JAEA-Review
2007-015

JP0750187

JAEA-Review

Annual Report of R&D Activities in Center for Promotion of Computational Science and Engineering and Center for Computational Science & e-Systems from April 1, 2005 to March 31, 2006

Center for Computational Science & e-Systems

March 2007

Japan Atomic Energy Agency

日本原子力研究開発機構

本レポートは日本原子力研究開発機構が不定期に発行する成果報告書です。
本レポートの入手並びに著作権利用に関するお問い合わせは、下記あてにお問い合わせ下さい。
なお、本レポートの全文は日本原子力研究開発機構ホームページ（http://www.jaea.go.jp/index.shtml）より発信されています。このほか財団法人原子力弘済会資料センター*では実費による複写頒布を行っております。

〒319-1195　茨城県那珂郡東海村白方白根2番地4
日本原子力研究開発機構　研究技術情報部　研究技術情報課
電話 029-282-6387, Fax 029-282-5920

*〒319-1195　茨城県那珂郡東海村白方白根2番地4　日本原子力研究開発機構内

This report is issued irregularly by Japan Atomic Energy Agency
Inquiries about availability and/or copyright of this report should be addressed to
Intellectual Resources Section, Intellectual Resources Department,
Japan Atomic Energy Agency
2-4 Shirakata Shirane, Tokai-mura, Naka-gun, Ibaraki-ken 319-1195 Japan
Tel +81-29-282-6387, Fax +81-29-282-5920

JAEA-Review 2007-015

Annual Report of R&D Activities in Center for Promotion of Computational Science and Engineering and Center for Computational Science & e-Systems from April 1, 2005 to March 31, 2006

Center for Computational Science & e-Systems

Japan Atomic Energy Agency
Tokai-mura, Naka-gun, Ibaraki-ken

(Received January 22, 2007)

This report provides an overview of research and development activities in Center for Computational Science and Engineering (CCSE), JAERI in the former half of the fiscal year 2005 (April 1, 2005 – Sep. 30, 2006) and those in Center for Computational Science & e-Systems (CCSE), JAEA, in the latter half of the fiscal year 2005(Oct 1, 2005 – March 31, 2006). In the former half term, the activities have been performed by 5 research groups, 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. At the beginning of the latter half term, these 5 groups were integrated into two offices, Simulation Technology Research and Development Office and Computer Science Research and Development Office at the moment of the unification of JNC(Japan Nuclear Cycle Development Institute) and JAERI(Japan Atomic Energy Research Institute), and the latter-half term activities were operated by the two offices. A big project, ITBL (Information Technology Based Laboratory) project and fundamental computational research for atomic energy plant were performed mainly by two groups, the R&D Group for Computer Science and the Research Group for Computational Science in Atomic Energy in the former half term and their integrated office, Computer Science Research and Development Office in the latter half one, respectively. The main result was verification by using structure analysis for real plant executable on the Grid environment, and received Honorable Mentions of Analytic Challenge in the conference "Supercomputing (SC05)". The materials science and bioinformatics in atomic energy research field were carried out by three groups, 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 the former half term and the one integrated office, Simulation Technology Research and Development Office and Computer Science Research in the latter half term, respectively. Through the 2005 fiscal year, main topics studied intensively in materials science and bioinformatics were as follows; a first-principle calculation to examine embrittlement effects of the grain boundaries for more than 10 impurity elements, a semi-first principle simulation to explore non-equilibrium superconducting dynamics after the neutron capture in neutron detector device using MgB2 superconductor, a molecular dynamics simulation of DNA replication/repair protein with DNA to analyze its atomic detail for realizing its function, and so on. The remarkable issue in these researches was that large-scale simulation technique developments on the Earth Simulator was selected as "Gordon Bell Prize finalist" in the conference "Supercomputing (SC05)".

Keywords: R&D Activities, CCSE, ITBL Project, Computer Technology for Atomic Energy Research, Computational Materials Science, Computational Quantum Bioinformatics

JAEA-Review 2007-015

平成17年度　システム計算科学センター　研究開発年報

日本原子力研究開発機構
システム計算科学センター

(2007年1月22日受理)

本報告書では、平成17年度4月1日～9月30日までの期間における日本原子力研究所・計算科学技術推進センター（CCSE）と平成17年度10月1日～3月31日までの日本原子力研究開発機構・システム計算科学センターにおける一年間（平成17年度）の研究開発活動について報告する。これらの研究開発は、平成17年度前期、CCSEにおける５つの研究グループ、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、同17年度後期は、２つに統合された高度計算科学技術開発室とシミュレーション技術開発室により執り行われた。高度計算科学を代表するITBL計画と原子力エネルギーシミュレーション基盤研究は主として、17年度前期、２つの研究グループ（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）、後半は、それらを統合した高度計算科学技術開発室によって遂行された。その結果として、ITBL基盤ソフトウエアと独グリッド環境の相互利用を可能とした他、グリッド計算機環境で動作する大規模構造解析技術を実プラントデータで実証し、世界最大の高性能計算機科学国際会議Supercomputing（SC05)で”Honorable Mention”を受けた。一方、原子力分野における物質材料シミュレーションや、生体及びDNA損傷修復機構解明のためのシミュレーションは、17年度前期、３つの研究グループ（原子力物性計算科学研究グループ、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）、17年度後期、それらを１つに統合したシミュレーション技術開発室によって執り行われた。その結果、原子炉鋼材の10種以上の不純物に対する粒界脆化度の第一原理計算による定量的評価結果と超伝導中性子デバイスの中性子衝突後の非平衡ダイナミクスによる時空間分解能予測結果が示された他、生体分子動力学シミュレーションによるDNA複製修復タンパク質の機能解析が展開できた。また、これらの一連の研究を通して研鑽した並列計算技術は、上記国際会議SC05にてゴードンベル賞のファイナリストに選出された。

原子力科学研究所(駐在)：〒319-1195 茨城県那珂郡東海村白方白根2-4

This is a blank page.

Contents

Foreword

1. Overview of CCSE R&D ---------- 1

2. CCSE Research and Development Activities ---------- 3

2.1 Fundamental Computer Technology for Atomic Energy Research (ITBL Project) ---------- 3

2.1.1 Research and Development of ITBL middleware ---------- 3

2.1.2 Visualization System for Grid Environment ---------- 5

2.1.3 Developments of high performance finite elements for structural analysis -- 6

2.1.4 Wave propagation of piping structures under impulsive load ---------- 7

2.1.5 Complementary study of phase properties and interaction force of acoustic bubbles ---------- 9

2.1.6 Avoided crossings in triple-bubble systems ---------- 12

2.2 Computational Materials Science for Atomic Energy Research ---------- 15

2.2.1 First-Principles Analysis for the Effects of More Than 10 Solute Elements on Grain Boundary Embrittlement of Nuclear-Reactor Materials ---------- 17

2.2.2 Mesoscopic modeling of the rim-structure formation of UO2 fuel pellets -- 19

2.2.3 Mesoscopic Modeling of Intergranular Crack-Propagation in Polycrystalline Nuclear Reactor Materials ---------- 21

2.2.4 Accuracy Enhancement in the Simulation Model for Superconducting Neutron Detector ---------- 23

2.3 Computational Quantum Bioinformatics for Atomic Energy Research ---- 25

2.3.1 Computational Predictions of Genes and DNA/RNA interfaces of Proteins for Repair Related Genes/Proteins ---------- 25

2.3.2 Fast Molecular Dynamics Simulation Programs for Studying Repair Mechanisms of Damaged DNA ---------- 28

2.3.3 Development of IMAGINE, the Dose Calculation System for Remotely Supporting X-ray Radiotherapy ---------- 30

3. Research Achievements ---------- 33

3.1 Publication & Presentation List ---------- 33

3.2 Staff List ---------- 47

目　次

前書き

1.　CCSE 研究・開発部門の概要 ---- 1

2.　CCSE 研究・開発活動 ---- 3
2.1　原子力研究のための並列処理基本システムの研究開発 ---- 3
2.1.1　ITBL 基盤ソフトウエアの研究開発 ---- 3
2.1.2　グリッド環境における可視化技術 ---- 5
2.1.3　高性能有限要素構造解析手法の開発 ---- 6
2.1.4　衝撃力を受ける配管系構造物の波動伝播シミュレーション ---- 7
2.1.5　音響的に相互作用する複数気泡の位相特性と相互作用力に関する補完的検討 ---- 9
2.1.6　三気泡系に現れる擬交差 ---- 12
2.2　原子力計算材料科学 ---- 15
2.2.1　原子炉材・粒界脆化に対する 10 種以上の不純物効果の第一原理計算による解析 ---- 17
2.2.2　酸化ウラン燃料ペレットのリム組織形成メゾスケール・モデリング 19
2.2.3　原子炉材・多結晶体における粒界割れき裂進展のメゾモデリング ---- 21
2.2.4　超伝導中性子検出器シミュレーションモデルの高精度化 ---- 23
2.3　原子力計算量子生命科学 ---- 25
2.3.1　ＤＮＡ／ＲＮＡ修復関連遺伝子と蛋白質のＤＮＡ／ＲＮＡ界面予測 ---- 25
2.3.2　高速大規模生体分子シミュレーションによる損傷ＤＮＡの修復機構研究 ---- 28
2.3.3　Ｘ線治療用線量計算遠隔支援システムＩＭＡＧＩＮＥの開発 ---- 30

3.　研究業績 ---- 33
3.1　研究論文及び研究発表リスト ---- 33
3.2　スタッフ・リスト ---- 47

Acronyms

AVS	Application Visualization System
CCSE	Center for Promotion of Computational Science and Engineering
CCSE	Center for Computational Science & e-Systems
FEM	Finite Element Method
GB	Grain Boundary
GUI	Graphical User Interface
HLRS	High Performance Computing Center in Stuttgart
IMAGINE	IT-based Medical Aiding Gear for Instantaneous Numeration of Energy Deposition Distribution System
IT	Information Technology
ITBL	IT Based Laboratory
ITER	International Thermonuclear Experimental Reactor
JAEA	Japan Atomic Energy Agency
JAERI	Japan Atomic Energy Research Institute
JAXA	Japan Aerospace Exploration Agency
JST	Japan Science and Technology Agency
LHC	Large Hadron Collider
MD	Molecular Dynamics
NIED	National Institute foe Earth Science and Disaster Prevention
NIMS	National Institute for Materials Science
RPV	Reactor Pressure Vessel
SC05	International Conference for High-performance computing, Networking, Storage and Analysis
SCC	Stress Corrosion Cracking
STAMPI	Seamless Thinking Aid Message Passing Interface
STARPC	Seamless Thinking Aid Remote Procedure Call
SCUBA	Simulation Codes for Huge Biomolecular Assembly
TME	Task Mapping Editor
UNICORE	Uniform Interface to Computing Resources
VASP	Vienna Ab initio Simulation Package

Foreword

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

At the beginning of the last half term in the fiscal year 2005, Japan Nuclear Cycle Development Institute (JNC) and Japan Atomic Energy Research Institute (JAERI) were unified into an organization, Japan Atomic Energy Agency (JAEA), CCSE was simultaneously renamed the Center for Computational Science & e-Systems (CCSE) to match the name with its activities, and 5 research groups were integrated into two research offices. Since the reorganization, the new CCSE has further concentrated on joint studies with other research sections in JAEA.

Throughout the fiscal year 2005, CCSE has carried out and completed the ITBL(Information Technology Based Laboratory) project in cooperation with 90 organizations. The goal of ITBL project is to establish a virtual research laboratory in which researchers in various disciplines can collaboratively develop highly sophisticated simulation systems by fully utilizing computer resources located inside high-speed network. We successfully realized the virtual research laboratory based on ITBL middleware developed in CCSE.

Large-scale simulation is now an essential tool in atomic energy research field as well as other scientific and engineering fields. The research potential of CCSE covers plant analysis, materials and biological science, and its application toward atomic energy research is promising. Several joint researches with other research sections inside JAEA are now ongoing by utilizing the wide potential.

It is our pleasure to publish the annual report of our research and development activities in the fiscal year of 2005. We believe that the research and development in CCSE becomes quite fruitful through cooperative interactions with other research sections in JAEA and other organizations.

Genki Yagawa
Director
Center for Computational Science and e-Systems,
JAEA

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. These five groups are integrated into two offices: (1) Simulation Technology Research and (2) Development Office and Computer Science Research and Development Office at the beginning of the latter half term of the fiscal year 2005. The R&D activity of these groups and offices in both CCSE is described in Chapter II. Here, we summarize the main results of their activities.

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 supercomputers located all over Japan, and by sharing the relevant computer hardware, software including database resources. Its main result in the fiscal year 2005 was structure analysis for real plant executable on the Grid environment. The research work received Honorable Mentions of "Analytic Challenge" in the conference "Supercomputing (SC05)".

A small amount of impurity elements brings about a drastic change in the mechanical properties of metals. It is well known that phosphorous (P), which is included in reactor pressure vessel (RPV) steels, is a weak embrittler for iron grain boundaries. We quantitatively study its impurity embrittlement effect for the iron grain boundaries by performing large-scale first-principle calculations. The research result was published in a commercial based magazine "Science".

When polycrystalline steel is subjected to both corrosive environment and tensile stress, it exhibits so-called "stress corrosion cracking (SCC)" which is known to be the most critical cause of degradation of nuclear reactor structural materials. In order to reproduce the crack propagating pattern and understand why such a pattern emerges in nuclear reactor materials, we have developed a coarse-grained simulation model of SCC and succeeded in identifying the origin of the pattern.

In studies on material properties in nano-scale structures, the superconducting non-equilibrium dynamics have been simulated on the Earth Simulator to clarify how the superconducting radiation detector behaves after a neutron capture and how the detector system gives a signal for detection of a neutron. The parallelization techniques and the large-scale

simulation results related to these researches were selected as a finalist of Gordon Bell Prize in the conference "Supercomputing (SC05)".

In application of ITBL to bioinformatics analyses, development of tools to analyze static and dynamic structures of biomolecules has been continued. We could develop a prototype of a tool to predict RNA interface of proteins that can be extended to atomic function prediction for DNA/RNA repair related proteins and an efficient molecular dynamics simulation program making much use of computational power of ITBL and other parallel computer resources. We have also developed an image-processing tool for medical application of ITBL.

2. CCSE Research and Development Activities

2.1 Fundamental Computer Technology for Atomic Energy Research (ITBL Project)

2.1.1 Research and Development of ITBL middleware[2.1.1-1]

Recently, there are some scientific global projects such as the International Thermonuclear Experimental Reactor (ITER) as well as the Large Hadron Collider (LHC). As the increase of global projects, the worldwide science grid environment, which enables to use such a large-scale experimental facility world-widely, becomes more necessary. To construct such an environment, the interoperability among different science grid systems is indispensable.

Under such consideration, Center for Computational Science & e-Systems of Japan Atomic Energy Agency (CCSE/JAEA) has achieved an interoperability between UNiform Interface to COmputing REsources (UNICORE) middleware of High Performance Computing Center Stuttgart (HLRS) and Information Technology Based Laboratory (ITBL) middleware (Fig.1).

ITBL project is a national project placed as one of the e-Japan Priority Policy Program to realize the e-Japan Strategy which sets goals to make Japan the world's most advanced IT nation. ITBL project was launched at April 2001 by six institutes: NIMS, NIED, JAXA, RIKEN, JST and JAEA and had been carried out up to March 2006 as 5 years' plan. The objective of ITBL project is to establish virtual laboratories in which researchers in various disciplines can collaboratively develop highly sophisticated simulation systems by fully utilizing computer resources located inside high-speed network. At the end of the ITBL project, 680 researchers from 90 organizations participate in ITBL project and ITBL middleware integrates 57TFlops computer resources. These resources consist of 26 computers from 13 sites (Fig.2). CCSE/JAEA keeps operating ITBL middleware (Fig.3) to maintain the ITBL environment and contributes to the establishment of a backbone grid environment in Japan.

