>
<td>PDB</td>
<td>Protein Data Bank</td>
</tr>
<tr>
<td>PST</td>
<td>Parallel Support Toolkit</td>
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<tr>
<td>SCC</td>
<td>Stress Corrosion Cracking</td>
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<tr>
<td>SFT</td>
<td>Stacking Fault Tetrahedron</td>
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<tr>
<td>STA</td>
<td>Seamless Thinking Aid</td>
</tr>
<tr>
<td>STAMPI</td>
<td>Seamless Thinking Aid Message Passing Interface</td>
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<tr>
<td>STARPC</td>
<td>Seamless Thinking Aid Remote Procedure Call</td>
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<tr>
<td>TDGP</td>
<td>Time-Dependent Gross-Pitaevskii</td>
</tr>
<tr>
<td>TME</td>
<td>Task Mapping Editor</td>
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<td>VR</td>
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Foreword

The Center for Promotion of Computational Science and Engineering (CCSE) has been conducting research and development activities such as development of a series of the parallel processing basic software for complex and large scale computational simulations in the science and engineering field. The CCSE has also made efforts to construct computational science and engineering related cooperative establishments in JAERI, in Japan and in the world.

The ITBL (Information Technology Based Laboratory) project is to establish high-speed networking supercomputers to be distributed in different research organizations so that computational resources such as software, databases and computational power can be shared by all organization in Japan. ITBL can realize so called virtual research laboratory. According to the mid-term evaluation for the ITBL project conducted by the MEXT, the achievement of the ITBL infrastructure software developed by JAERI has been remarked as outstanding at the 13th Information Science and Technology Committee in the Subdivision on R&D Planning and Evaluation of the Council for Science and Technology on April 26th, 2004.

It is our pleasure to publish the annual report of our research and development activities in the fiscal year of 2004. We believe the research and development of in CCSE on a common technological basis of parallel processing for scientific computations through cooperative interactions with other research organizations under MEXT disseminates the fruits thereof in a proper fashion to the public domain as well as to other research and development activities in JAERI.

Genki Yagawa
Director
Center for Promotion of Computational Science and Engineering,
JAERI
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1. Overview of CCSE R&D

The JAERI CCSE (Center for Promotion of Computational Science and Engineering) has five R & D groups: (1) Research Group for Computational Science in Atomic Energy, (2) Research Group for Computational Material Science in Atomic Energy, (3) R&D Group for Computer Science, (4) R&D Group for Numerical Experiments, and (5) Quantum Bioinformatics Group. The R&D activity of each group in CCSE is described in Chapter II. Here we summarize the main results of each group.

The ITBL (Information Technology Based Laboratory) project, aligned with the national e-Japan Priority Policy Program, aims to provide a highly efficient and virtually unified research environment on the nation-wide distributed laboratories basis by inter-connecting super computers located all over Japan, and by sharing the relevant computer hardware, software and database resources. According to the mid-term evaluation for the ITBL project conducted by the MEXT, the achievement of the ITBL infrastructure software developed by JAERI is remarked as outstanding at the 13th Information Science and Technology Committee in the Subdivision on R&D Planning and Evaluation of the Council for Science and Technology on April 26th, 2004.

Simulation studies on the material properties in nano-scale clarified a condition under which a system confined inside nano-scale area exhibits superfluidity, and also showed the condition can be easily verified by using Fermi atomic gas loaded on an optical lattice created by laser beam.

For the research on the development of parallel algorithms, a mesoscopic model to simulate grain boundary fractures is successfully developed to realize complex fracture patterns with branches observed in the experiments of stress corrosion cracking.

For the research on the computational science in nuclear engineering fields, a new first-principles calculation method is developed to simulate the atomic bonding states of materials under the tensile test conditions. Using this method, it is found that the embrittlement of nickel (Ni) grain boundary occurs due to the presence of segregated sulfur (S) impurity atoms, where a large grain-boundary expansion is caused by a short-range overlap repulsion among densely segregated and neighboring sulfur atoms.

In application of ITBL to bioinformatics analyses, development of integrated systems has been continued for computational analysis tools named BAAQ (Bioinformatics: Ask Any Questions). Specifically, a method has been developed to predict RNA interfaces of proteins including repair enzymes and it was applied to an enzyme for protein synthesis.
2. CCSE Research and Development Activities

2.1 ITBL Project

ITBL is a project started in 2001 with the objective of realizing a virtual joint research environment using information technology (IT). ITBL aims to connect 100 or more supercomputers located in Japan over SuperSINET so that they can be shared, and to build a system enabling joint use over the Internet of large-scale experimental facilities and the like. The project will also develop and provide software utilizing databases and supercomputers, promoting a variety of types of R&D and improving usage efficiency of various facilities, including supercomputers. Currently ITBL has six member institutions, which are Japan Atomic Energy Research Institute, RIKEN, National Institute for Materials Science (NIMS), National Aerospace Laboratory of Japan (NAL), National Research Institute for Earth Science and Disaster Prevention (NIED), and Japan Science and Technology Corporation (JST). Among these institutions, JAERI and RIKEN are handling the development of the common basic technology required for implementing the ITBL plan. Each of the six research institutions is handling different aspects of the development of application software that can be used through ITBL.

According to the mid-term evaluation for the ITBL project conducted by the MEXT, the achievement of ITBL infrastructure software developed by JAERI is remarked as outstanding at the 13th Information Science and Technology Committee which belongs to R&D Planning and Evaluation Subdivision of Council for Science and Technology, on April 26th, 2004. The ITBL infrastructure software has accomplished its functions of grid computing environment needed for researches, and is the leading technology in the world.

Cooperation : National Institute of Informatics（The provision of a high-speed network named SuperSINET）

2.1.1 Research and Development of Parallel Basic Software System[2.1-1]

Since the alpha prototype of the ITBL Infrastructure Software was released at the end of the 2001 fiscal year, we have operated and maintained the latest version of software. We have also promoted to join various researchers and research groups on the ITBL network and supported them in various ways. Now the ITBL network has grown to 33 high-end computers from 12 organizations including 11 supercomputers, totaling to
19.4 TFLOPS of computing power and 19 Tera-byte memory capacities (Fig.1, 2). The ITBL has gathered over 500 registered users from 36 organizations. We accepted and answered approximately 86 questions, performed 39 bug fixes, and also, we installed the ITBL Infrastructure Software on 11 computer systems.