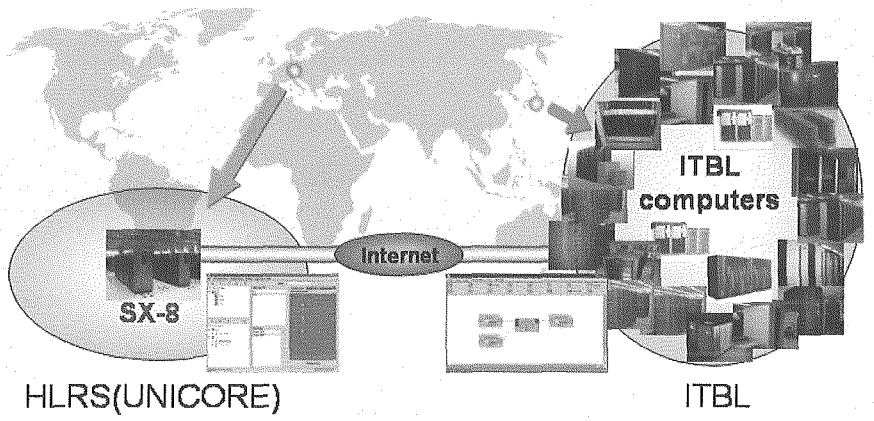


Fig.1 Interoperability between UNICORE and ITBL

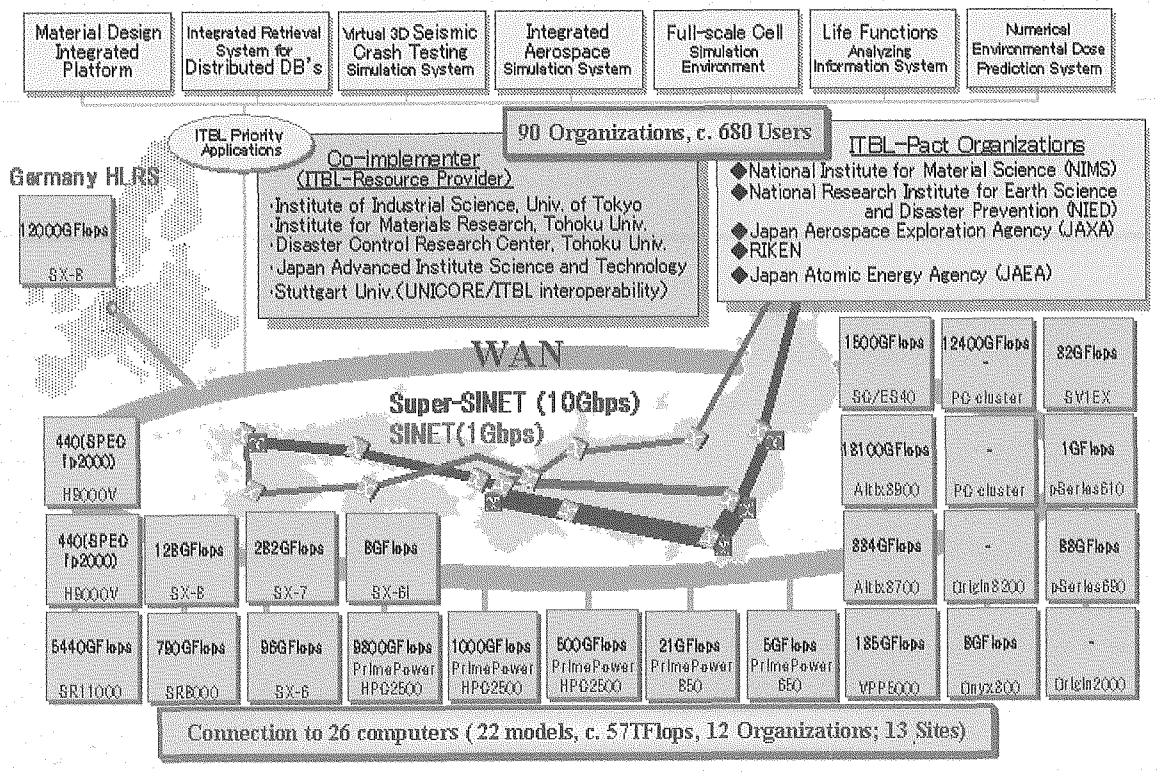


Fig.2 Status of ITBL (as of Mar. 31, 2006)

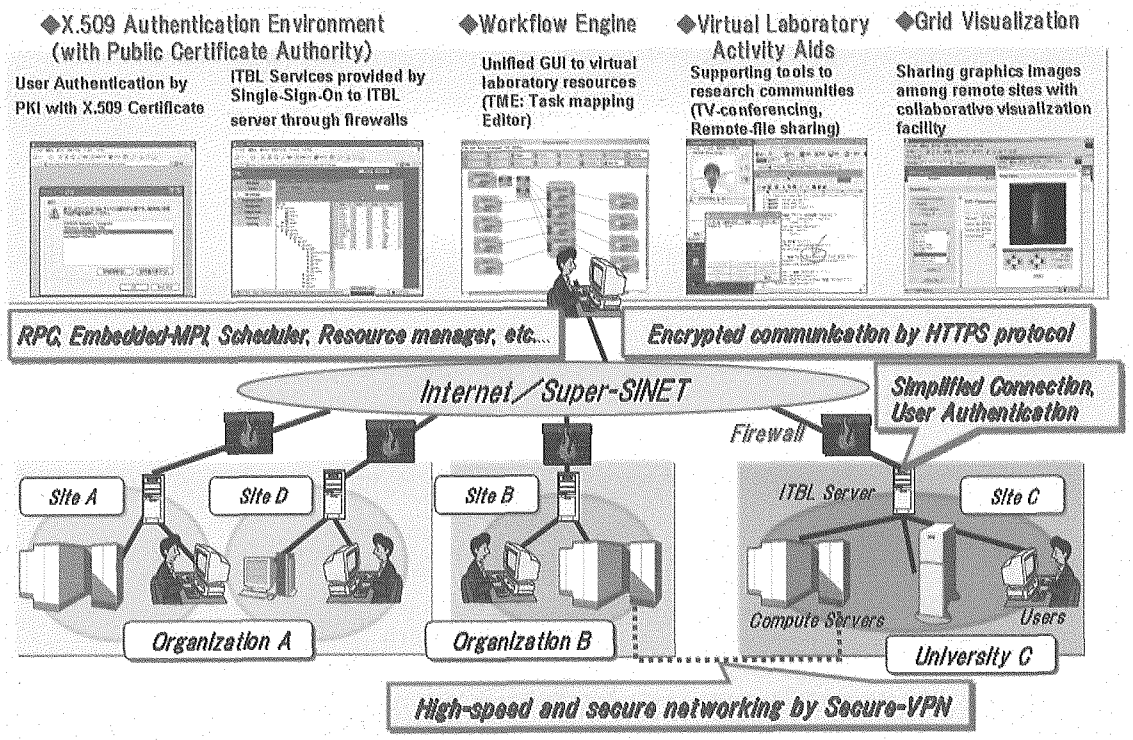


Fig.3 Main function of ITBL middleware

2.1.2 Visualization System for Grid Environment[2.1.2-1]

CCSE/JAEA has developed ITBL middleware as ITBL system infrastructure software and operated it since April 2003. Tools of ITBL middleware enable secure communication among plural supercomputers via internet (STARPC: Seamless Thinking Aid Remote Procedure Call), parallel computation between different types of supercomputer (STAMPI: Seamless Thinking Aide Message Passing Interface), job control on distributed computational environment (TME: Task Mapping Editor), parallel and distributed visualization (AVS/ITBL) and so on. Researchers can use these tools on the Web browser as shown in Fig.4.

AVS/ITBL has been developed aiming at constructing a visualization system suitable for grid environment. It works in cooperation with AVS/Express (commercial software). It displays, controls and shares an image using Web GUI (authentication using X.509). It enables remote data read. It accelerates visualization using parallel and distributed processing (PST: Parallel Support Toolkit has been developed by CCSE/JAEA).

PST has three kinds of parallelism: data parallelism (each module itself executes in parallel), task parallelism (Independent modules execute in parallel), and pipeline parallelism (series of modules execute in parallel). These parallelisms work on one server / two or more servers.

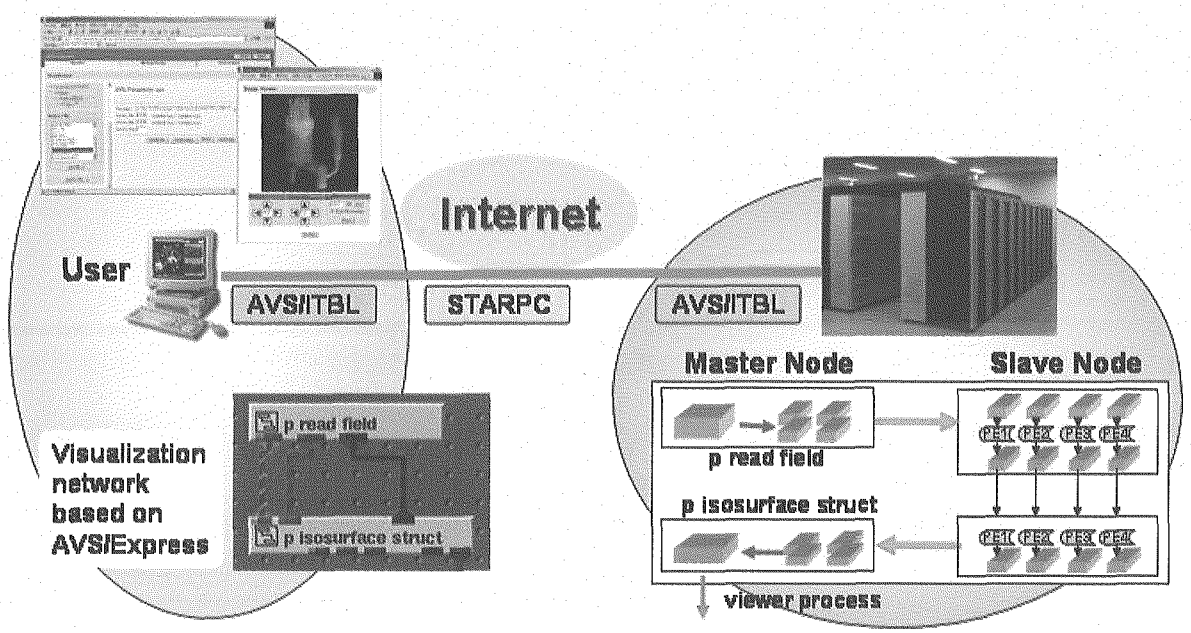


Fig.4 Visualization System developed on ITBL middleware

2.1.3 Developments of high performance finite elements for structural analysis[2.1.3-1]

The recent advances in both computer hardware and parallel-computing software techniques have enabled the finite-element method (FEM) to become widely used in a variety of large-scale structural analyses. However, if the geometry of the domain is very complex, and the number of degrees of freedom of the computational model is extremely large, the preparation of input data for large-scale FEM analysis remains a difficult, time-consuming process. Because of their suitability for arbitrarily complex geometries and fully automatic mesh generations, tetrahedrons with only corner nodes and high accuracy are favorable in the complex finite element structural analyses.

We developed a 4-node quadratic tetrahedral element. Figure 5 shows a typical cantilever benchmark of the new developed element GNTet4. Its numerical performance is compared with conventional elements TET4, TET10, and HEX20. See the figure for the meaning of these abbreviations. TET10 and HEX20 are two excellent general purpose solid elements in finite element structural analysis but are relatively difficult in mesh generation due to the midside nodes included. It is demonstrated that GNTet4 significantly improves TET4 and achieves comparable accuracy as TET10 and HEX20 for the same computational effort while keeping mesh generation extremely simple.

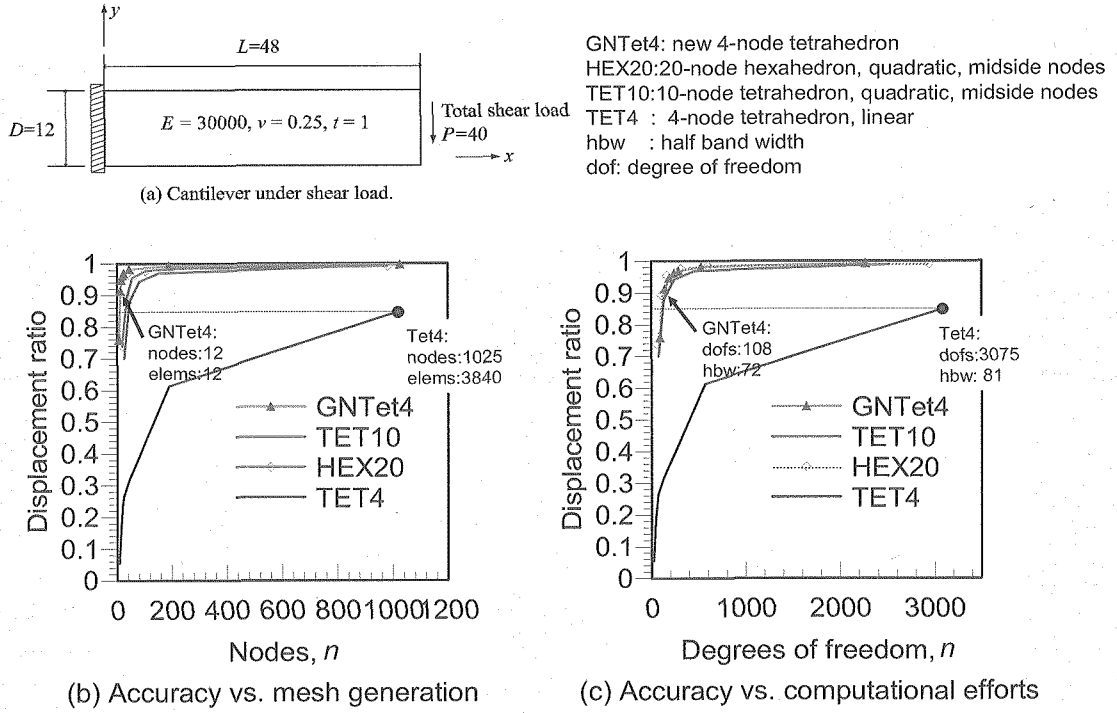


Fig. 5 Developments of high performance finite elements for structural analysis: test results of performance of new finite element.

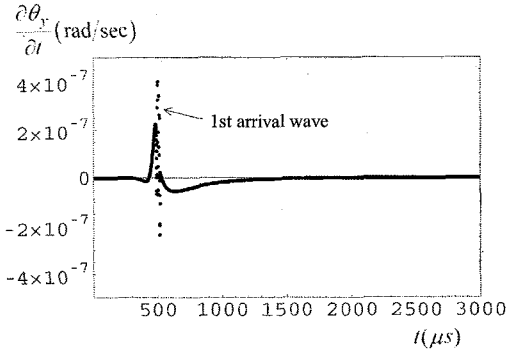
2.1.4 Wave propagation of piping structures under impulsive load[2.1.4-1]

Since it is generally difficult to predict the occurrence of natural disasters such as earthquakes, a performance management system is required to constantly maintain the safety and functionality of structures, particularly critical structures such as nuclear power plants. In order to realize such a system, it is important to perform detailed modeling procedures and analyses for gaining a better understanding of actual phenomena. Such details are essential for explaining the phenomena that occur in frame structures such as piping systems, which are considered to be one of the weakest and most vulnerable components of nuclear power plants. Accidents such as fractures caused by fluid elastic vibration in small tubes used for heat transfer from steam generators and cracks in welded parts of the piping caused by the cyclic stress of the piping vibration have recently occurred in nuclear power plants. It is crucial to clarify the dynamic behavior of the piping structure during operation in order to avoid these accidents.

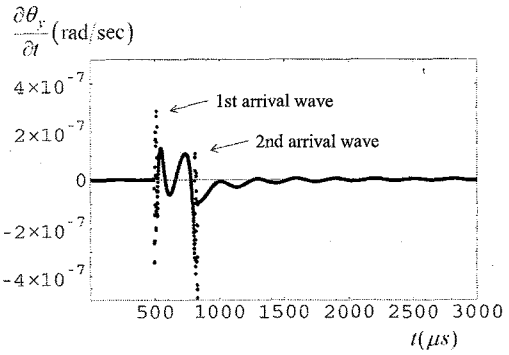
The aim of this study is to determine the dynamic behavior of piping systems, particularly the wave propagation phenomena under impulsive loads, in nuclear power plants, which are complicated assemblages of different parts. For this purpose, the spectral element method is adopted, and a formulation considering shear deformation independently for a three-dimensional frame element is described. The Timoshenko beam theory is introduced for developing this formulation.

In this study, the Timoshenko beam theory was compared with the conventional Bernoulli-Euler beam theory in terms of the propagation speed, and the application limit of the latter was specified [2.2-2]. Fig.6 shows the results obtained by using both the theories. The impulsive load and the infinite steel pipe model used for the analysis are shown in Fig.7 and the time history of the load is shown in Fig.8. In the case of the steel pipe used in this example, two peaks were observed by using the Timoshenko beam theory whereas only one peak was observed by using the conventional beam theory and were able to confirm that the second arrived wave in the higher frequency domain could be represented. In the case of this model, two peaks were observed in the plot obtained by the Timoshenko beam theory, whereas only one peak was observed in that obtained by the conventional beam theory. This confirmed that the second arrival wave in the high frequency domain could be represented by using the Timoshenko beam theory. Thus, by using the spectral element based on the Timoshenko beam theory, it is possible to represent the wave propagation phenomena of piping systems including high frequency modes, and the dynamic properties of these systems under impulsive loads could be clarified.

For future study, we intend to perform a numerical simulation of the piping system in the nuclear reactor system of the high temperature engineering test reactor (HTTR) located in the Oarai R&D Center, JAEA.