The 5th ITBL symposium was held on November 26th, 2004 at National Museum of Emerging Science and Innovation (Tokyo), and ITBL building at Kansai Laboratory of JAERI with outside broadcasting on ITBL video conference. The symposium was conducted by 6 organizations of the ITBL project, and reported the recent achievement.

Fig.1 Computers on ITBL
2.1.2 Visualization with Grid Technology

The ITBL project aims at the construction of a virtual research environment which shares various resources and which supports researchers in remote location to communicate with others [2.1-2]. In the project, AVS/ITBL has been developed as a tool to share visualization results of the simulations. The AVS/ITBL offers a function to visualize any data on web browser by remote operations. It proposes a data streaming and pipeline-parallelized communication technology for the visualization. In order to mature the remote and collaborative visualization, we have added the following functions [2.1-3, 2.1-4]: (1) Remote import function, (2) Web client visualization function, (3) AVS batch-style visualization function, and (4) Collaborative visualization function. Figure 3 shows the simulation result of the diffusion of the air pollutant on web browser, where the calculation is done with VPP5000 in the Tokai laboratory while making to visible is done by GP400S at CCSE in Ueno. This vision was prepared for users who are apart from each others, to share the discussion on the results.
2.1.3 A Technique of Evaluating a Similarity between Critical Point Graphs and its Application [2.1-5]

To mechanically search and classify a large volume data in a voluminous dataset, an evaluating method for global similarity in the given dataset is proposed. In the method, the local characteristic of the volume data is identified by searching the critical points of the field. The critical point graph is generated by linking the stream lines adjacent to the critical points. The similarity of the volume data is measured by comparing the spatial routings of the critical point graphs.

The function module of the introduced method is commercialized in the AVS/Express visualization software package as an analysis tool.

A scalar field volume data of a temperature distribution is analyzed by the software to exemplify the capability of identifying the statistical similarity of the two different critical point graphs whose stream lines are generated by 2\textsuperscript{nd} and 4\textsuperscript{th} order Runge-Kutta formula (Fig.4); the graphical similarity between (a) and (b) is illustrated in Fig.5 and statistical similarity is shown in Fig.6.
(a) Stream lines are generated by 2nd order Runge-Kutta
(b) Stream lines are generated by 4th order Runge-Kutta

Fig. 4 Critical point graphs of temperature distribution

Red: Similar, Blue, or Green: Not similar
Fig. 5 Graphical similarity between (a) and (b)

Fig. 6 Statistical similarity between (a) and (b)
2.1.4 Introducing Topological Attributes for Objective-based Visualization [2.1-6]

Quality of the volume-rendered image highly depends on the type of transfer function (TF) to be used. A conventional one-dimensional TF cannot render details of inside structure of a volume data with optically-nested information characteristics. A multi-dimensional TF with topological attributes has been designed for such a type of volume rendering that some specific area with respect to the information depth of the volume data will be selectively emphasized so as to accommodate with an observer’s objective. Topological attributes, such as inclusion level, isosurface-trajectory distances, and isosurface genus, are derived from an abstract level-set-graph, VST (Volume Skeleton Tree). By proper selection of topological attributes to a given volume data, the multi-dimensional TF generates objective-based visualization such as Fig.7.

(a) Volume Skeleton Tree which expresses topological changes of field
(b) one dimensional function for opacity
(c) two dimensional transfer function for opacity
(d) two dimensional transfer function for opacity to emphasize only the inside the nest.

Fig. 7 Visualizing simulated implosion in laser fusion
2.1.5 Designing Multi-dimensional Transfer Functions with Topological Attributes [2.1-7]

Volume rendering is to project all the optically-encoded samples onto the screen at once to allow us to peer into the inner structure of a volume data, where the voxel's field value is translated to color or transparency by a transfer function (TF). It has been known that the multiply nested inner structure of a 3D simulation dataset cannot be clearly peered into by using the traditional one-dimensional TF. It has been proposed to use a multi-dimensional TF with the set of topological attributes, in order to emphasize a specific region of information out of 3D simulation result. Designing principle of the multi-dimensional TF has been shown, and the method has been applied to visualize datasets from simulations such as density distribution of implosion of laser fusion, molecular wave function of Iron protein, and charge distribution of two-body nucleon system. Through these visualization results, detailed inner structures of volume data have been clearly peered and effectiveness of our approach has been well demonstrated (Fig.8).

Upper: Topologically-accentuated 1D opacity TF, Lower: 2D opacity TF
Fig.8 Visualizing HIPIP (High Potential Iron Protein) dataset
2.1.6 Research and Development of Spherical Sampling Volume Renderer [2.1-8]

In recent years, an immersive VR system has been used as one of the visualization techniques for analyzing various complicated phenomena in computational science fields, and the volume rendering method is widely used for the intuitively understanding of 3-D distributed physical quantities. However, a plane slice sampling method in the volume rendering method has a downside problem of image in the immersive projection system. To resolve this problem a sphere slice sampling method is applied. The quality of image and the display speed are compared between these two methods in Fig.9. Three techniques (Optimization of sampling plane, High speed-Visualization and shading) have been used to apply the volume rendering method to the immersive VR system. Sampling planes are optimized by centering on centers of right and left both eyes and using a vertical sampling side for the direction of the glance. Speeding up and weight saving of visualization is realized by Mapping RGB color to texture color table. Shading is used by developing the texture that various some texture techniques. Deteriorate image was improved by using a sphere slice sampling method applied to immersive VR system. Display speed of this method is not far removed from a plane slice sampling method. It can be concluded that a sphere slice sampling method can display with higher resolution than a plane slice sampling method.

![Images](a) plane sampling (b) spherical surface sampling

Fig. 9  Comparison of image quality between plane sampling, and spherical surface sampling.

2.1.7 Parallel Volume Rendering on Immersive Projection Technology [2.1-9]

Visualizing complicated objects on immersive projection device (CAVE) is an effective way to understand the inside structure of complicated objects. However it is important to give an enough frame rate to visualize those objects because an immersive projection device tries to render the images whenever the sensor of the immersive projection
device detects a change of the location on the objects. This research interest is to implement volume rendering on CAVE with an enough frame rate. For example the frame rate of volume rendering declines when the view point is close to the data, and images projected to the screens become bigger. We have developed an effective algorithm for volume rendering without declining the frame rate of volume rendering on CAVE. The algorithm takes the Shear-Warp method to improve the frame rate of volume rendering with parallelization. And the method enables high speed rendering by generating both images for left-eye and right-eye at a time. This volume rendering algorithm is applied to the void fraction of boiling flow to observe the phenomena of the boiling flow to evaluate the quality of the algorithm and its rendering speed. Figure 10 shows the void fraction of the boiling water in a metal container. The blue area shows the void fraction is zero, and the red area shows the high void fraction with a lot of steam. By using the cave, the detail behavior can be observed, although a 2D display may not. This algorithm generates images with the speed of 5 frames per second on Onyx with 7 CPUs for a datasets of 128x128x128 meshes shown in Fig.10. This frame rate is smooth enough to visualize the test dataset. In addition, the size of a dataset does not give much influence to rendering speed when the new algorithm is used. Texture mapping algorithm that is commonly used for volume rendering has a decline of the frame rate when it tries to visualize 256x256x256 meshes, on the other hand, the new method shows almost the same frame rate as the 128x128x128 case.

Fig.10 Void Fraction of Boiling Flow
Reference


2.2 Computational Science Research in Atomic Energy

The Research Group for Computational Science in Atomic Energy, formed in April 2004, performs research and development regarding structural, fluid, and heat problems arising in the fields of nuclear science and engineering, by the use of high-performance computing technologies, e.g., parallel and distributed computing systems and next-generation IT infrastructures. One of our ultimate goals is to establish a 3D full-scale simulation system for nuclear facilities, including atomic energy plants, nuclear reactors, and accelerators, to be used for their safety and reliability maintenance. Toward this end, we are currently performing basic studies on numerical methods, physical modeling, parallel processing, and code design, all of which are essential for large-scale, realistic computer simulation of, not only nuclear facilities, but also generic build-up structures.

In the following, we present three of our recent achievements. A theoretical study of the Gaussian filtered Navier–Stokes equations is to detect the underlying cause of the numerical instability observed frequently in large eddy simulations (LES) of turbulence; it also provides a refined answer to our previous question as to whether a numerically stable LES model can be ideally accurate. Next, the examination of dynamics of gas bubbles pulsating in water, where a basic system of equations for fluids is solved, aims at gaining rich insights into cavitation problems and bubbly flows, and also aims at developing a fine physical model of clusters of dynamically oscillating and interacting bubbles. Finally, an integrated simulation infrastructure for distributed computing systems realizes the parallel computation of coupled fluid–structure problems based on the concurrent use of different kinds of computers. These achievements would be utilized as fundamental components of the 3D full-scale simulation system.

2.2.1 Underlying Mechanism of Numerical Instability in Large Eddy Simulation of Turbulent Flows

Turbulence is one of the unsolved problems of physics. Because a complete theoretical description has not yet been achieved even for a relatively simple flow configuration, numerical simulations are commonly used to analyze it. One of the typical numerical approaches is the large eddy simulation (LES), which directly solves the large scales but models the small-scale eddies by employing a model. One of the major problems of LES is numerical instability. As is already known, several existing LES models have a numerically unstable property, and hence some artificial numerical treatments have been incorporated so as to guarantee numerical stability. Recently, we claimed based on a
theoretical investigation that the filter operation, which is the most fundamental component of LES, itself seems to be the underlying origin of the numerical instability, raising a question as to whether a numerically stable LES model can be complete. In the present study [2.2-1], we have extended our previous work [M. Ida and N. Taniguchi, Phys. Rev. E 68, 036705 (2003)] so as to gain a refined understanding. Our discussion uses the Gaussian filtered Navier–Stokes (NS) equations as the governing equations, and assumes that the time averaged streamwise velocity, not depending on time, is linearly proportional to the distance from a plane wall, an assumption that corresponds to the case of the viscous sublayer in plane channel flows. As we have shown, in this situation a numerically unstable term appear in the filtered equation for the streamwise velocity, a term that has a time-independent coefficient and can be decomposed into positive and negative diffusion terms. We have suggested that if a condition is not fulfilled, the filtered NS equations should be numerically unstable. In the case of plane channel flow, this condition corresponds to $\Delta^* \leq 2\sqrt{6}$, where $\Delta^*$ denotes the filter width in the wall units. This result implies that at least several grid points are needed in the viscous sublayer to guarantee numerical stability, which is a formidable restriction in high-Reynolds-number practical applications, and it also indicates a significant difficulty in developing an excellent LES model that can provide satisfactory (i.e., not only stable but also accurate) solutions even with large wall-normal filter widths.

2.2.2 Investigation of Transition Frequencies of two Acoustically Coupled Bubbles using a Direct Numerical Simulation Technique

The secondary Bjerknes force is an interaction force acting between pulsating gas bubbles. In recent studies it has been shown that the force can reverse its own direction as the distance between the bubbles changes. Recently, we claimed that this phenomenon cannot be explained by observing the resonance frequencies and the transition frequencies must be observed at which the oscillation phase of a bubble inverts. Our theory predicted that the sign reversal takes place around the transition frequencies that do not correspond to the resonance frequencies. We have verified this suggestion by a direct numerical simulation technique (Fig. 1) [2.2-2, 2.2-3]. Figure 2 displays the sign of the force (a), determined by observing the direction of the bubbles' translation, and the bubbles' pulsation amplitudes (b and c). The equilibrium radii of the bubbles are $(R_{10}, R_{20}) = (5 \mu m, 9 \mu m)$, and the initial distance between them is $20 \mu m$. From this figure, one knows that the smaller bubble has two resonance frequencies, the higher of which is higher than $\omega_{10}$ and the lower of which is lower than $\omega_{20}$ ($\approx 0.53\omega_{10}$), where $\omega_{ij}$ is the partial resonance frequency of bubble $j$. The sign of
the force changed twice in the frequency region considered. The reversal at a low frequency clearly indicates that a kind of characteristic frequency should exist in the frequency region between the partial resonance frequencies. It is evident that this characteristic frequency is not the resonance frequency of the larger bubble, which is much lower. This result is in opposition to the conjecture by Doinikov and Zavtrak that the resonance frequencies of both bubbles rise as the bubbles approach each other. This characteristic frequency is, arguably, the second highest transition frequency of bubble 1, which cannot be derived by resonance frequency analysis.