(a) Plot obtained by the Bernoulli-Euler beam theory



(b) Plot obtained by the Timoshenko

Fig.6 Rotation velocity at x = 2 m

[Reprinted from "JSME International Journal Series B, 49, No.2, p360-367(2006)"]

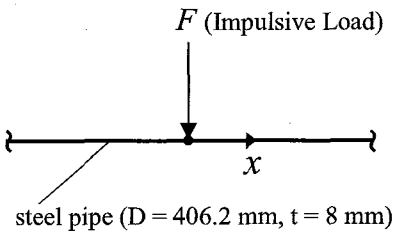


Fig.7 Frame model impacted at the center

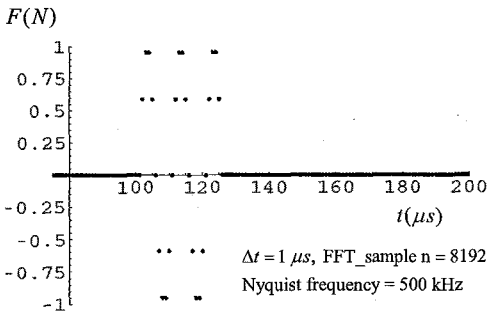


Fig.8 Input load characteristics: time history

2.1.5 Complementary study of phase properties and interaction force of acoustic bubbles[2.1.5-1]

Bubbles in a liquid are familiar objects to us. One can simply produce and observe many bubbles by only shaking a water-filled bottle. Also, bubbles emerge in diverse fields including nuclear and chemical engineering and medicine. Cavitation bubbles emerging in a depressurized liquid, for example, have a strong impact force that sometimes destroys fluid machinery such as nuclear plants. Despite their familiarity, bubbles still have many unsolved problems. Recently, by examining the pulsation phases of bubbles pulsating and interacting with each other through sound, we have found theoretically and numerically an unknown characteristic frequency, which we now call it a "transition frequency." Some of the transition frequencies invert a bubble's pulsation phase (e.g., from in phase to out of phase with the driving sound) without resonance, and are thus essentially different from the resonance frequency which is also known to invert the pulsation phase. In a following study, we have found that the transition frequency plays an important role in the sign reversal of the secondary Bjerknes force, an interaction force acting between pulsating bubbles. Based on transition-frequency analysis we have clarified that the sign reversal takes place around the transition frequencies that do not correspond to the resonance frequencies, an interpretation which disproves the previous explanations of the phenomenon given based on resonance-frequency analysis, see Fig. 9. We are now performing additional investigations to clarify similarities and differences between the transition frequency and known characteristic frequencies. The transition frequencies and the resonance (and anti-resonance) frequencies in a double-bubble case are shown in Fig. 10, where one can see a similarity in their maximum numbers, three, and a difference in their values. The results given in our study would be useful tools for understanding multibubble phenomena, such as the collapse of cavitation bubbles and the stable structure formation of bubble clusters.

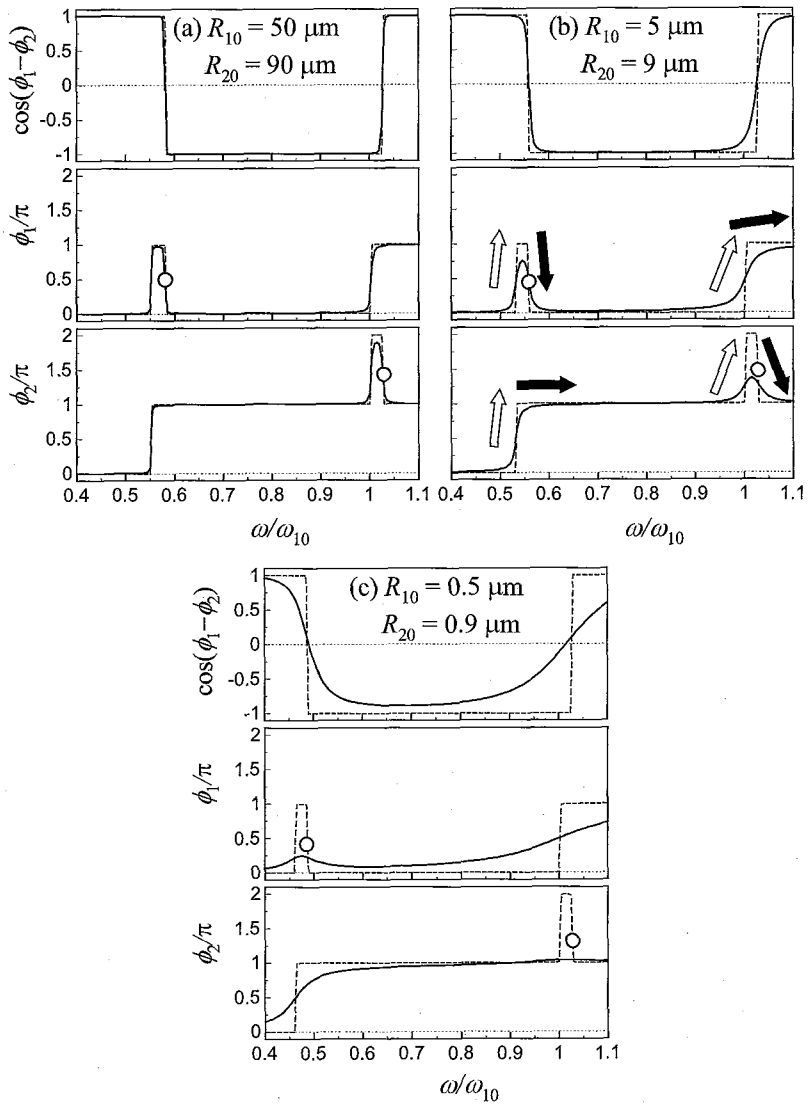


Fig. 9 Phases of two interacting bubbles measured from the phase of driving sound, $\phi_{1,2}$, and the sign of the interaction force, $\cos(\phi_1-\phi_2)$, for bubble pairs of different equilibrium radii R_{j0} as functions of the driving angular frequency. The positive value of $\cos(\phi_1-\phi_2)$ indicates attraction and the negative indicates repulsion. The solid and dashed lines denote results for finite and zero damping, respectively. At the transition frequencies that do not correspond to the resonance frequencies, only one phase shifts as indicated by a circle, which results in the sign reversal of the force. However, at the other transition frequencies, both two phases shift almost simultaneously, not resulting in the sign reversal. This result is obviously inconsistent with the previous explanation that the sign reversal takes place at the resonance frequencies.

[Reprinted from "Physics of Fluids 17, 097017 (2005)"]

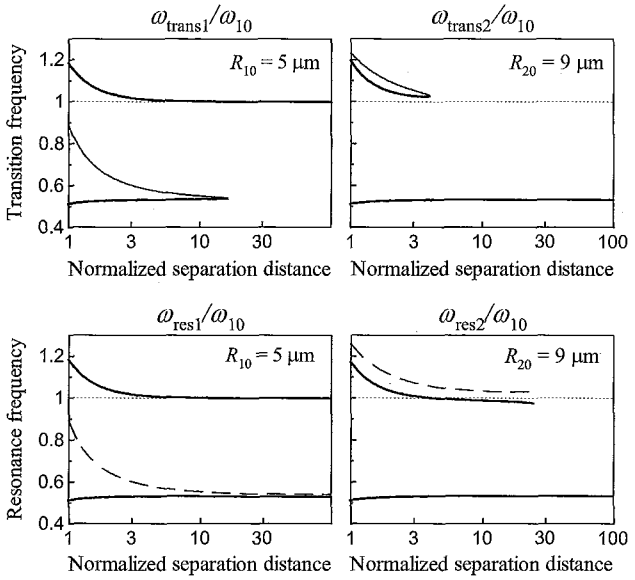


Fig. 10 Transition frequencies (upper) and resonance and anti-resonance frequencies (lower) of a double-bubble system as functions of the separation distance between the centers of bubbles normalized by the bubble radii. The solid and the dashed lines in the lower panels denote the resonance and anti-resonance frequencies, respectively, the later of which minimizes the oscillation amplitude of the corresponding bubble. The maximum number of transition frequencies, three, is equal to the sum of the numbers of resonance and anti-resonance frequencies, which is a similarity of them. However, the values of those frequencies are obviously different from each other, a difference between them.

2.1.6 Avoided crossings in triple-bubble systems[2.1.6-1]

Gas or vapor bubbles emerging through cavitation will pulsate violently and sometimes destroy the flow channels of nuclear plants by emitting high-speed liquid jets which focus the kinetic energy of bubbles in a very narrow region. In a cavitating liquid, a huge number of pulsating bubbles emerge and interact with each other through acoustic and hydrodynamic forces, and hence bubbles constitute a kind of system of interacting oscillators, that is, a "coupled oscillator system." We have recently been studying the dynamics of multiple bubbles as a coupled oscillator system and have discovered a strange phenomenon "avoided crossing." Avoided crossings have been studied in several research fields including quantum chemistry and chaos dynamics, and have been found in a number of physical systems involving multiple eigenvalues (e.g., eigenenergies, natural frequencies, Lyapunov exponents). In the case of bubbles, avoided crossings appear in the resonance frequencies. The solid lines in Fig. 11 denote the avoided crossing resonance frequencies of a system of three bubbles aligned in-line (Fig. 12). The resonance frequencies that crossed when a bubble (bubble 3) was decoupled exhibit avoided crossing when all three bubbles are coupled. Carefully examining this result, we have found that in the avoided crossing region, two of the transition frequencies (at which the pulsation phase of a bubble inverts) cross with each other and the bubbles act as if they exchange their oscillation states with each other. Our paper is the first to report such a behavior of bubbles. Our finding appears to reveal a bubble's hidden complexity.

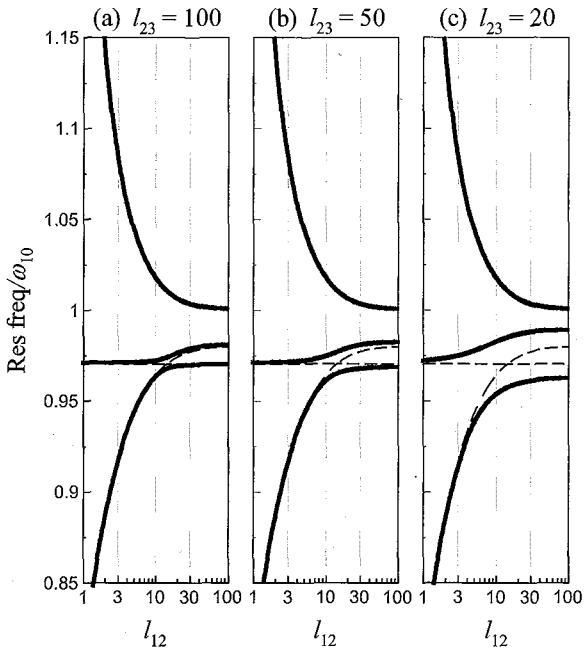


Fig. 11 Avoided crossing found in a triple-bubble system. Shown are the resonance frequencies of the system when bubble 3 is decoupled (the dashed lines) and when all three bubbles are coupled (the solid lines). l_{ij} are the separation distances between bubbles i and j ($i,j=1,2,3$, $i\neq j$). When all bubbles are coupled, the intersecting point appearing in the decoupled case vanishes and the resonance frequencies connect smoothly, without crossing, around the intersecting point. The avoided crossing becomes broader as bubble 3 approaches to the other bubbles (i.e., as l_{23} becomes smaller).

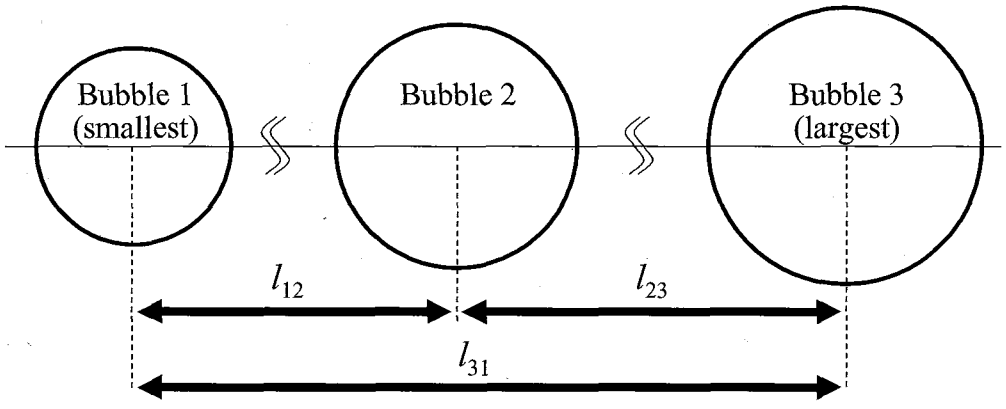


Fig. 12 Arrangement of bubbles. The three bubbles are aligned on a line. The equilibrium radii of them are $(R_{10},R_{20},R_{30})=(50\ \mu m, 51\ \mu m, 51.5\ \mu m)$.

References

[2.1.1-1] Y. Suzuki, T. Minami, M. Tani, N. Nakajima, R. Keller, T. Beisel, "Interoperability between UNICORE and ITBL," *Proceedings of WCGC'2006 (Workshop on Computational Grids and Clusters)* (Rio De Janeiro, Brazil, July 10-14, 2006).CDROM.

[2.1.2-1] O. Hazama, H. Matsubara, R. Tian, A. Nishida, Y. Suzuki, M. Tani and N. Nakajima, "Towards Construction of a Numerical Testbed for Nuclear Power Plants," *7th MpCCI User Forum*, (Sankt Augustin, Germany, 21-22, February 2006) Proceedings of 7th MpCCI User Forum (2006) pp.132-137.

[2.1.3-1] R. Tian, H. Matsubara, A. Nishida, N. Nakajima, G. Yagawa. "A formulation of generalized node, a quadratic tetrahedron/triangle with only corners, and meshfree approximation with rotational degrees of freedom", *Proceedings (CDs) of the Eighth U.S. National Congress on Computational Mechanics* (USNCCM VIII), July 24-28, 2005, Austin, Texas, USA(2005).

[2.1.4-1]A. Nishida, "Wave Propagation Properties of Frame Structures—Formulation for Three-Dimensional Frame Structures," *JSME International Journal, Series B*, **49**, No.2, p.360-367(2006).

[2.1.5-1] M. Ida, "Phase properties and interaction force of acoustically interacting bubbles: A complementary study of the transition frequency," *Physics of Fluids* **17**, 097107 (2005).

[2.1.6-1] M. Ida, "Avoided crossings in three coupled oscillators as a model system of acoustic bubbles," *Physical Review E* **72**, 036306 (2005).

2.2 Computational Materials Science for Atomic Energy Research

Throughout the fiscal year 2005, materials scientists in CCSE have faced the following three topics, which are currently important in nuclear energy science and engineering: i) crack propagation in nuclear reactor materials, ii) rim structure formation in nuclear fuel, and iii) nano-scale device design for atomic-energy research. In these three topics, our final goal is to develop multiscale simulation techniques to solve those intrinsically multiscale problems as shown in Fig.13(an image of materials science research in CCSE).