![Fig. 1](image.png)

Fig. 1 A DNS result of two microbubbles in a sound wave. The pulsating bubbles attract each other, resulting finally in coalescence. The floor under the bubbles is a virtual object for visualization.

![Fig. 2](image.png)

Fig. 2 DNS results: (a) Sign of the force, (b) pulsation amplitude of bubble 1, and (c) that of bubble 2, as functions of the driving frequency. The amplitudes were measured for \( t < 5 \mu s \) (open circles), and for \( t < 10 \mu s \) but until the coalescence has been observed (filled circles).
2.2.3 Development of an Integrated Numerical Simulation System for Parallel Fluid-structure Coupled Simulations

It is now widely recognized that coupled multi-physics simulations are important and necessary to reflect reality into the simulations carried out. Most physical phenomena around us occur as a result of interactions with other phenomena, and hence it is natural to consider the events simultaneously, rather than independently. An “integrated numerical simulation infrastructure” (Figs.3 and 4) for multi-disciplinary and multi-physics simulations has been developed under the international collaborative efforts between JAERI and Fraunhofer SCAI [2.2-4]. The infrastructure is based on the MpCCI (Mesh-based Parallel Code Coupling Interface) and STAMPI libraries, which perform interpolation between different computational domains and communication between different computers, respectively, and it is used to solve multi-disciplinary problems in meta- and grid-computing environments by coupling two different arbitrary simulation codes which have in general different mesh structures and applicable computers. In order to verify the performance of the developed infrastructure, a simple validation test is carried out. A laminar flow in a three-dimensional steel pipe is considered (Fig.5) where the Navier–Stokes equation and a linear elastic model are used as the governing equations of the fluid and solid phases, respectively. This sample test has been carried out in a meta-computing environment to verify the functionality of the infrastructure to handle communications between computers in such environments. A Linux PC and an IBM pSeries690 workstation are used to solve the solid and fluid phases, respectively. Since nearly no deformation should be seen in the pipe, the flow should develop and converge closely to the Hagen–Poiseuille flow. Figure 6 illustrates the flow velocity profile near the inlet and outlet. The velocity profile along the vertical axis at the outlet is in good agreement with that predicted by the Hagen–Poiseuille theory.
Fig. 3 An image of an "integrated numerical simulation system."

Fig. 4 Data exchange and interpolation at shared surface, used in our system.
Fig. 5 Set up of a pipe.

Fig. 6 Fluid velocity profile at pipe inlet and at outlet.

References


2.3 Computational Material Science

The research activities of our group during the fiscal year of 2004 are roughly classified into two topics: developments of numerical simulation techniques for materials science and simulation studies for mechanical properties of materials. In the former one, we applied the Algebraic Multi Grid method and the Splitting Scheme for the Ginzburg-Landau Equation which describes superconducting states in superconductors and found that both methods were quite useful to perform fast calculations keeping high precision. Moreover, we have developed a simulation code to study the three-dimensional dynamics of Bose-Einstein condensates in atomic Bose gases by using splitting-Fourier method which is the splitting scheme coupled with the Fourier spectral method. In the numerical technique studies on the Earth Simulator, we have developed a new algorithm for the diagonalization of huge matrices to study strongly correlated Fermion systems. Our method (Preconditioned Conjugate Gradient) showed much more excellent performance than the traditional method (the Lanczos method). By employing the method, we explored a possibility of novel superconductivity on superconductors confined in nano-scale sizes and found superconductivity peculiar to the confined potential. As for the latter topic, we have studied the mechanical behavior of polycrystalline metals/alloys under stress via microscopic molecular dynamics simulation and mesoscopic simulation of intergranular crack propagation. We have developed a new molecular dynamics which enabled us to successfully simulate the grain boundary migration process of polycrystalline nickel. We have also developed and simulated a mesoscopic model of realistic intergranular crack propagation in three-dimensions, and found that cracks tends to branch under certain conditions owing to the general geometric instability which is universal in three-dimensions. We developed the materials tensile test simulation method, based on the first principles calculation, to evaluate the embrittlement potency of the grain boundary due to the segregation of impurity atoms for the nuclear model materials. We studied the nickel-sulfur system, where sulfur atoms have been known experimentally to cause a strong embrittlement of nickel, and found its atomistic mechanism of grain boundary embrittlement. We have also started a new project to study the formation of the rim structure, which is the high porosity microstructure near the rim region of the high burn-up UO2 fuel pellet, by developing mesoscale modeling method, such as cellular automata or phase field methods.
2.3.1 Application of Algebraic Multi Grid (AMG) Method and Splitting Scheme for the Ginzburg-Landau Equation in Superconductors

The Algebraic Multi Grid (AMG) method is applied to numerically solve the Ginzburg-Landau and Maxwell equations which describe superconductivity in materials [2.3-1]. Numerical efficiency are compared between the AMG and the Conjugate Gradient method. In a certain parameter region, i.e., in large Ginzburg-Landau parameter (the ratio of the magnetic penetration depth to the superconducting coherence length), it is found that the AMG method shows an outstanding performance compared to the Conjugate Gradient method. In addition, the splitting scheme, which has been used for energy conserved systems, is applied to numerically solve the time dependent Ginzburg-Landau and Maxwell equations which describe non-equilibrium superconducting states in materials. We systematically examine its numerical stability by performing various numerical simulations. Consequently, we find that the splitting scheme is quite useful for large-scale numerical simulations since the scheme guarantees the highest efficiency if the precision is fixed.

2.3.2 Large-scale Numerical Simulations for 3-D Dynamics of Bose-Einstein Condensates in Atomic Bose Gases

We numerically integrate the 3-D Gross-Pitaevskii equation to investigate dynamical changes of the trapped Bose-Einstein condensate (BEC) from an initial non-vortex state to a steady vortex lattice state after the trigger of the rotation[2.3-2]. We use the splitting-Fourier method as a numerical scheme to perform stable 3-D numerical simulations with high computational efficiency[2.3-3]. Consequently, we find that characteristic 3-D non-steady dynamics of vortices are sequentially divided into three stages, i.e., the vortex initiation, the stochastic vortex wandering, and the vortex lattice vibration. This classification is consistent with experimental observations. This consistency clearly indicates that the 3-D Gross-Pitaevskii equation well describes the dynamics of the condensate while the present numerical scheme is quite useful to precisely examine the condensate dynamics.

2.3.3 High Performance Computing for Ultra Large-scale Eigenvalue Problems on the Earth Simulator

Non-blocking communication in the MPI standard is supposed to provide us with a
functionality to overlap communications with calculations. However, the MPI libraries installed on the Earth Simulator, HITACHI SR8000 and Compaq AlphaServer ES40 do not actually cover overlaps between communications and calculations. Whether the MPI functionality is activated or not depends on installation levels by vendors. Thus, we propose a novel communication strategy to perform the communications and the calculations simultaneously using the intra-node parallelization operation. The exact diagonalization method adopting the strategy solves an eigenvalue problem 1.4 times faster than the method without the strategy[2.3-4].

2.3.4 Novel Superfluidity in Nano-structured Condensed Matter and Trapped Atomic Fermi Gas

An ultra-cold atom gas placed in an optical lattice is an outstanding experimental achievement, which enables to experimentally approach the Hubbard model. Since the discovery of high-Tc cuprate superconductors, the Hubbard model has been a key model to investigate superconductivity originating from the Coulomb repulsion. However, it is still unclear how the repulsive interaction really leads to Cooper pairing which can bring about high-Tc superconductivity. In this year, we therefore investigated a possibility of high-Tc superconductivity confined inside a nano-structured matter. This situation is equivalent to a trapped gas of Fermi atoms with a repulsive interaction in the presence of an optical lattice. Applying the exact diagonalization method to a one-dimensional Hubbard model including the trap potential which has a role to confine Fermi particles, we found that, when the strength of the repulsive interaction exceeds a critical value, the binding energy of two Fermi particles becomes “negative” below the half-filling case (the averaged Fermi- particle number is 1 per site), indicating that an attractive interaction effectively works between Fermi atoms and superfluidity emerges[2.3-5]. In this case, a "Mott core" (showing that the particle occupation is 1 per site) appears in the center of the trap, and the Cooper-pair correlation strongly develops between atoms in the left and right hand sides of this core. In order to clarify an origin of the attractive force, we computed pseudo spin correlation between neighboring sites. As a result, we find that a creation of a singlet pair between both sides of the Mott core is strongly coupled with a pseudo-spin singlet reformation leading to an energy gain process, namely “negative” binding energy.
2.3.5 A Mesoscopic Simulation of Crack Propagation

When polycrystalline steel is subjected to both corrosive environment and tensile stress, it exhibits inter-granular fracture in which crack propagates through grain boundaries. In such cases, which is known as "stress corrosion cracking (SCC)", the shape of the crack often shows intricate branching pattern. We are developing a simple computer model which reproduces this behavior[2.3-6]. The shape of polycrystalline grains is generated by random Voronoi tessellation of the simulation cell. Then the tensile stress is applied to the system and the local stress is calculated by finite-element method. In this model, inter-granular crack front proceeds via the successive failures of grain boundaries; The crack front proceeds through the grain boundary which is adjacent to the crack front and under the strongest tensile stress perpendicular to its surface. This way, the grain boundaries break one by one and the stress distribution is re-calculated at each step. Although this propagation rule forbids the explicit branching at the grain boundary triple junctions (because we only choose a grain boundary which is adjacent to the crack front), the resultant crack shape shows many branches as shown by Fig.1, and strikingly reproduces the experimentally observed branching shape[2.3-6].

We have found that this branching behavior is typical phenomena in three dimensions, and never occurs in the two dimensional models. Figure 2 schematically depicts the mechanism of this branching, which is expected in general cases of crack propagation in three dimensions:

(a) The sloped section is lagged behind, owing to the weak mode-I stress at the crack front.
(b) The left and the right side of the segment bulge inward.
(c) The bulged segments further proceed and eventually overlap each other. Then one part shields the stress and continues to proceed, while the other slows down.
(d) Owing to mode-II stress induced by the interaction between the crack front segments of overlapped parts, each part gets closer and eventually intersects.
(e) Here a segment of the triple junction, or a root of a branch, is formed.
(f) A branched 'tongue' is left behind and the crack front (now intact) proceeds further. In this way, many small branches are left behind the sweeping crack front in three dimensions. This insight on the crack branching mechanism, which is applicable to a wide range of crack propagation models, greatly helps both the physical studies of crack morphology and the engineering studies of structural analysis[2.3-6].
Fig. 1 Crosssection of experimentally observed SCC fracture (left) and the result of simulation (right), which strikingly reproduces the observed branching shapes.

Fig. 2 Schematic depiction of branching mechanism inferred from the result of the simulation. Bold solid lines and bold dotted lines are the crack tip and crack tip under the fracture surface, respectively. The dashed line denotes the triple junction of fracture surface.
2.3.6 Molecular Dynamics Simulation of Grain Boundary Sliding

Molecular simulations are sometimes seriously time consuming when they are used to study mechanical properties of solid materials, such as stress-strain relation or Born stability criterion from elastic constants. In order to resolve this problem, we have proposed a new simulation approach under constant external stress and temperature, modifying Parrinello-Rahman method using the state-of-the-art efficient sampling techniques [2.3-7].

The mechanism of stress-assisted sliding in a Ni symmetrical tilt grain boundary (GB) is investigated by the modified Parrinello-Rahman molecular dynamics [2.3-8]. It has been found that the grain boundary can slide in the direction perpendicular to the tilt axis with the aid of shear stress in that direction. This sliding is coupled to the diffusive motion of the grain boundary involving a collective rearrangement of atoms near the boundary. The critical stress necessary to move the grain boundary damps almost exponentially as the temperature is increased. At temperatures above about a half of the melting point, random walk of GB diffusion occurs without the assistance of stress. On the other hand, it is only at much higher stress that the grain boundary can slide in the direction parallel to the tilt axis whereas the sliding is not coupled to the GB diffusion.