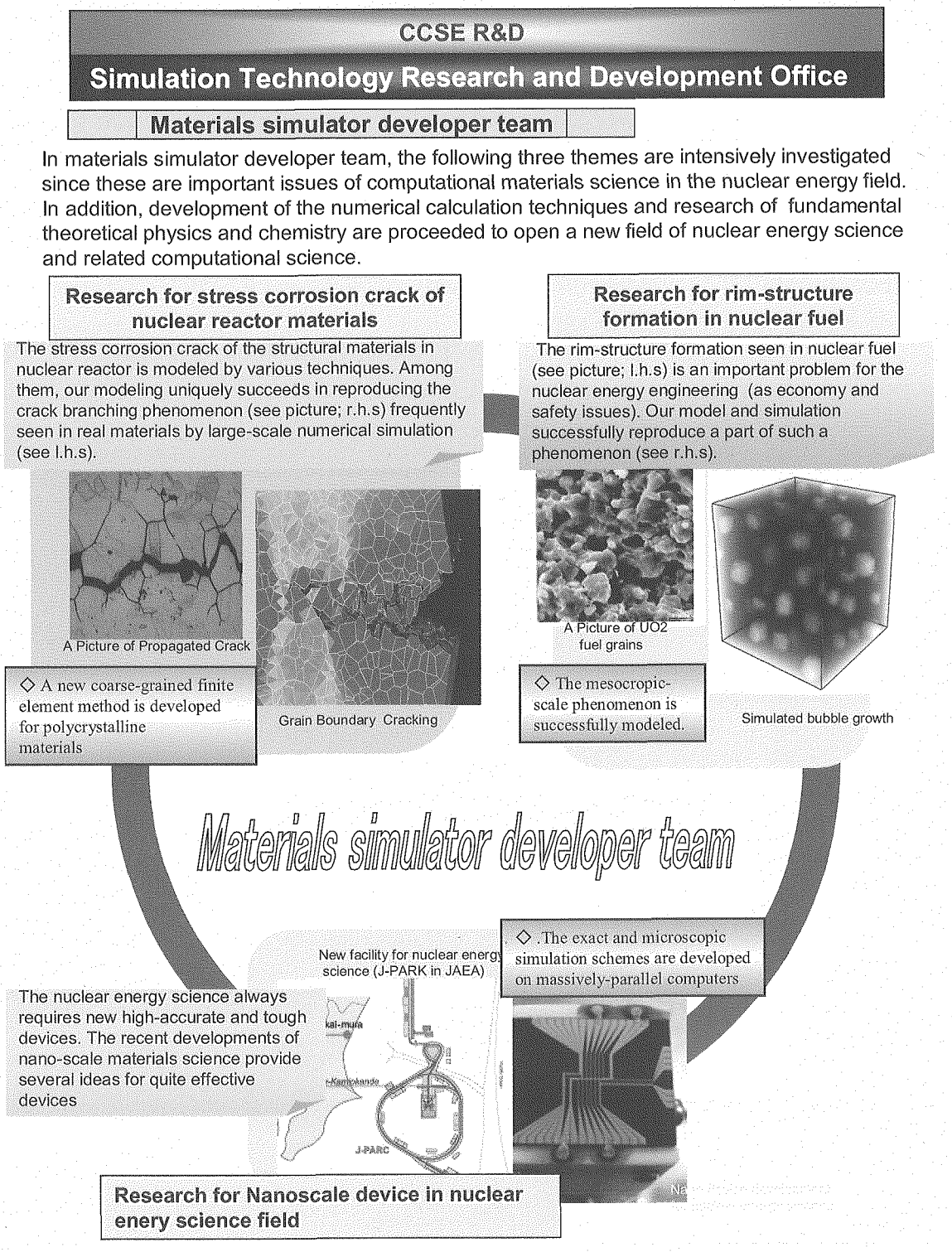


Fig. 13 Purpose, theme, and target of materials science research in CCSE.

2.2.1 First-Principles Analysis for the Effects of More Than 10 Solute Elements on Grain Boundary Embrittlement of Nuclear-Reactor Materials

A small amount of impurity elements brings about a drastic change in the mechanical properties of metals [2.2.1-1]. It is well known that phosphorous (P), which is included in reactor pressure vessel (RPV) steels, is a weak embrittler for iron grain boundaries. However, the mechanism of the embrittlement is not well understood. To clarify the mechanism of the grain boundary weakening (or strengthening), we simulate the solute segregation and cohesion/decohesion in an iron grain boundary by progressively adding various solute elements.

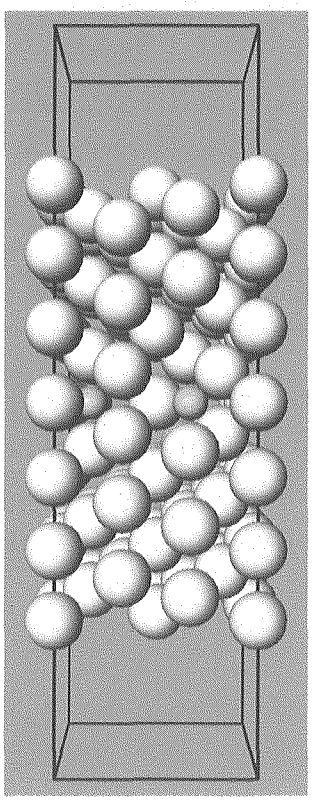


Fig. 14 4 Modelling of bcc Fe Σ3 symmetrical tilt grain boundary.

We use bcc Fe Σ3 symmetrical tilt grain boundary as shown in Fig. 14. This unit cell contains 76 Fe atoms. Grey spheres indicate iron (Fe) atoms, yellow ones grain boundary vacancy sites. Vacuum regions are introduced to allow grain boundary sliding in the upper and lower regions of the cell. We use VASP (Vienna Ab initio Simulation Package) code.

The calculated results are shown in Fig. 15. These calculated results are consistent with the experimental facts.

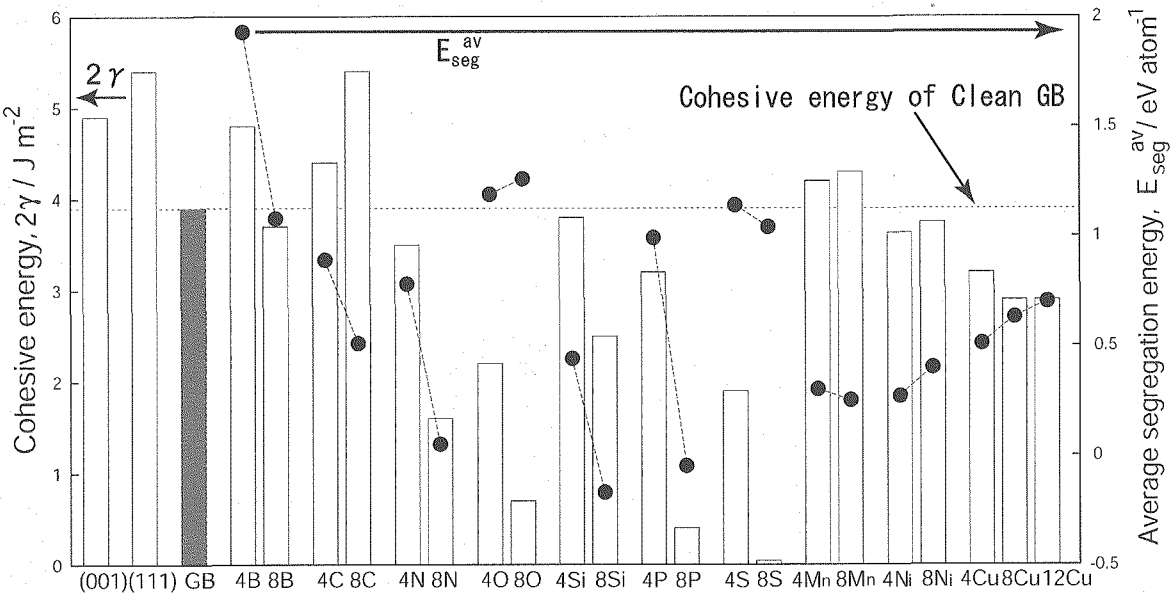


Fig. 15 Calculated average segregation energy (E_{seg}^{av}, right), cohesive energy (2γ, left). "(001)" indicates the cleavage plane of bcc Fe, "(111)" the plane parallel to GB Σ3(111) plane, "GB" the clean GB case (no segregation). "4B(8B)" indicates that 4(8) boron atoms are introduced to the GB region of the unit cell (Fig. 1), and so on. (4(8) atom/unitcell = 7.2(14.4) atom/nm^2).

2.2.2 Mesoscopic modeling of the rim-structure formation of UO2 fuel pellets

The thermal and mechanical properties of Uranium-dioxide (UO_2) fuel have been studied in order to seek safer and more economic operation of nuclear power plants. An important safety-related requirement is to confine the highly-radioactive fission products within the fuel pellet. It is, however, known that a typical microstructural change, also called the rim-structure formation, occurs at the peripheral region of fuel pellets over some critical value of the burnup ~60 MWd/kgU, that is, nano-sized bubbles containing fission-gas atoms such as Xe atoms aggregate and form large bubbles with the diameter of ~2μm. This change might promote the swelling of the pellet and the gas-release, both of which are not desirable to the safe operation of reactors.

To computationally study the bubble growth described above, an innovative three-dimensional Monte-Carlo method was proposed: Each small lattice element carries variables that determine its state. The state of each element assumes either a bubble, a void, or a matrix state. A lattice element with the bubble state represent a cluster composed of vacancies and inert gas atoms. The inert gas we consider here is Xe. The element with the void state represents a cluster composed of vacancies.

The energy functional used for the algorithm is composed of two kinds of energy: the bubble/matrix interface energy and the void formation energy. Figure 16 shows a typical result from the prototype calculations mimicking the porous structure. A bi-modal bubble size distribution, which is typically observed in the bubble growth experiments, is also given in our numerical results. (See Fig. 17). We have confirmed the methodology we adopted has a sufficient modeling capability for the general bubble growth.

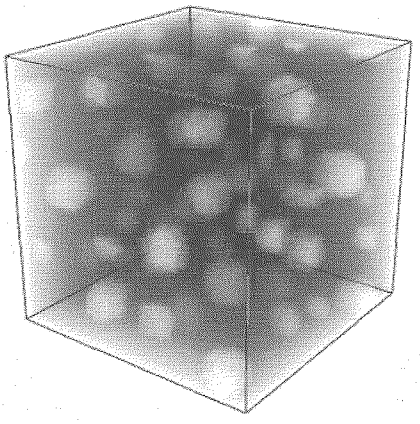


Fig. 16 A calculation results of the 3-dimensional bubble formation model: The bright parts are the pores.

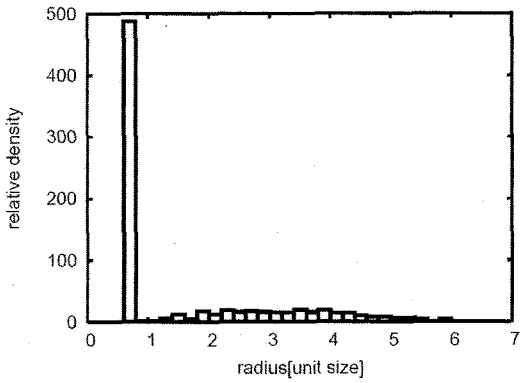


Fig. 17 A bi-modal distribution obtained by the simulation study.

2.2.3 Mesoscopic Modeling of Intergranular Crack-Propagation in Polycrystalline Nuclear Reactor Materials

When polycrystalline steel is subjected to both corrosive environment and tensile stress, it exhibits so-called "stress corrosion cracking (SCC)" which is known to be the most critical cause of degradation of nuclear reactor structural materials. One of typical features of SCC is its complicated crack shape, making conventional fracture mechanics analysis difficult to apply. This unique feature is believed to result from the interaction between stress concentration and diffusion of corrosive agent around a crack tip, and identification of the mechanism by which this complicated crack shape is generated is a key to a full understanding of SCC, which will lead to SCC-resistant materials. Thus, we have developed a simulation model of SCC [2.2.3-1], in which the irregular shapes of grains are incorporated. In this model, as the first step, we only used stress concentration as a cause of crack propagation, which is modeled as a sequence of discrete events of grain boundary failure, rather than continuous propagation of crack front. This simplification is based on a speculation of SCC process inferred from experimental observations: a rich amount of oxygen is usually observed in grain boundaries ahead of crack tips. These grain boundaries are oxidized and become far more brittle than unoxidized ones. Thus, we speculated the SCC process as follows: (1) a grain boundary next to the crack tip is opened by a small amount owing to tensile stress concentration, and becomes diffusion channel for oxygen atoms (2) oxygen atoms from corrosive environment rapidly diffuse through this grain boundary, making it brittle, as shown in Fig.18a (3) oxidized brittle grain boundary fails and failure stops at grain boundary triple junction, owing to crack tip blunting caused by grain boundary slide, as shown in Fig.18b. From these assumptions, we modeled the SCC process as successive failures of grain boundary which is next to the crack tip and under the strongest tensile stress. Despite its simplicity, this model could reproduce the typical crack shape of SCC to some extent as shown in Fig. 19. As the second step, we have developed a theoretical model which also incorporates the diffusion of corrosive agent around a crack tip, and simulation of the model is in progress.

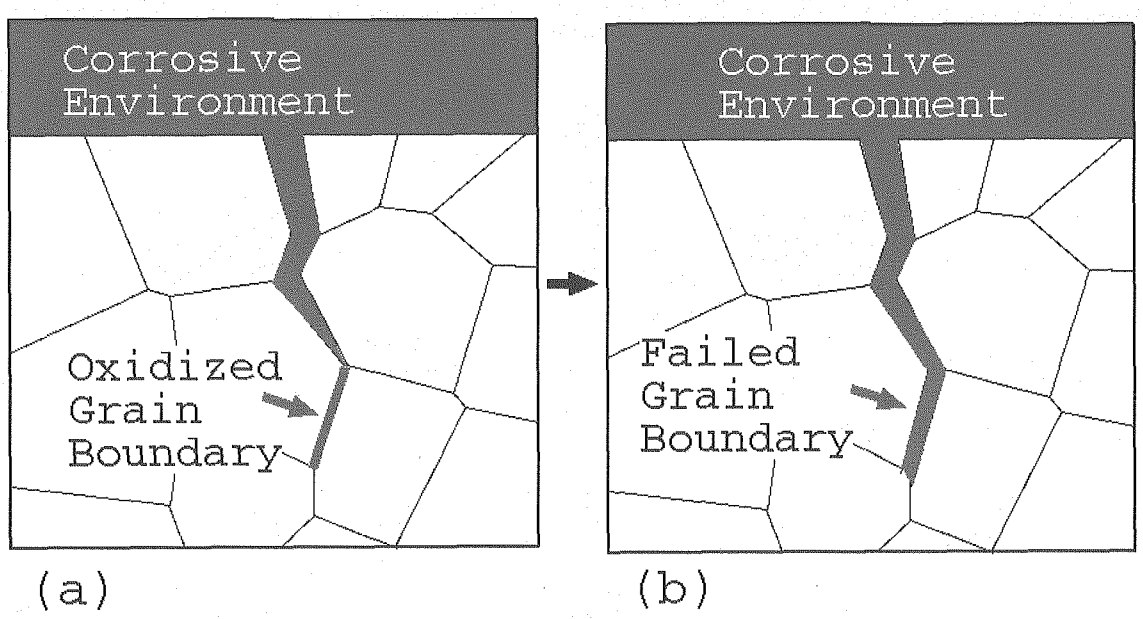


Fig. 18 A schematic depiction of SCC scenario we assumed in the present work. (a) Grain boundaries next to the crack tip is oxidized and embrittled (b) An embritlled grain boundary fails and the crack tip proceeds to a triple junction.

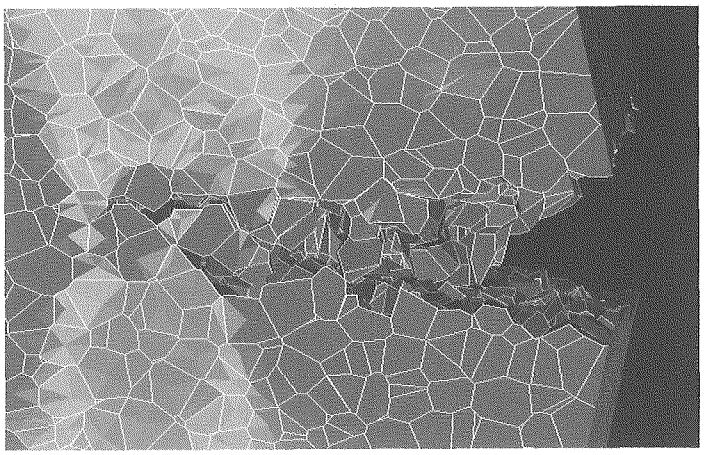


Fig. 19 A snapshot of a dynamical simulation by our SCC model for the grain boundary cracking.

2.2.4 Accuracy Enhancement in the Simulation Model for Superconducting Neutron Detector

The one of final plan of our team is to construct a multiscale simulation technique which contributes to develop nanoscale devices [2.2.4-1～6] in nuclear energy science and engineering field. Toward to the goal, the fiscal 2005 year plan was to develop a new simulation code in order to simulate real non-equilibrium dynamics after neutron capture in undertaking superconducting neutron-detector. After the completion of the code, we will design a new neutron detector which may be used under high neutron flux beam like J-PARK. However, since it was proved to require about ten times accuracy enhancement in its time-resolution when using the present prototype code adopting the conventional time-evolutional scheme, we started with implementing an alternative time-evolutional scheme to the prototype code. Thus, the fiscal 2005 year achievements are as follows: i) for the time-dependent Ginzburg-Landau equation and the Maxwell equations which describe superconducting dynamical phenomena [2.2.4-1～2], we developed an original splitting method [2.2.4-3～4] instead of the conventional Euler method. ii) We implemented the scheme on the simulation code and confirmed that the scheme can generally result in an order of CPU time reduction for various dynamical simulations. This result indicates that one can enhance an order of the simulation precision for the same CPU time period. Consequently, we have succeeded in performing systematic and realistic non-equilibrium dynamics after neutron captures by using the improved code. The typical simulation results of the non-equilibrium dynamics are shown in Fig.20.