2.3.7 First-principles Study on the Grain-boundary Embrittlement of Nickel by Sulfur Segregation

Since 1925, it has been well known that the addition of sulfur to many metals and alloys causes them to become brittle. Metallic materials consist of crystal grains several tens of micrometers in size. The boundary between the crystal grains is called the “grain boundary”. In the 1970’s, it was found that sulfur atoms gather at the grain boundaries by heating, etc., and thereby metallic materials break easily at the grain boundaries. However, it was not well understood why and how the sulfur weakened the grain boundaries.

We simulated this phenomenon on a supercomputer using a first-principles calculation, which is the method to numerically solve the basic equation (Schrödinger equation) of quantum mechanics and thereby clarify the properties of materials at the electronic level. We applied this method to a nickel system. First, we investigated the extent the sulfur atoms can gather at the grain boundary by calculating the energy difference between the two cases; the sulfur atom is in the inner bulk region and in the
As a result, we have shown that the sulfur atoms can gather at the grain boundary even when the sulfur concentration in inner bulk region is 25 atomic parts per million. Although this had been clarified by experiments, we found that the sulfur atoms can be adjacent to each other but then they cannot make strong bonds owing to the stronger bonds between nickel and sulfur atoms. This leads to a long S-S bonding distance that forces apart the two nickel crystal grains. From first-principles tensile test calculations, we found that the maximum tensile strength is reduced by one order of magnitude by the repulsive interactions among sulfur atoms (Fig. 3). Thus, we have concluded that the repulsive interactions between segregated sulfur atoms cause metals to become brittle[2.3-9].

Fig. 3 Tensile test calculations from first principles. The 2-monolayer segregation of sulfur at sites 0 and 2 reduces the tensile strength by one order of magnitude.
2.3.8 A Mesoscopic Model to Simulate the Formation of the Rim-structure in UO$_2$ Fuel Pellets.

We have kicked off a new five-year project to computationally investigate the microstructure of UO$_2$ fuel. The project especially examines the development of the so-called rim-structure, i.e., a porous microstructure at the periphery of high-burnup fuel pellets. These pores are bubbles including the highly insoluble gaseous atoms such as Xenon or Krypton, which are caused by the nuclear fissions and the following radioactive decay processes. Such gaseous atoms inside the fuel are therefore mobile and their dynamics are critical for ensuring the confinement of radioactive fission products.

For this computational modeling purpose, the usage of a cellular automaton was proposed, and as a first step a prototype was developed in order to assess its modeling capability. The prototype is a two-dimensional dynamical system [2.2-10], adopting a simplified local interaction model between gaseous atoms and vacancy sites. Figure 4 shows a snapshot from the prototype calculations mimicking the porous structure.

We have confirmed the cellular automaton methodology has a sufficient modeling capability for this purpose. The next step is to develop more realistic three-dimensional model so that the mechanism of the formation of such characteristic microstructures can be investigated in detail.

![Image](a) A porous microstructure of UO$_2$ fuel, and (b) a simulation by the two-dimensional cellular automaton: The dark parts are the pores in which the black cells denotes the inert gaseous atoms.
References


2.4 Quantum Bioinformatics Research

The group covers a wide range of computational biology, including bioinformatics and macromolecular simulation. Bioinformatics is the field to analyze huge amounts of data emerging out of genome sequencing and structural genomics projects. Macromolecular simulation deals with large size biomolecules, such as protein complexes binding to DNA/RNA. It is not common to find a single group working in these two fields of computational biology. The difficulty in forming a group like ours lies in the fact that each member is required to have wide knowledge in some of the following fields: biology, physics, chemistry, mathematics, evolution, statistics, and computation.

Bioinformatics, one of the main topics in the group, is defined as a field to develop new methods to extract information from genome/proteome information and to build integrated tools/databases to expand our knowledge. Macromolecular simulation, the other aim in the group, is to develop new computational techniques to study the dynamic structures of proteins and nucleic acids and to reveal the molecular mechanisms that realize their biological functions.

The research in this group is a basic science and aims to expand knowledge on biology, developing new ideas and techniques. However, the knowledge we will gain will easily be applied to pharmaceutical science for development of new drugs to cure diseases, to agricultural science, and to other fields.

2.4.1 Development of Protein Information Databases and Analysis Tools

Emergence of whole genome sequences of more than 200 species from different kingdoms of life has laid an enormous impact on our view toward life. In addition, three-dimensional (3D) structures of the representative proteins are getting obtained. However, the information must be converted so that they are understandable. There are a lot of software available on the Internet to retrieve meaningful information from the genome sequences and proteome structures. However, the variety in methods and data formats precludes us from deep analyses of the genome sequences. The current obstacles are as follows; 1) There exists no overviews for the state-of-the-art software for bioinformatics, 2) There are so many software to handle a single data that no one can tell which software should be used to meet the end, and 3) There are so many data formats for input and output that conversion between different formats is getting a most time consuming job.

We have initiated, in 2002, developing a system named BAAQ (Bioinformatics: Ask
Any Questions) that realize easy analyses of these data. BAAQ works on GUI named TME (Task Mapping Editor) developed by CCSE. On TME any data and software are visualized as icons, and data flow as lines connecting icons[2.4-1]. For the widespread use of the system, it is important for BAAQ to run on personal computers as well as on grid computing system. For this purpose, we developed the installers and conducted porting experiments on various kinds of Linux OS in 2004. We have also started to expand the system in such a way that user can share combinations of bioinformatics tools (scenarios) and search for appropriate scenarios. Furthermore, we continued to work on increasing the number of the bioinformatics tools to BAAQ for preparation of genome annotation of radiation resistant bacterium. Prototypes of the new scenarios have been built based on researches of human genome annotation [2.4-2] and electrostatic potential calculation for protein structures [2.4-3]. This work has been carried out in collaboration with Bioinformatics Unit at Nara Institute of Science and Technology.