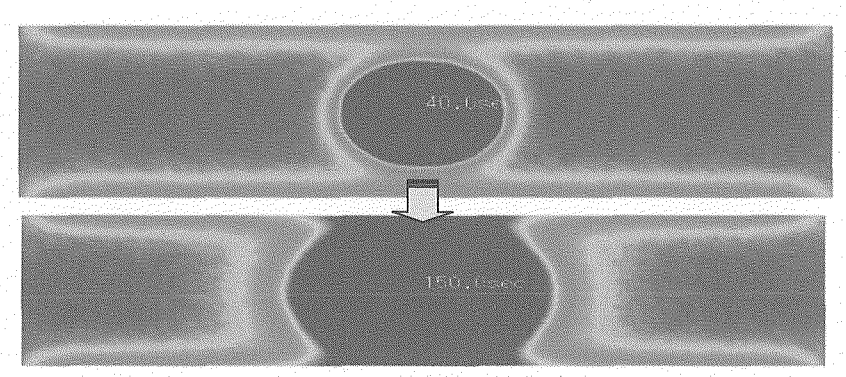


Fig. 20. Two typical snapshots of the superconducting electron density profile
Fig. 20 ıclear reaction at the central region. The arrow indicates an order of the time sequence

References

[2.2.1-1] M. Yamaguchi, M. Shiga, and H. Kaburaki, "Grain-boundary decohesion by impurity segregation in a nickel-sulfur system ", *Science* **307**, 393-397 (2005).

[2.2.1-2] M. Yamaguchi, M. Shiga, and H. Kaburaki, "Response to Comment on 'Grain-boundary decohesion by impurity segregation in a nickel-sulfur system'", *Science* **307**, 1677d (2 pages) (2005).

[2.2.2-1] M. Itakura, H. Kaburaki, and C. Arawaka, "Branching mechanism of intergranular crack propagation in three dimensions," *Phys. Rev. E* **71**(2005), 055102 (R)

[2.2.4-1] M. Machida, T. Koyama, M. Kato and T. Ishida, "Direct numerical simulations for non-equilibrium superconduting dynamics and related neutron detection in MgB2," *Physica C* 426-431, 169-173(2005).

[2.2.4-2] M. Machida, T. Koyama, M. Kato, and T. Ishida, "Josephson Half-quantized Vortices in Long Square pi Junctions around d-dot," *Physica C* 426-431, 1566-1571(2005).

[2.2.4-3] N. Sasa, M. Machida, and H. Matsumoto, "3-Dimensional Dynamics of Vortices in a Rotating Bose-Einstein Condensate," *J. Low Temp. Phys.* 138 (2005).

[2.2.4-4] M. Machida, N. Sasa, and H. Matsumoto, "coexistence of Vortex Liquid and Solid in Rotating Bose-Einstein Condensate," *J. Low Temp. Phys.* 138 (2005).

[2.2.4-5] M.Machida, S.Yamada, Y.Ohashi, and H.Matsumoto, "Reply to Comment on Novel Superfluidity in a Trapped Gas of Fermi Atoms with Repulsive Interaction Loaded on an Optical Lattice," *Phys. Rev. Lett.* 95 , 218902 (2005).

[2.2.4-6] M.Machida and T. Koyama, "Structure of a Quantized Vortex near the BCS-BEC Crossover in an Atomic Fermi Gas", *Phys. Rev. Lett.* 94, 140401(2005).

2.3 Computational Quantum Bioinformatics for Atomic Energy Research

2.3.1 Computational Predictions of Genes and DNA/RNA interfaces of Proteins for Repair Related Genes/Proteins [2.3.1-1~3]

Organisms are under constant exposure of radiation including ultraviolet light. Irradiation on organisms is known to damage their DNA and RNA. High-energy light as well as oxygen is the known cause of the damage. These damages are considered as one of the causes of cancer and aging. To undo those damages, the organisms have mechanisms to repair DNA/RNA damages. Molecular mechanisms for DNA/RNA repair, therefore, attract interest of a number of researchers and extensive studies have been carried out.

We have been studying molecular mechanisms of DNA/RNA repair by finding genes for DNA/RNA repair out of the whole DNA sequences and by predicting structures of the proteins at the time of DNA/RNA repair. DNA sequences of the human genome were all determined by the start of the 21st century, and we now have a blueprint for a human. However, the question we face now is how to read the blueprint. DNA sequences of human genome are equivalent to a string of 3 billion letters written with only four types of characters, and we need to 'decipher' the string. The process of deciphering is a collaboration of biology and computational science, and this new field is called bioinformatics. The bioinformatics research we are advancing here is specifically a study to discover a DNA/RNA repair related protein by deciphering DNA sequences.

This year, we started to develop a method to find sub-structure of proteins from their sequences, to discover functionally important metal-binding site, and to predict DNA/RNA-binding sites on proteins. Finding out locations on the proteins for DNA/RNA interactions is one of the first steps for studying DNA/RNA repair. Many researchers have elucidated a lot of structures of protein that bind to a target RNA. We have gathered structural data of RNA-protein complexes and built a database (Fig. 21). Using this database, we carried out many types of statistical analyses to find characteristics of RNA interface on proteins, such as size of RNA interfaces and characteristic atoms appearing in RNA interfaces. With these statistically derived characteristics, one can perform prediction of RNA interfaces on a protein not yet observed to bin RNA. We are developing new statistical methods and are trying to predict the interfaces with high quality (Fig. 22). By RNA interfaces on proteins with

high quality, we can design biochemical experiments to determine RNA interfaces. A collaboration of biological and computational sciences is now getting to elucidate mechanisms of molecules that sustain life.

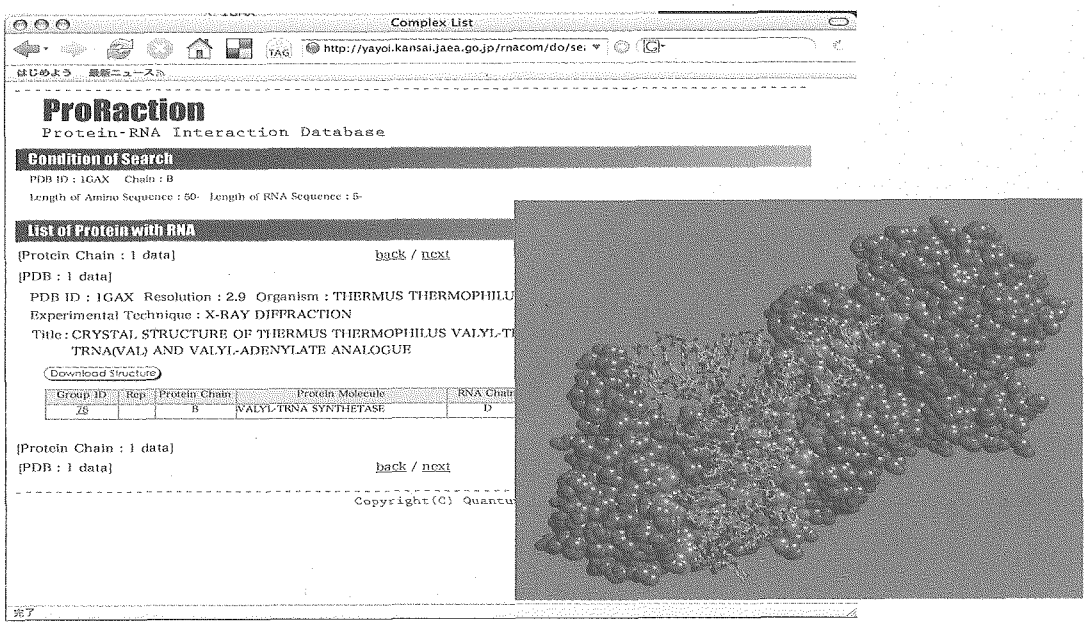


Fig. 21 Database for RNA-protein complex structures

To understand how proteins interact with RNA, coordinate data of RNA-protein complex were gathered and stored in a database. In this database, one can observe the atomic structure of a specific protein in complex with RNA. A set of solid balls in blue, red and green represents a protein three-dimensional structure and a set of wires represents an RNA molecule. Protein surfaces in red and green are the interfaces. RNA interfaces on a protein are predicted based on statistical characteristics of protein surface derived from the database. A set of balls (protein) in orange to red is the predicted RNA interface and a set of wires is an RNA molecule.

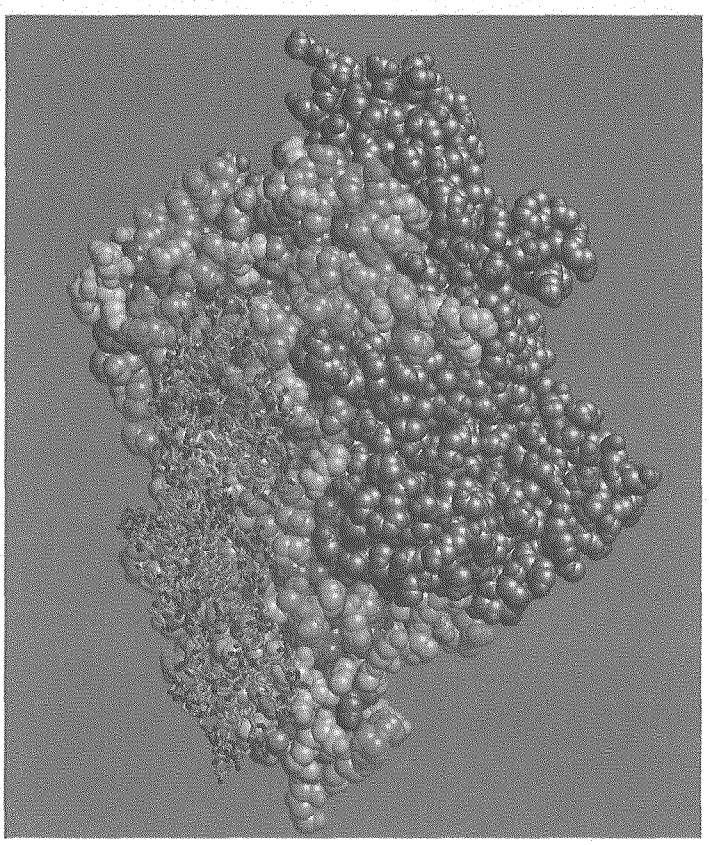


Fig. 22 A result of RNA interface prediction

2.3.2 Fast Molecular Dynamics Simulation Programs for Studying Repair Mechanisms of Damaged DNA[2.3.2-4~5]

Molecular dynamics (MD) simulation not only provides dynamic descriptions of molecules on the atomic scale, but also provides valuable information for the interpretation of experimental data. The rapid development of faster computer and the elucidation of the structures of biological macromolecules by X-ray crystallography and other experiments have enabled us to perform large-scale MD simulations of biological huge molecules.

We are developing an integrated molecular simulation system for biological macromolecules, called SCUBA (Simulation Codes for hUge Biomolecular Assembly), which is designed to run a system composed of more than a million particles efficiently on parallel computers. SCUBA has many special features, and listed below are the several of them.

- High performance
  SCUBA achieves both a high parallelization efficiency ratio and a high vectorization ratio.
- Reduction of the amount of communication
  In the conventional method, each processor needs to evaluate the interactions between atoms in a cell and the surrounding 26 neighboring cells. SCUBA employs a method for minimizing communication between processors, in which each processor evaluates the interactions of atoms with only seven surrounding cells.
- Vectorization
  In order to improve the performance of SCUBA, the algorithm to calculate the interactions among the atoms is intensively vectorized.
- Dynamic load balance
  A dynamic load-balancing algorithm is implemented to optimize the number of processors assigned for several different types of calculation during the simulations.

SCUBA achieved a parallelization efficiency ratio of 75.8 %, even when 360 processors were used as shown in Fig. 23. The vectorization ratio of 96.2% was achieved for the same number of processors, which is due to the intense vectorization for the calculation of atomic interactions.

We have carried out a benchmark test of SCUBA. The physical system for this test was chosen to be RuvAB-Holliday junction complex, as shown in Fig. 24. The size of the system was 274.0Å×142.2 Å×148.9 Å, and the cutoff length for the van der Waals

interactions was chosen to be 8 Å. On the basis of the cutoff length the system was divided into 31×16×16 = 7,936 sub-cells. The parallelization efficiency ratio and vectorization ratio are plotted in red and blue, respectively, with respect to the number of processors used in the calculation.

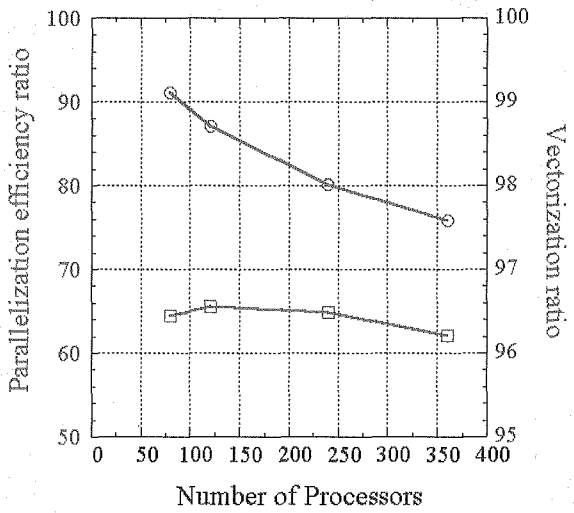


Fig. 23 Performance of SCUBA

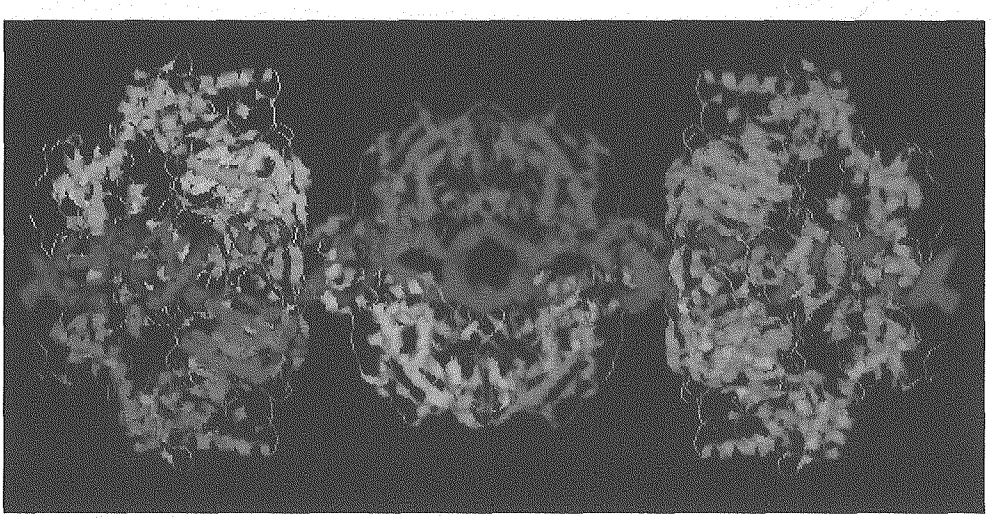


Fig. 24 RuvAB protein - Holliday junction DNA complex, the system for the benchmark test. The system is a biomolecular complex consisting of twenty protein molecules and of four strands of DNA The set of proteins executes recombination of homologous DNA strands. The size of the system and the number of atoms in the system are 274.0Å×142.2 Å×148.9 Å and 546,725 atoms, respectively.

2.3.3 Development of IMAGINE, the Dose Calculation System for Remotely Supporting X-ray Radiotherapy[2.3.3-6~7]

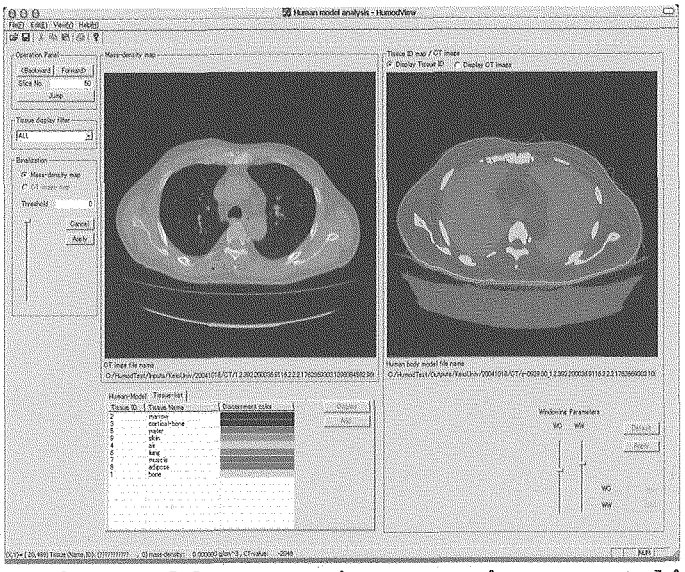


Fig. 25. Automatic patient model construction system incorporated into the IMAGINE system.

The algorithm for the automatic construction of a patient model from CT data has been improved. An example of the automatic construction is shown in Fig.25: the right colored model was constructed from the left CT image. The couch was separately recognized from the patient body, and the patient body was segmented into six different media having different elemental compositions. Using this algorithm, 99% of artificial structures other than patient bodies can be properly recognized. Usually, a patient model can be constructed within a few minutes.

A prototype of the IMAGINE system was completed and the on-line test was carried out being connected with the ITBL computer. Proper functioning of the system was verified by this test. Figure 26 shows the comparison of dose distribution for two-field irradiation of a tumor in a lung by 10 MV X-rays. The dose distribution calculated by the IMAGINE system was compared with that by the superposition method currently used in commercial treatment planning systems. They showed obvious difference which is considered due to the electron non-equilibrium, suggesting the Monte Carlo calculation should be used for the treatment planning in the case where the density changes steeply according to position in the body.

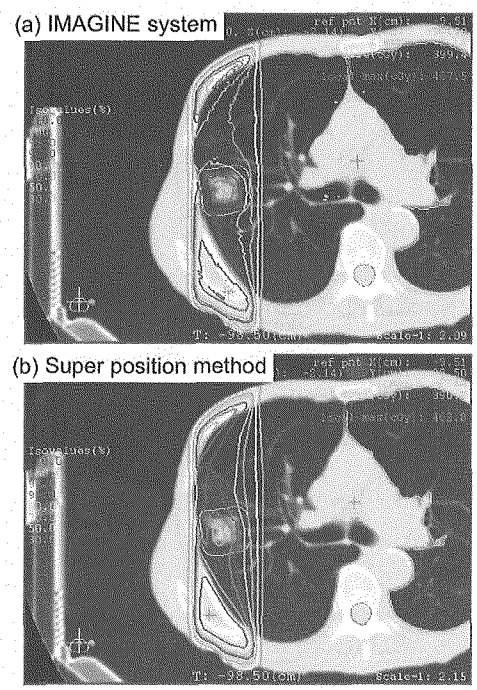


Fig. 26 Comparison of dose distributions for two-field irradiation of a tumor in a lung..

References

[2.3.1-1] Metsugi, S., Uenoyama, A., Adan-Kubo, J., Miyata, M., Yura, K., Kono, H., and Go, N., "Sequence analysis of the gliding protein Gli349 in Mycoplasma mobile", BIOPHYSICS 1, 33-43 (2005).

[2.3.1-2] Nakamura, K. and Go, N., "Function and molecular evolution of multicopper blue proteins", Cellular and Molecular Life Science 62, 2050-2066 (2005).

[2.3.1-3] Yura, K., "Protein Function Prediction based on the Three-Dimensional Structure: In Case of DNA Repair Related Proteins", The 5th Annual Meeting of the Protein Science Society of Japan, June, 30- July 2 (2005)(Invited talk).

[2.3.2-1] Metsugi, S., "Influence of Multidimensionality on Convergence of Sampling in Protein Simulation", J. Phys. Soc. Jpn. 74, 1865-1870 (2005).

[2.3.2-2] Matsumoto, A. and Olson, W.K., "Effects of Sequence, Cyclization, and Superhelical Stress on the Internal Motions of DNA" in Normal Mode Analysis: Theory And Applications to Biological And Chemical Systems (Mathematical and Computational Biology) (Cui, Q. and Bahar, I. eds.) Crc. Pr. I. Llc. pp. 187-211 (2006).

[2.3.3-1] Saito, K., Kunieda, E., Narita, Y., Kimura, H., Hirai, M., Deloar, H. M., Kaneko, K., Ozaki, M., Fujisaki, T., Myojoyama, A., Saitoh, H., "Dose calculation system for remotely supporting radiotherapy," Radiation Protection Dosimetry 116, 190-195 (2006).

[2.3.3-2] Saito, K., Sato, K., Kinase, S., Noguchi, H., Funabiki, J., Takagi, S., Sato, O., Emoto, Y., Sukehiko, K., "Dose calculation using Japanese voxel phantoms for diverse exposure", Monte Carlo 2005 Topical Meeting, Chattanooga, Tennessee, April 17-21, 2005. , on CD-ROM, American Nuclear Society, LaGrange Park, IL (2005).(Invited talk).

3. Research Achievements

3.1 Publication & Presentation List

List of Paper

1) M. Ida, "Avoided crossings in three coupled oscillators as a model system of acoustic bubbles", *Physical Review E*, 72, 036306 (2005).
2) M. Ida, "Phase properties and interaction force of acoustically interacting bubbles: A Complementary study of the transition frequency", *Physics of Fluids*, 17, 097107 (2005).
3) Y. Suzuki, Y. Takeshima, N. Ohno, K. Koyamada, "Utilization of the volume rendering with spherical sampling method to immersive VR system", *Journal of Nippon Virtual Reality Society*, 10, 231 (2005) (in Japanese).
4) A. Nishida, K. Kawaguchi, "Experimental study on wave propagation behavior of lattice structures", *J. Struct. Constr. Eng., AIJ,* 597, 69 (2005) (in Japanese).
5) A. Nishida, "Wave propagation properties of framed structures based on the Timoshenko beam theory", *Kozo Kogaku Ronbunshu*, 52B, 119 (2006) (in Japanese).
6) R. Tian, G. Yagawa, "Generalized nodes and high-performance elements", *International Journal for Numerical Methods in Engineering*, 64, 2039 (2005).
7) Y. Shu, K. Furuta, "An Inference method of team situation awareness based on mutual awareness", *Cognition, Technology & Work*, 7, 272 (2005).
8) M. Shiga, "Heat capacity of water; Path integral molecular dynamics approach", *Bulletin of The molecular Simulation Society of Japan,* 7, 21 (2005).
9) S. Yamada, T. Imamura, M. Machida, T. Arakawa, "Novel communication strategy for distributed-shared memory parallel computer", *Transactions of the Japan Society for Computational Engineering and Science,* 7, 243 (2005).
10) M. Machida, T. Koyama, "Structure of a quantized vortex near the BCS-BEC crossover in atomic fermi gas", *Physical Review Letters*, 94, 140401 (2005).
11) M. Itakura, H. Kaburaki, T. Arakawa, "Branching mechanism of intergranular crack propagation in three dimensions", *Physical Review E,* 71, 055102 (2005).
12) Carty, G. J., M. Machida, Hampshire, D. P., "Numerical studies on the effect of normal-metal coatings on the magnetization characteristics of type-II superconductors", *Physical Review B,* 71, 144507 (2005).
13) A. Hayashi, M. Shiga, H. Tachikawa, "Ab initio path integral molecular dynamics simulation on the dihydrogen bonds", *Chemical Physics Letters*, 410, 54 (2005).
14) M. Machida, T. Koyama, M. Kato, T. Ishida, "Direct numerical simulation on

non-equilibrium superconducting dynamics after neutron capture in MgB2 superconductors", *Nuclear Instruments and Methods in Physics Research Section A* 559, 594(2006).

15) M. Machida, T. Koyama, Y. Ohashi, "Vortex structure from BCS to BEC Superfluid",*Physica C* 437-438, 190(2006).

16) . S. Yamada, M. Machida, T. Imamura, "Physics of strongly-correlated Fermi-Atom gases; Novel approach for material design", *Bulletin of the Japan Society for Industrial and Applied Mathematics*, 15, 153 (2005) (in Japanese).

17) H. Tachikawa, M. Shiga, "Geometrical H/D isotope effect on hydrogen bonds in charged water clusters", *Journal of the American Chemical Society*, 127, 11908 (2005).

18) M. Shiga , W. Shinoda, "Calculation of heat capacities of light and heavy water by path-integral molecular dynamics", *Journal of Chemical Physics*, 123, 134502 (2005).

19) M. Yamaguchi, M. Shiga, H. Kaburaki, "Response to comment on "Grain Boundary Decohesion by Impurity Segregation in a Nickel-Sulfur System", *Science*, 309, 1677d (2005).

20) S. Metsugui, "Influence of multidimensionality on convergence of sampling in protein simulation", *Journal of the Physical Society of Japan*, 74, 1865 (2005).

21) S. Metsugui, A. Uenoyama, J. Adan-Kubo, M. Miyata, K. Yura, H. Kono, N. Go, "Sequence analysis of the gliding protein Gli349 in *Mycoplasma mobile*", *Biophysics*, 1, 33 (2005).

22) Y. Yonetani, "A Severe artifact in simulation of liquid water using a long cut-off length; Appearance of a strange layer structure", *Chemical Physics Letters*, 406, 49 (2005).

23) M. Machida, "Edge boundary effect for Josephson vortices in finite-size layered high-Tc superconductors", *Physical Review Letters*, 96, 097002 (2006).

24) M. Machida, S. Yamada, Y. Ohashi, H. Matsumoto, "Reply to comment on ""Novel superfluidity in a trapped gas of fermi atoms with repulsive interaction loaded on an optical lattice""", *Physical Review Letters*, 95, 218902 (2005).

25) K. Nakamura, N. Go, "Function and molecular evolution of multicopper blue proteins", *Cellular and Molecular Life Sciences*, 62, 2050 (2005).

26) N.Yamamoto, F.Shimizu, M.Yokokawa, S.Sekiguchi, H.Kaburaki, M.Kurokawa, and R.Himeno, "Web-based Grid PSE for MD Simulations using Grid PSE Builder", *International Journal of Information Technology*, 11, 59 (2005).

27) S.Ogata, F.Shimizu, J.Li, M.Wakeda, and Y.Shibutani, "Atomistic Simulation of

Shear Localization in Zr-Cu Bulk Metallic Glass", *Intermetallics*, 14, 1033 (2006).
28) K. Ebihara, "Dynamical Pressure Anisotropy in Liquid-Gas Model of Lattice-Gas", *International Journal of Modern Physics* C, 17, 53 (2006).

List of Research Report and Book

1) K. Ebihara, "Introduction of lattice boltzmann simulation for interfacial growth and deformation in horizontal stratified two-phase flow", *RIST News*, 40, 30 (2005).
2) H. Kaburaki, "Themal transport process by the molecular dynamics method", *Handbook of Materials Modeling*, S. Yip ed. Springer, 763 (2005).
3) Y. Hoshi, E. Kume, "Report on processing speed for visualization of large-scale data", *JAERI-Data/Code*, 48 (2005).
4) S. Tokuda, "Annual report of R&D activities in Center for Promotion of Computational Science and Engineering from April 1, 2004 to March 31, 2005", *JAERI-Review*,. (2005).
5) K. Matsumoto, "Summaries of research and development Activities by using JAERI computer system in FY2004; April 1, 2004-March 31, 2005", *JAERI-Review* (2005).
6) N. Nakajima, "A Technique to manage and control the data security on the network computing", *2005-annual report of Toyo University, Center for Computational Mechanics Research*, 46 (2006).
7) N. Nakajima, "A Technique to manage communication on network computing by a data control method", *2005-annual report of Toyo University, Center for Computational Mechanics Research*, 44 (2006).
8) A. Matsumoto, W.K. Olson, "Effects of Sequence, Cyclization, and Superhelical Stress on the Internal Motions of DNA", *Normal Mode Analysis: Theory And Applications to Biological And Chemical Systems (Mathematical and Computational Biology)* (Cui, Q. and Bahar, I. eds.) Crc. Pr. I. Llc. pp. 187-211 (2006).

List of Proceedings

1) A. Miyazaki, "Wave propagation properties of frame structures; Formulation for three dimensional frame structures", *13th International Conference on Nuclear Engineering (ICONE-13)*, (Pekin, China, May. 2005) pp.6..

2) Tian, R., N. Nakajima, M. Yagawa, "Numerical investigation into the linear dependence problem of partition of unity based generalized finite element methods ", *10th Conference on Computational Engineering and Science, JSCES*, (Tokyo, Japan, May. 2005), Vol.10, No.1, pp393.

3) Tian, R., N. Nakajima, M. Yagawa, "Nodal arrangements for boundary treatment in EFGM", *10th Conference on Computational Engineering and Science, JSCES*, (Tokyo, Japan, May. 2005), Vol.10, No.1, pp397.

4) A. Inami, H. Matsubara, S. Iranami, Y. Kanda, "Design of the anchor wall using 3D finite element method", *JCI Annual Convention*, (Nagoya, Japan, Jun. 2005), 27, No2, pp1663.

5) S. Shinohara, Y. Okuda, S. Ito, N. Nakajima, M. Ida, "Shape optimization using adjoint variable method for reducing pressure drag and its application to ITBL", *10th Conference on Computational Engineering and Science, JSCES*, (Tokyo, Japan, May. 2005), Vol.10, No.2, pp692.

6) Y. Shu, N. Nakajima, "Building plant quake-proof information inference system based on hybrid data mining approach", *1st International Workshop on Risk Management System with Intelligent Data Analysis (RMDA 2005) in Conjunction with 19th Annual Conference of the Japanese Society for Artificial Intelligence (JSAI 2005)*, (Kitakyushu, Japan, Jun. 2005), pp35.

7) O. Hazama, N. Nakajima, "Development of a coupler for parallel simulations of weakly coupled systems on the grid-computing environment", *10th Conference on Computational Engineering and Science, JSCES*, (Tokyo, Japan, May. 2005), 10, No.1, pp259.

8) Y. Shu, N. Nakajima, "Development of a quake-proof information inference system by using data mining technology", *11th International Conference on Human-Computer Interaction (HCI International 2005)*, (Las Vegas, U.S.A, Jul. 2005), pp9.

9) N. Nakajima, T. Aoyagi, Y. Tsujita, R. Arima, M. Yamazaki, K. Idemitsu, "An Approach to realize a large-scale simulation for nuclear plant's materials by molecular dynamics", *Joint Conference of Electrical and Electronics Engineers in Chugoku*, (Hiroshima, Japan, Oct. 2005).

10) M. Ida, "Avoided crossings observed in three coupled oscillators as a model of acoustically coupled bubbles," *2005 Annual Meeting of Japan Society of Fluid Mechanics*, (Tokyo, Japan, Sep. 2005).

11) S. Shinohara, Y. Okuda, N. Nakajima, M. Ida, "Shape optimization using parameter-survey-type parallel adjoint variable method," *The 18th Computational Mechanics Conference*, (Sendai, Japan, Nov. 2005).

12) S. Shinohara, Y. Okuda, S. Ito, N. Nakajima, M. Ida, "Shape optimization technique using adjoint variable method," *The 19th Symposium on Computational Fluid Dynamics*, (Tokyo, Japan, Dec. 2005).

13) S. Tokuda, M. Furukawa, Y. Yoshida, " Regularization method in magnetohydrodynamic stability problems with continuous spectra," *2005 Annual Meeting of Japan Society of Fluid Mechanics*, (Tokyo, Japan, Sep. 2005).

14) M. Machida, "Numerical simulations for non-equilibrium superconducting dynamics in neutron and X-ray detection", *4th JSIAM-SIMAI Seminar on Industrial and Applied Mathematics*, (Hayama, Japan, May. 2005).

15) M. Machida, "Vortex structure and dynamics in fermi superfluids: From superconductivity to fermi atom gas", *Ryukoku Workshop on Mathematical Aspects of Pattern Formation and Dynamics in Dissipative Systems*, (Seta, Japan, Jul. 2005).

16) M. Machida, T. Koyama, H. Oohashi, "Structure change of a quantized vortex in fermi atom gas", *24th International Conference on Low Temperature Physics (LT24),* (Orlando, U.S.A, Aug. 2005).

17) T. Watanabe, "Numerical simulation of droplet dynamics using level set method", *11th International Topical Meeting on Nuclear Reactor Thermal Hydraulics (NURETH-11),* (Avignon, France, Oct. 2005), pp8-8.

18) K. Ebihara, H. Kaburaki, "Lattice boltzmann simulation of solution chemistry for crevice corrosion", *14th International Conference on Discrete Simulation of Fluid Dynamics in Complex Systems*, (Kyoto, Japan, Aug. 2005).

19) M. Itakura, H. Kaburaki, T. Suzudo, S. Suzuki, "Mesoscopic simulations on the evolution of a system of dislocations in the presence of a grain boundary", *Micromechanics and Microstructure Evolution*, (Madrid, Spain, Sep. 2005).

20) M. Machida, T. Imamura, S. Yamada, "16.447 Tflop /s and 159-Billion-Dimensional Exact Diagonalization for Trapped Fermion-Hubbard Model on the Earth Simulator", *The International Conference for High Performance Computing, Networking and Storage*, (Seattle, U.S.A, Nov. 2005).