2.4.2 Development of DNA Repair Protein Databases

DNA molecules carry genetic information. The information is copied to proteins at the appropriate time at the appropriate places. The information retrieval system is also made from proteins and those proteins are well tuned to maintain the organisms [2.4-4]. If DNA get damaged by radiation, the organisms repair the damages. Without DNA repair systems, DNA sequence would change frequently and genetic information would not be delivered from generation to generation. Thus, DNA repair is one of the essential mechanisms for any organisms and is carried out by so-called DNA repair proteins through a series of chemical reactions. Each DNA repair protein works for a specific type of DNA damage.

In 2004, we started to update our DNA repair databases. It is getting known that the living organisms repair not only DNA but also RNA. Thus, we tried to update the DNA repair protein databases by adding the information about three-dimensional structures of RNA repair proteins. However, there is not so much structural information about the interaction between the proteins and the RNA at the atomic resolution. We, therefore, developed a method to predict the interactions between the RNA-binding proteins and the RNA using ITBL computers. By analyzing the small number of experimental data statistically, we derived the tendency of the interactions between the amino acid residues and the RNA, and developed empirical rules for the interaction [2.4-5]. Based on the rules, it will become possible to predict which part of the protein
interacts with the RNA.

We have also developed a new database on SNPs (Single Nucleotide Polymorphisms) to understand the effect on proteins of the point mutations, which escaped the DNA repair systems. By the use of the database, we are able to predict the effect of the SNPs on the three-dimensional structure of the proteins. This prediction will be valuable to understand the mechanism of the formation of the genetic diseases due to the SNPs.

2.4.3 Development of the Dose Calculation System IMAGINE for Remotely Supporting Radiotherapy using Photons

A dose calculation system for providing accurate dose distribution in a patient body is under development for supporting radiotherapy using photons and electrons. In this system, a sophisticated human model, a precise accelerator head model, and Monte Carlo calculations are utilized to perform realistic simulation. The dose distribution is calculated by this system on the ITBL high-performance computer at the dose calculation center located at the JAERI Kansai establishment, and the related data are transferred through a network.

First, the CT images and treatment parameters are sent from a hospital to the center; a human model for the patient is constructed rapidly; the dose distribution is calculated with super-parallel computing; and the calculated results are sent back to the hospital. This system is intended to support the quality assurance of a great number of current treatments carried out in Japan. Further, this system is planned to apply to advanced radiotherapy such as IMRT (Intensity Modulated Radiation Therapy) and CTRTx (CT Radiotherapy).

A prototype of the multipurpose IMAGINE system was completed in fiscal year 2004. The system showed a proper performance in the test where a therapy planning system at the Keio university hospital was connected to the ITBL computer through servers consisting the system. An important problem left is how to simulate the effect of multi-leaf collimators (MLC) properly in a short time. The problem is expected to be solved by the MLC calculation engine under development. The multi-purpose IMAGINE system is planned to be completed in 2007 after a certain number of practical tests in collaboration with several medical facilities [2.4-6].
2.4.4 Development of Molecular Dynamics Simulation System

A large number of structures of biological macromolecules are solved by X-ray crystallography and other experimental methods, and the need for large-scale molecular dynamics simulations is increasing [2.4-7, 2.4-8, 2.4-9]. To meet this need, using the ITBL computer as well as other computers available in JAERI, we are developing a molecular dynamics simulation system, called PABIOS, designed to study a system composed of more than a million particles efficiently on parallel computers.

In 2003, we developed a code equipped with the Particle-Particle Particle-Mesh (PPPM) method, which is one of the molecular dynamics calculation modules and computes long-range interactions accurately and efficiently. In 2004, we continued to work on the improvement of the vectorization ratio of the PPPM algorithm. Moreover, a dynamic load-balancing algorithm was developed to optimize the load balance among the processors. In the PPPM method, the parallel efficiency ratio tends to be lower as the number of processors increases. We could mitigate this effect by limiting the number of processors for the PM calculation and assigning the rest of the processors to other calculations. By these efforts, we successfully improved the parallel efficiency of our program.

In order to improve the performance of PABIOS on the Earth Simulator, the algorithm to calculate short-range interactions (PP interactions) was intensively vectorized. A benchmark test was carried out using the system of a RuvA-Holliday junction DNA complex, which consisted of 166,177 atoms. At present, PABIOS has achieved a parallel efficiency ratio of 55.0%, and a vectorization ratio of 97.5%, even when as many as 15 nodes (120 processors) were used. As a result, the speed of calculation was about twice as fast as that in the last year.
References


3 Research Achievements

3.1 Publication List (April 2004 – March 2005)

Papers published in journals


22) Kim, T.P.O., Yura, K., Go, N., and Harumoto, T.: Newly sequenced eRF1s from ciliates: the diversity of stop codon usage and the molecular surfaces that are important for stop codon interactions., Gene, 346, 277 (2005).


Papers published in conference proceedings


9) Kenji Higuchi, Hiroshi Maesako, Tetsuo Aoyagi, Yukihiro Hasegawa, Nobuhiro Yamagishi, Norihiro Nakajima, and Genki Yagawa, “Current Status of ITBL Project and Basic Middleware,” (Tokyo Japan, May.24-26, 2004), Vol9,No.2,
pp609-612 [in Japanese].


Oral / Poster presentations


4) M. Machida, and N. Sasa, “Quantized Vortex Dynamics in Bose-Einstein Condensate: Role of Microscopic Dissipation,” 54-th Meeting of Theoretical and Applied Mechanics, (Tokyo, Japan, Jan 8-9, 2005).


2005).


21) M. Shiga, and W. Shinoda, “A study on grain boundary sliding by molecular


33) Kim, T. P. O, Yura, K., Go, N. and Harumoto, T.: Computational analyses of eRF1 molecular surface that is important for stop codon interactions, The 42nd Annual meeting of biophysical society of Japan, Kyoto, Japan, Dec. 2004

34) Ishida, H., and Go, N.: Umbrella sampling simulation of branch migration in a model of Holliday junction, Biophysical Society 49th annual Meeting, California, USA, Feb. 2005

Workshops and symposium


HLRS, (Stuttgart, Germany, Mar. 2005).