List of Oral Presentation

1) A. Miyazaki, "Wave propagation properties of frame structures; Formulation for three dimensional frame structures", *13th International Conference on Nuclear Engineering (ICONE-13)*, (Pekin, China, May. 2005).
2) Tian, R., N. Nakajima, M. Yagawa, "Numerical investigation into the linear dependence problem of partition of unity based generalized finite element methods ", *10th Conference on Computational Engineering and Science, JSCES*, (Tokyo, Japan, May. 2005).
3) Tian, R., N. Nakajima, M. Yagawa, "Nodal arrangements for boundary treatment in EFGM", *10th Conference on Computational Engineering and Science, JSCES*, (Tokyo, Japan, May. 2005).
4) A. Inami, H. Matsubara, S. Iranami, Y. Kanda, "Design of the anchor wall using 3D finite element method", *JCI Annual Convention*, (Nagoya, Japan, Jun. 2005).
5) S. Shinohara, Y. Okuda, S. Ito, N. Nakajima, M. Ida, "Shape optimization using adjoint variable method for reducing pressure drag and its application to ITBL", *10th Conference on Computational Engineering and Science, JSCES*, (Tokyo, Japan, May. 2005).
6) Y. Shu, N. Nakajima, "Building plant quake-proof information inference system based on hybrid data mining approach", *1st International Workshop on Risk Management System with Intelligent Data Analysis (RMDA 2005) in Conjunction with 19th Annual Conference of the Japanese Society for Artificial Intelligence (JSAI 2005)*", (Kitakyushu, Japan, Jun. 2005).
7) O. Hazama, N. Nakajima, "Development of a coupler for parallel simulations of weakly coupled systems on the grid-computing environment", *10th Conference on Computational Engineering and Science, JSCES*, (Tokyo, Japan, May. 2005).
8) Y. Shu, N. Nakajima, "Development of a quake-proof information inference system by using data mining technology", *11th International Conference on Human-Computer Interaction (HCI International 2005)*, (Las Vegas, U.S.A, Jul. 2005).
9) N. Nakajima, T. Aoyagi, Y. Tsujita, R. Arima, M. Yamazaki, K. Idemitsu, "An Approach to realize a large-scale simulation for nuclear plant's materials by molecular dynamics", *Joint Conference of Electrical and Electronics Engineers in Chugoku*, (Hiroshima, Japan, Oct. 2005).
10) O. Hazama, N. Nakajima, Post, P.,Wolf, K., "Development of a generic coupler for parallel and distributed multi-disciplinary simulations on the Japanese ITBL grid

infrastructure", *8th US National Congress on Computational Mechanics (USNCCM-8)*, (Austin, U.S.A, Jul. 2005).

11) M. Ida, "Avoided crossings observed in three coupled oscillators as a model of acoustically coupled bubbles", *2005 Annual Meeting of Japan Society of Fluid Mechanics*, (Tokyo, Japan, Sep. 2005).

12) S. Shinohara, Y. Okuda, N. Nakajima, M. Ida, "Shape optimization using parameter-survey-type parallel adjoint variable method", *The 18th Computational Mechanics Conference*, (Sendai, Japan, Nov. 2005).

13) E. Kume, T. Kitamura, K. Takase, Y. Ose, "Numerical visualization of herted liquid film flow behavior around a spacer in a narrow channel", *National Symposium on Visualization, Visualization society of Japan*, (Niigata, Japan, Oct. 2005).

14) O. Hazama, H. Matsubara, Tian. R, A. Nishida, Y. Suzuki, M. Tani,N. Nakajima, "Towards construction of a numerical testbed for nuclear power plants", *7th MpCCI User Forum*, (Sankt Augustin, Germany, Feb. 2006).

15) S. Shinohara, Y. Okuda, S. Ito, N. Nakajima, M. Ida, "Shape optimization technique using adjoint variable method", *The 19th Symposium on Computational Fluid Dynamics*, (Tokyo, Japan, Dec. 2005).

16) S. Tokuda, M. Furukawa, Y. Yoshida, "Regularization method in magnetohydrodynamic stability problems with continuous spectra", *2005 Annual Meeting of Japan Society of Fluid Mechanics,* (Tokyo, Japan, Sep. 2005).

17) S. Tokuda, N. Aiba, I. Minami, "Parallel computing method for monitoring the MHD stability of a fusion plasma", *The 2005 annual conference of the Japan Society for Industrial and Applied Mathematics*, (Sendai, Japan, Sep. 2005).

18) N. Nakajima, "Visualization technique in ITBL and strategy",*Seminar for Advanced Visualization*, (Tokyo, Japan, Jun. 2006).

19) N. Nakajima, "Visualization technique in ITBL and strategy", *The 4th VizGrid Symposium*, (Tokyo, Japan, Jun. 2006).

20) Tian, R., A. Miyazaki, N. Nakajima, M. Yagawa, "Tian, R., "Nodal arrangement for boundary treatments in the EFGM", *8th US National Congress on Computational Mechanics (USNCCM-8)*, (Austin, U.S.A, Jul. 2005).

21) Tian, R., H. Matsubara, A. Miyazaki, N. Nakajima, M. Yagawa",A Formulation of generalized node, a quadratic tetrahedron/triangle with only corners, and meshfree approximations with rotational dofs", *8th US National Congress on Computational Mechanics (USNCCM-8)*, (Austin, U.S.A, Jul. 2005).

22) Tian, R., A. Miyazaki, N. Nakajima, M. Yagawa, "Some numerical studies on linear dependence problems in partition-of-unity based generalized finite element

methods", *8th US National Congress on Computational Mechanics (USNCCM-8)*, (Austin, U.S.A, Jul. 2005).

23) S. Shinohara, Y. Okuda, S. Ito, N. Nakajima, M. Ida, "Shape optimization using parallel adjoint variable method in ITBL environment", *The 2005 annual conference of the Japan Society for Industrial and Applied Mathematics*, (Sendai, Japan, Sep. 2005).

24) T. Hirayama, "For development of nuclear fusion power reactor; Future of plasma simulation", *Symposium on Computational Science and Tchnology*, (Tokyo, Japan, Sep. 2005).

25) M. Tani, Y. Suzuki, A. Nishida, N. Nakajima, "The ITBL middleware and its applications", *International Conference for High Performance Computing, Networking and Storage (SC '05)*, (seattle, U.S.A, Nov. 2005).

26) Y. Suzuki, N. Matsumoto, K. Nakajima, M. Tani, N. Nakajima, "R&D for visualization tool in ITBL middleware", *International Conference for High Performance Computing, Networking and Storage (SC '05)*, (seattle, U.S.A, Nov. 2005).

27) H. Matsubara, T. Minami, O. Hazama, A. Miyazaki, Tian, R, N. Nakajima, M. Tani, "The Large-scale Numerical Analysis of Nuclear Power Plant in Distributed Computational Environment", *International Conference for High Performance Computing, Networking and Storage (SC '05)*, (seattle, U.S.A, Nov. 2005).

28) A. Miyazaki, Tian, R, H. Matsubara, N. Nakajima, M. Tani , "The Large-scale numerical simulation of nuclear power plant on ITBL grid infrastructure, 2; Numerical simulation results", *International Symposium on Structures under Impulsive Loading (IB '05)*, (Nagoya, Japan, Nov. 2005).

29) Y. Suzuki, "Utilization of ITBL to fusion grid", *2006 NIFS Collaborative Research, "Study of the Next Generation System for Data Analysis of Nuclear Fusion Experiments"*, (Toki, Japan, Feb. 2006).

30) N. Nakajima, "A Nuclear engineering application for analytic challenge award", *International Conference for High Performance Computing, Networking and Storage (SC '05)*, (seattle, U.S.A, Nov. 2005).

31) S. Shinohara, Y. Okuda, S. Ito, N. Nakajima, M. Ida, "Shape optimization using adjoint variable method and its application to ITBL grid", *Symposium on High Performance Computing and Computational Science (HPCS 2006)*, (Tokyo, Japan, Jan. 2006).

32) N. Yamagishi, T. Aoyagi, S. Hasegawa, N. Nakajima, M. Tani, "Development of communication mechanism in ITBL middleware", *International Conference for High*

Performance Computing, Networking and Storage (SC '05), (seattle, U.S.A, Nov. 2005).

33) M. Ida, "Multibubble dynamics; Phase shift, transition frequency, and avoided crossing", *American Physical Society 58th Annual Meeting of the Division of Fluid Dynamics*, (Chicago, U.S.A, Nov. 2005).

34) M. Machida, "Numerical simulations for non-equilibrium superconducting dynamics in neutron and X-ray detection", *4th JSIAM-SIMAI Seminar on Industrial and Applied Mathematics*, (Hayama, Japan, May. 2005).

35) M. Machida, "Vortex structure and dynamics in fermi superfluids; From superconductivity to fermi atom gas", *Ryukoku Workshop on Mathematical Aspects of Pattern Formation and Dynamics in Dissipative Systems*, (Seta, Japan, Jul. 2005).

36) M. Machida, T. Koyama, H. Oohashi, "Structure change of a quantized vortex in fermi atom gas", *24th International Conference on Low Temperature Physics (LT24)*, (Oland, U.S.A, Aug. 2005).

37) M. Machida, T. Koyama, M. Kato, T. Ishida, "Direct numerical simulation on non-equilibrium superconducting dynamics after neutron capture in MgB2 superconductors", *11th International Workshop on Low Temperature Detectors (LTD-11)*, (Tokyo, Japan, Jul. 2005).

38) M. Machida, T. Koyama, H. Oohashi, "Vortex structure from BCS to BEC Superfluid", *Joint JSPS and ESF Conference on Vortex Matter in Nanostructured Superconductors (VORTEX-4)*, (Crete, Greece, Sep. 2005).

39) M. Watanabe, "Numerical simulation of droplet dynamics using level set method", *11th International Topical Meeting on Nuclear Reactor Thermal Hydraulics (NURETH-11)*, (Avignon, France, Oct. 2005).

40) K. Ebihara, H. Kaburaki, "Lattice boltzmann simulation of solution chemistry for crevice corrosion", *14th International Conference on Discrete Simulation of Fluid Dynamics in Complex Systems*, (Kyoto, Japan, Aug. 2005).

41) M. Itakura, H. Kaburaki, T. Suzudo, S. Suzuki, "Mesoscopic simulations on the evolution of a system of dislocations in the presence of a grain boundary", *Micromechanics and Microstructure Evolution*, (Madrid, Spain, Sep. 2005).

42) M. Machida, S. Yamada , H. Oohash, H. Matsumoto, "Superfluidity and pseudo-spin magnetism of trapped fermi atoms on an optical lattice", *14th International Laser Physics Workshop (LPHYS '05)*, (KeihannaPlaza, Japan, Jul. 2005).

43) M. Itakura, "The Branching mechanism of intergranular crack propagation",

Advanced Numerical Analysis for Solving Dynamics of interface phenomena and Its Application II, (Kobe, Japan, Jul. 2005).

44) S. Yamada, T. Imamura, M. Machida, "Preconditioned conjugate gradient method for eigenvalue problems of ultra large-scale matrix", *The 2005 annual conference of the Japan Society for Industrial and Applied Mathematics*, (Sendai, Japan, 2005).

45) S. Yamada, T. Imamura, M. Machida, "16.14 TFLOPS eigenvalue solver on the earth simulator; Exact diagonalization for ultra largescale hamiltonian matrix", *6th International Symposium on High Performance Computing (ISHPC-6)*, (Nara, Japan, Sep. 2005).

46) M. Shiga, "Perturbative QM/MM molecular dynamics-theory", *Annual Meeting of the Molecular Science Society of Japan*, (Tokyo, Japan, Sep. 2005).

47) M. Machida, S. Yamada, H. Oohash, H. Matsumoto, "On Pseudo-spin magnetism and superfluidity in trapped atomic fermi gas placed in an optical lattice", *2005 Autumn Meeting of the Physical Society of Japan*, (Kyoto, Japan, Sep. 2005).

48) M. Machida, T. Koyama, M. Kato, T. Ishida, "A Confirmation of string formation (Kibble-Zurek mechanism) by quenching superconducting thin films with hole arrays", *2005 Autumn Meeting of the Physical Society of Japan*, (Kyoto, Japan, Sep. 2005).

49) N. Sasa, J. Ieda, "Hirota's method for 3-component NLS equation in Spinor BEC", *The 2005 annual conference of the Japan Society for Industrial and Applied Mathematics*, (Sendai, Japan, Sep. 2005).

50) N. Sasa, M. Machida, K. Kasamatsu, M. Tsubota, "Energy disspation and turbulence in a rotating BEC", *2005 Autumn Meeting of the Physical Society of Japan*, (Kyoto, Japan, Sep. 2005).

51) N. Sasa, "Application of symplectic integrator for BEC system", *RIMS Conference "From Soliton Theory to a Mathematics of Integrable Systems"*, (Kyoto, Japan, Aug. 2005).

52) T. Szudo, H. Kaburaki, M. Itakura, "Cellular automaton model of fission gas behavior in nuclear fuel", *Micromechanics and Microstructure Evolution*, (Madrid, Spain, Sep. 2005).

53) K. Ebihara, "A Study on interfacial growth and deformation in horizontal stratified two-phase flow using lattice Boltzmann method", *Doctor Forum 2005, AESJ*, (Hachinohe, Japan, Sep. 2005).

54) M. Watanabe, "Interfacial dynamics of levitated droplet", *The 18th Computational Mechanics Conference, JSME*, (Tsukuba, Japan, Nov. 2005).

55) K. Yura, "Protein structural bioinformatics for protein function prediction; Studies

of DNA repair related proteins", *The 5th Annual Meeting of the Protein Science Society of Japan*, (Fukuoka, Japan, Jun. 2005).

56) Kim. T. P. O., K. Yura, N. Go, "Structure-based bioinformatics analyses of protein-RNA interface toward the understanding of RNA interface on proteins", *The 5th Annual Meeting of the Protein Science Society of Japan,* (Fukuoka, Japan, Jun. 2005).

57) Y. Yoneya, "On the treatment of the long-range interactions in biomolecular simulations", *2005 Autumn Meeting of the Physical Society of Japan*, (Kyoto, Japan, Sep. 2005).

58) M. Itakura, T. Kadoyoshi, H. Kaburaki, S. Jutsukawa, "Molecular dynamics and quasi-two dimensional dislocation dynamics simulations on the hardening mechanism of FCC metals", *Materials Research Society 2005 Fall Meeting,* (Boston, U.S.A, Nov. 2005).

59) M. Yamaguchi, H. Nishiyama, M. Shiga, H. Kaburaki, "First-principles calculations on the embrittlement mechanism of bcc iron grain boundaries by impurity segregation", *Materials Research Society 2005 Fall Meeting*, (Boston, U.S.A, Nov. 2005).

60) N. Nakajima, "A Nuclear Engineering Application for Analytic Challenge Award", *The International Conference for High Performance Computing, Networking And Storage(2005)*, (Seattle, U.S.A, Nov. 2005).

61) M. Machida, T. Koyama, H. Oohashi, "Vortex structure in weak to strong coupling superconductors: Crossover from BCS to BEC", *18-th International Symposium on Superconductivity,* (Tsukuba, Japan, Oct. 2005).

62) M. Yamaguchi, M. Shiga, H. Kaburaki, "Grain boundary embrittlement of iron by phosphorous segregation- A first-principles study", *CRIEPI, Meeting for irradiation damage mechanisms on water reactor materials*, (Tokyo, Japan, Oct. 2005).

63) T. Suzudo, M. Itakura, H. Kaburaki, "Meso-Scale Approaches to the Simuration of the Microstructure Formation Observed at Higi-Burnup", *New Crossover Workshop-2*, (Kyoto, Japan, Oct. 2005) .

64) T. Suzudo, M. Itakura, H. Kaburaki, "A Monte-Carlo simulation of bubble nucleation and growth", *Topical meeting on irradiation damage mechanism of LWR materials, CRIEPI*, (Tokyo, Japan, Oct. 2005).

65) Kim. T. P. O, K. Yura, "Database analysis of interfaces 3D structures between protein and RNA", *The 43nd Annual meeting of biophysical society of Japan*, (Sapporo, Japan, Nov. 2005).

66) K. Yura, "Supramolecular database for deducing higi resolntion structure", *The*

43nd Annual meeting of biophysical society of Japan, (Sapporo, Japan, Nov. 2005).

67) A. Matsumoto, "The effect of local nuclotide structure on the global flexibility of circular DNA deduced from noramal mode analysis", *The 43nd Annual meeting of biophysical society of Japan*, (Sapporo, Japan, Nov. 2005).

68) M. Machida, T. Imamura, S. Yamada, "16.447 Tflop /s and 159-Billion-Dimensional Exact Diagonalization for Trapped Fermion-Hubbard Model on the Earth Simulator", *The International Conference for High Performance Computing, Networking and Storage*, (Seattle, U.S.A, Nov. 2005).

69) S. Yamada, T. Imamura, M. Machida, "A challenge to largest-scale eigenvelue problem on the Earth Simulator", *The 18th Computational Mechanics Conference*, (Tsukuba, Japan, Oct. 2005).

70) T. Suzudo, M. Itakura, H. Kaburaki, "Meso-Scale Approaches to the Simuration of the Microstructure Formation Observed at Higi-Burnup", *Innovative Nanoscale Approach to Dynamic Studies of Materials*, (Okinawa, Japan, Jan. 2006).

71) M. Machida, "Numerical Simulations for Superconducting Radiation Detector and Novel Nano-scale Superconductivity", *Annual Meeting for research projects in FY 2005*, (Yokohama, Japan, Jan. 2006) .

72) T. Suzudo, M. Itakura, H. Kaburaki, E. Iwai, "Three-Dimonsional Monte-Carlo Simulation of the Nuclation and Growth of Bubbles", *2006 Spring Meeting of Atomic Energy Society of Japan*, (Ooarai, Japan, Mar. 2006).