17) Matsumoto, A: Dynamic property of DNA structure, The 10th CCSE workshop, Tokyo, Jan. 2005
3.2 Staff List in Center for promotion of Computational Science and Engineering (April 2004 – March 2005)

Director: Genki Yagawa
Vice Director: Toshio Hirayama

Research Group for Computational Science in Atomic Energy
Group Leader: Norihiro Nakajima
Senior Engineer: Kenji Higuchi
Research Scientist: Masato Ida
Staff (Engineer): Hideo Kimura
Researcher (Term Limited): Akemi Nishida
Rong Tian
Post-Doctoral Fellow: Osamu Hazama
Yufei Shu
Fellow of Advanced Science: Kazunori Shinohara

Research Group for Computational Materials Science in Atomic Energy
Group Reader, Principal Scientist: Masahiko Machida
Research Scientist: Narimasa Sasa
Futoshi Shimizu
Mitsuhiro Itakura
Susumu Yamada
Motoyuki Shiga
Cooperative Staff: Tomoko Kadoyoshi
Visiting Researcher: Chuichi Arakawa

R&D Group for Numerical Experiments
Group Leader, Principal Scientist: Hideo Kaburaki
Senior Engineer: Tomoaki Suzudo
Senior Scientist: Masatake Yamaguchi
Research Engineer: Ken-ichi Ebihara
Quantum Bioinformatics Group

Group Leader: Nobuhiro Go
Senior Scientist: Kei Yura
Research Scientist: Atsushi Matsumoto

Kensuke Nakamura
Post-Doctoral Fellow: Yoshiteru Yonetani

Oanh T.P. Kim
Fellow of Advanced Science: Shoichi Metsugi

Masataka Oikawa
Principal Scientist: Kimiaki Saito
Senior Scientist: Hidetoshi Kono
Research Scientist: Hisashi Ishida
Invited Researcher: Akio Kitao
### 国際単位系（SI）と換算表

#### 表１ SI基本単位および補助単位

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#### 表２ SIと併用される単位

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<td>グル</td>
<td>J/s</td>
</tr>
<tr>
<td>クロロン</td>
<td>C</td>
</tr>
<tr>
<td>ヴェルト</td>
<td>V</td>
</tr>
<tr>
<td>ウバ</td>
<td>W</td>
</tr>
<tr>
<td>ウバ</td>
<td>W</td>
</tr>
<tr>
<td>ジェルム</td>
<td>Wb</td>
</tr>
<tr>
<td>シャス</td>
<td>T</td>
</tr>
<tr>
<td>シャス</td>
<td>T</td>
</tr>
<tr>
<td>セルシウス度</td>
<td>°C</td>
</tr>
<tr>
<td>エルム</td>
<td>lm</td>
</tr>
<tr>
<td>ルクス</td>
<td>lm/m²</td>
</tr>
<tr>
<td>ベクレル</td>
<td>Bq</td>
</tr>
<tr>
<td>グレイ</td>
<td>Gy</td>
</tr>
<tr>
<td>シーベルト</td>
<td>Sv</td>
</tr>
</tbody>
</table>

#### 表４ SIと共に暫定的に維持される単位

<table>
<thead>
<tr>
<th>名称</th>
<th>記号</th>
</tr>
</thead>
<tbody>
<tr>
<td>アンギストローム</td>
<td>Å</td>
</tr>
<tr>
<td>バー</td>
<td>b</td>
</tr>
<tr>
<td>バール</td>
<td>bar</td>
</tr>
<tr>
<td>ガル</td>
<td>Gal</td>
</tr>
<tr>
<td>クリ</td>
<td>Ci</td>
</tr>
<tr>
<td>レントゲン</td>
<td>R</td>
</tr>
<tr>
<td>レイ</td>
<td>rem</td>
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</tbody>
</table>

#### 表５ SI換算表

<table>
<thead>
<tr>
<th>名称</th>
<th>記号</th>
</tr>
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<tbody>
<tr>
<td>10^-1</td>
<td>エクサ</td>
</tr>
<tr>
<td>10^-10</td>
<td>ペタ</td>
</tr>
<tr>
<td>10^-12</td>
<td>テラ</td>
</tr>
<tr>
<td>10^-15</td>
<td>テラ</td>
</tr>
<tr>
<td>10^-18</td>
<td>デカ</td>
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(1) 表１－５は「国際単位系」第5版、国際度量衡局1985年刊行による。ただし、1eV の値はCODATAの1986年推薦値によった。

2. 表４には海里、ノット、アール、ヘクタールも含まれているが日常の単位なのでここでは省略した。

3. バーは、J/S では流体の圧力を表す場合に限り表2のカテゴリに分類されている。

4. E.C国際議事録指令ではbar, barsおよび「圧の単位」mmHgを表2のカテゴリーに入れている。

### 計算表

<table>
<thead>
<tr>
<th>名称</th>
<th>MPa（10bar）</th>
<th>kgf/cm²</th>
<th>atm</th>
<th>mmHg(Torr)</th>
<th>lbf/in²（psi）</th>
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</thead>
<tbody>
<tr>
<td>1</td>
<td>10.1972</td>
<td>9.86923</td>
<td>71.0602×10²</td>
<td>145.038</td>
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</tr>
<tr>
<td>9.80656</td>
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<td>9.86923</td>
<td>71.0602×10²</td>
<td>145.038</td>
<td></td>
</tr>
<tr>
<td>4.48822</td>
<td>0.45592</td>
<td>1</td>
<td>71.0602×10²</td>
<td>145.038</td>
<td></td>
</tr>
</tbody>
</table>

### 計算表

<table>
<thead>
<tr>
<th>名称</th>
<th>J(10⁶ erg)</th>
<th>kgf*cm</th>
<th>kW-h</th>
<th>cal (US)</th>
<th>Btu</th>
<th>ft-lbf</th>
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</thead>
<tbody>
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<td>2.7777×10⁻¹⁰</td>
<td>2.7777×10⁻¹⁰</td>
<td>2.7777×10⁻¹⁰</td>
<td>1.01872</td>
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<td>2.7777×10⁻¹⁰</td>
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<td>1</td>
<td>71.0602×10²</td>
<td>145.038</td>
<td></td>
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</tr>
</tbody>
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### 計算表

<table>
<thead>
<tr>
<th>名称</th>
<th>Bq</th>
<th>Ci</th>
</tr>
</thead>
<tbody>
<tr>
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<td>1.00</td>
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<td>3.7×10⁹</td>
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</table>

(86年12月26日現在)