73) N. Sasa, "Turbulence and Vortex Lattice in a Rotating BEC", *The 55th Conference for Theoretical and Applied Mechanics*, (Kyoto, Japan, Feb. 2006).

74) M. Machida, H. Oohashi, T. Koyama , "Vortex Structure and Dynamics in Fermi Superfluid Gas", *2006 American Physical Society Marchi Meeting*, (Baltimore, U.S.A, Mar. 2006).

75) M. Machida, H. Oohashi, T. Koyama, "Turbulencd and Vortex Lattice in a Rotating BEC", *Spring Meeting of Physical Society of Japan*, (Matsuyama, Japan, Mar, 2006).

76) M. Machida, "Vortex Structure in Atomic Fermi Gas : Vortex Under Extreme Situations", *Seminar on the Strong-Coupling Modeling Group, NIMS-CMSC*, (Tsukuba, Japan, Feb. 2006).

77) M. Yamaguchi, H. Nishiyama, M. Shiga, H. Kaburaki, "Iron grain boundary embrittlement by phosphorous or sulfur segregation - A first-principles study -", *Meeting of Japan Institute of Metals 2006 Spring*, (Tokyo, Japan, Mar. 2006).

78) M. Machida, "Huge-Space-Time and Large-Scale Simulation in Atomic Power Field", *The 13th workshop of CCSE* (Tokyo, Japan, Feb. 2006).

79) M. Yamaguchi, "Grain boundary embrittlement by impurity segregation – A first-

principles study", *The 13th workshop of CCSE*, (Tokyo, Japan, Feb. 2006).

80) S. Yamada, T. Imamura, M. Machida, "Novel Numerical method for ultra-large-scale sparse matrix on full nodes of the Earth Simulator", *The 12th meeting of the Japan Society of Mechanical Engineers*, (Kawagoe, Japan, Mar. 2006).

81) S. Yamada, T. Imamura, M. Machida, "Preconditoned conjugate gradient method for eigenvalue problem of quantum problem", *The joint meeting of the Japan Society for Industrial and Applied Mathematics*, (Tokyo, Japan, Mar. 2006).

82) S. Ogata, F. Shimizu, J. Li, M. Wakeda, Y. Shibuya, "Atomistic Simulation of Shear Localization in Zr-Cu Bulk Metallic Glass", *The fourth International Bulk Metallic Glasses Conference*, (Gatlinburg, U.S.A, May. 2005).

83) F. Shimizu, N. Ogata, J. Li, H. Kaburaki, "Approaching the Universal Yield of Metallic Glasses From Molecular Dynamics Simulations", *Materials Research Society 2005 Fall Meeting*, (Boston, U.S.A, Nov. 2005).

84) F. Shimizu, N. Ogata,, H. Kimizuka, T. Kano, H. Kaburaki, "First-principles Study on the Core Structure of Dislocation in BCC -An Accurate Calculation using Earth Simulator", *The 13th CCSE Workshop*, (Tokyo, Japan, Feb. 2006).

85) K. Yura, "Characteristics of subunit inerfaces in biosupramolecules", *Seminar in Institute for Protein Research Osaka University, "Decoding biomolecular functions based on time and space dimension"*, (Oosaka, Japan, Mar. 2006).

86) Li. Ju, F. Shimizu, N. Ogata, H. Kaburaki, "Approaching the Universal Yield of Metallic Glasses From Molecular Dynamics Simulations", *TMS 2006 : 135 t h Annual Meeting and Exhibition*, (San Antonio, U.S.A, Mar. 2006).

87) N. Nakajima, "An approach to manege and control the communication quality and security in service", *Project of the Ministry of Education, Culture, Sports, Science and Technology for Private School in Toyo University,* External Assessment of the Research Center for Numerical Mechanics, (Tokyo, Japan, Apr. 2006).

88) N. Sasa, M. Machida, "Vortex Lattice in Optical Lattice", *Spring Meeting of Physical Society of Japan*, (Matsuyama, Japan, Mar. 2006).

89) N. Nakajima, "A Virtual Plant Shaker on ITBL Grid Computing Environment", *2006 Spring Meeting of Atomic Energy Society of Japan*, (Ooarai, Japan, Mar. 2006).

3.2 Staff List in Center for Promotion Computational Science and Engineering (April 2005 – September 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 Miyazaki
	Rong Tian
Post-Doctor Fellow:	Osamu Hazama
	Yufei Shu
	Hitoshi Matubara
Fellow of Advanced Science:	Kazunori Shinohara

Research Group for Computational Material Science in Atomic Energy

Group Leader, Principal Scientist	Masahiko Machida
Research Scientist:	Narimasa Sasa
	Futoshi Shimizu
	Mituhiro Itakura
	Susumu Yamada
	Motoyuki Siga
Cooperative Staff:	Tomoko Kadoyoshi
Visiting Researcher:	Chuichi Arakawa

R&D Group for Computer Science

Division Leader:	Norihiro Nakajima
Principal Engineer:	Tetsuo Aoyagi
Principal Researcher:	Shinji Tokuda
Collaborating Engineer:	Nobuko Matumoto
	Nobuhiro Yamagishi
	Yukihiro Hasegawa
	Takahiro Minami

Kohei Nakajima

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:	Atushi Matumoto
	Kensuke Nakamura
Post-Doctor 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 Kitano

Staff List Center for Computational Science & e-Systems
(October 2005 - March 2006)

Director:	Genki Yagawa
Deputy Director	Toshio Hirayama

Computer Science Research and Development Office

Division Leader:	Norihiro Nakajima
Principal Engineer:	Tetsuo Aoyagi
Principal Researcher:	Shinji Tokuda
Assistant Principal Researcher:	Yoshio Suzuki
Assistant Principal Engineer:	Toshihiko Matsuura
Scientist:	Masato Ida
Staff (engineer):	Hideo Kimura
Collaborating Engineer:	Nobuko Matumoto
	Yukihiro Hasegawa
	Nobuhiro Yamagishi
	Takahiro Minami
	Kohei Nakajima
Senior Post-Doctor Fellow:	Osamu Hazama
	Akemi Miyazaki
	Rong Tian
	Noriyuki Kushida
Post-Doctor Fellow:	Hitoshi Matubara
	Yufei Shu

Simulation Technology Research and Development Office

Division Leader:	Masahiko Machida
Vice Division Leader	Kei Yura
Invited Researcher:	Chuichi Arakawa
Assistant Principal Researcher:	Tomoaki Suzudo
	Masatake Yamaguch
	Mituhiro Itakura
Scientist:	Narimasa Sasa

Futoshi Shimizu
Susumu Yamada
Motoyuki Siga
Atushi Matumoto
Research Engineer: Ken-ichi Ebihara
Collaborating Engineer: Tomoko Kadoyoshi
Senior Post-Doctor Fellow: Kensuke Nakamura
Fellow of Advanced Science: Masataka Oikawa

国際単位系（SI）

表１．SI 基本単位

基本量	SI 基本単位	
	名称	記号
長さ	メートル	m
質量	キログラム	kg
時間	秒	s
電流	アンペア	A
熱力学温度	ケルビン	K
物質量	モル	mol
光度	カンデラ	cd

表２．基本単位を用いて表されるSI組立単位の例

組立量	SI 基本単位	
	名称	記号
面積	平方メートル	m^2
体積	立法メートル	m^3
速さ，速度	メートル毎秒	m/s
加速度	メートル毎秒毎秒	m/s^2
波数	毎メートル	m^{-1}
密度（質量密度）	キログラム毎立法メートル	kg/m^3
質量体積（比体積）	立法メートル毎キログラム	m^3/kg
電流密度	アンペア毎平方メートル	A/m^2
磁界の強さ	アンペア毎メートル	A/m
（物質量の）濃度	モル毎立方メートル	mol/m^3
輝度	カンデラ毎平方メートル	cd/m^2
屈折率	（数の）1	1

表５．SI 接頭語

乗数	接頭語	記号	乗数	接頭語	記号
10^{24}	ヨタ	Y	10^{-1}	デシ	d
10^{21}	ゼタ	Z	10^{-2}	センチ	c
10^{18}	エクサ	E	10^{-3}	ミリ	m
10^{15}	ペタ	P	10^{-6}	マイクロ	μ
10^{12}	テラ	T	10^{-9}	ナノ	n
10^{9}	ギガ	G	10^{-12}	ピコ	p
10^{6}	メガ	M	10^{-15}	フェムト	f
10^{3}	キロ	k	10^{-18}	アト	a
10^{2}	ヘクト	h	10^{-21}	ゼプト	z
10^{1}	デカ	da	10^{-24}	ヨクト	y

表３．固有の名称とその独自の記号で表されるSI組立単位

組立量	SI 組立単位			
	名称	記号	他のSI単位による表し方	SI基本単位による表し方
平面角	ラジアン(a)	rad		$m \cdot m^{-1}=1$(b)
立体角	ステラジアン(a)	sr(c)		$m^2 \cdot m^{-2}=1$(b)
周波数	ヘルツ	Hz		s^{-1}
力	ニュートン	N		$m \cdot kg \cdot s^{-2}$
圧力，応力	パスカル	Pa	N/m^2	$m^{-1} \cdot kg \cdot s^{-2}$
エネルギー，仕事，熱量	ジュール	J	N・m	$m^2 \cdot kg \cdot s^{-2}$
工率，放射束	ワット	W	J/s	$m^2 \cdot kg \cdot s^{-3}$
電荷，電気量	クーロン	C		s・A
電位差（電圧），起電力	ボルト	V	W/A	$m^2 \cdot kg \cdot s^{-3} \cdot A^{-1}$
静電容量	ファラド	F	C/V	$m^{-2} \cdot kg^{-1} \cdot s^4 \cdot A^2$
電気抵抗	オーム	Ω	V/A	$m^2 \cdot kg \cdot s^{-3} \cdot A^{-2}$
コンダクタンス	ジーメンス	S	A/V	$m^{-2} \cdot kg^{-1} \cdot s^3 \cdot A^2$
磁束	ウエーバ	Wb	V・s	$m^2 \cdot kg \cdot s^{-2} \cdot A^{-1}$
磁束密度	テスラ	T	Wb/m^2	$kg \cdot s^{-2} \cdot A^{-1}$
インダクタンス	ヘンリー	H	Wb/A	$m^2 \cdot kg \cdot s^{-2} \cdot A^{-2}$
セルシウス温度	セルシウス度(d)	℃		K
光束	ルーメン	lm	cd・sr(c)	$m^2 \cdot m^{-2} \cdot cd=cd$
照度	ルクス	lx	lm/m^2	$m^2 \cdot m^{-4} \cdot cd=m^{-2} \cdot cd$
（放射性核種の）放射能	ベクレル	Bq		s^{-1}
吸収線量，質量エネルギー分与，カーマ	グレイ	Gy	J/kg	$m^2 \cdot s^{-2}$
線量当量，周辺線量当量，方向性線量当量，個人線量当量，組織線量当	シーベルト	Sv	J/kg	$m^2 \cdot s^{-2}$

(a)ラジアン及びステラジアンの使用は、同じ次元であっても異なった性質をもった量を区別するときの組立単位の表し方として利点がある。組立単位を形作るときのいくつかの用例は表４に示されている。
(b)実際には、使用する時には記号rad及びsrが用いられるが、習慣として組立単位としての記号“１”は明示されない。
(c)測光学では、ステラジアンの名称と記号srを単位の表し方の中にそのまま維持している。
(d)この単位は、例としてミリセルシウス度m℃のようにSI接頭語を伴って用いても良い。

表４．単位の中に固有の名称とその独自の記号を含むSI組立単位の例

組立量	SI 組立単位		
	名称	記号	SI 基本単位による表し方
粘度	パスカル秒	Pa・s	$m^{-1} \cdot kg \cdot s^{-1}$
力のモーメント	ニュートンメートル	N・m	$m^2 \cdot kg \cdot s^{-2}$
表面張力	ニュートン毎メートル	N/m	$kg \cdot s^{-2}$
角速度	ラジアン毎秒	rad/s	$m \cdot m^{-1} \cdot s^{-1}=s^{-1}$
角加速度	ラジアン毎平方秒	rad/s^2	$m \cdot m^{-1} \cdot s^{-2}=s^{-2}$
熱流密度，放射照度	ワット毎平方メートル	W/m^2	$kg \cdot s^{-3}$
熱容量，エントロピー	ジュール毎ケルビン	J/K	$m^2 \cdot kg \cdot s^{-2} \cdot K^{-1}$
質量熱容量（比熱容量），質量エントロピー	ジュール毎キログラム毎ケルビン	J/(kg・K)	$m^2 \cdot s^{-2} \cdot K^{-1}$
質量エネルギー（比エネルギー）	ジュール毎キログラム	J/kg	$m^2 \cdot s^{-2} \cdot K^{-1}$
熱伝導率	ワット毎メートル毎ケルビン	W/(m・K)	$m \cdot kg \cdot s^{-3} \cdot K^{-1}$
体積エネルギー	ジュール毎立方メートル	J/m^3	$m^{-1} \cdot kg \cdot s^{-2}$
電界の強さ	ボルト毎メートル	V/m	$m \cdot kg \cdot s^{-3} \cdot A^{-1}$
体積電荷	クーロン毎立方メートル	C/m^3	$m^{-3} \cdot s \cdot A$
電気変位	クーロン毎平方メートル	C/m^2	$m^{-2} \cdot s \cdot A$
誘電率	ファラド毎メートル	F/m	$m^{-3} \cdot kg^{-1} \cdot s^4 \cdot A^2$
透磁率	ヘンリー毎メートル	H/m	$m \cdot kg \cdot s^{-2} \cdot A^{-2}$
モルエネルギー	ジュール毎モル	J/mol	$m^2 \cdot kg \cdot s^{-2} \cdot mol^{-1}$
モルエントロピー，モル熱容量	ジュール毎モル毎ケルビン	J/(mol・K)	$m^2 \cdot kg \cdot s^{-2} \cdot K^{-1} \cdot mol^{-1}$
照射線量（X線及びγ線）	クーロン毎キログラム	C/kg	$kg^{-1} \cdot s \cdot A$
吸収線量率	グレイ毎秒	Gy/s	$m^2 \cdot s^{-3}$
放射強度	ワット毎ステラジアン	W/sr	$m^4 \cdot m^{-2} \cdot kg \cdot s^{-3}=m^2 \cdot kg \cdot s^{-3}$
放射輝度	ワット毎平方メートル毎ステラジアン	$W/(m^2 \cdot sr)$	$m^2 \cdot m^{-2} \cdot kg \cdot s^{-3}=kg \cdot s^{-3}$

表６．国際単位系と併用されるが国際単位系に属さない単位

名称	記号	SI 単位による値
分	min	1 min=60s
時	h	1h =60 min=3600 s
日	d	1 d=24 h=86400 s
度	°	1° =(π/180) rad
分	’	1’ =(1/60)° =(π/10800) rad
秒	”	1” =(1/60)’ =(π/648000) rad
リットル	l、L	1l=1 $dm^3=10^{-3}m^3$
トン	t	$1t=10^3$ kg
ネーパ	Np	1Np=1
ベル	B	1B=(1/2)ln10(Np)

表７．国際単位系と併用されこれに属さない単位でSI単位で表される数値が実験的に得られるもの

名称	記号	SI 単位であらわされる数値
電子ボルト	eV	$1eV=1.60217733(49) \times 10^{-19}$J
統一原子質量単位	u	$1u=1.6605402(10) \times 10^{-27}$kg
天文単位	ua	$1ua=1.49597870691(30) \times 10^{11}$m

表８．国際単位系に属さないが国際単位系と併用されるその他の単位

名称	記号	SI 単位であらわされる数値
海里		1海里=1852m
ノット		1ノット=1海里毎時=(1852/3600)m/s
アール	a	1a=1 $dam^2=10^2m^2$
ヘクタール	ha	1ha=1 $hm^2=10^4m^2$
バール	bar	1bar=0.1MPa=100kPa=1000hPa=10^5Pa
オングストローム	Å	1 Å=0.1nm=10^{-10}m
バーン	b	1b=100$fm^2=10^{-28}m^2$

表９．固有の名称を含むCGS組立単位

名称	記号	SI 単位であらわされる数値
エルグ	erg	1 erg=10^{-7} J
ダイン	dyn	1 dyn=10^{-5}N
ポアズ	P	1 P=1 dyn・s/cm^2=0.1Pa・s
ストークス	St	1 St =1$cm^2/s=10^{-4}m^2/s$
ガウス	G	1 G ^10^{-4}T
エルステッド	Oe	1 Oe ^(1000/4π)A/m
マクスウェル	Mx	1 Mx ^10^{-8}Wb
スチルブ	sb	1 sb =1cd/$cm^2=10^4cd/m^2$
ホト	ph	1 ph=10^4lx
ガル	Gal	1 Gal =1cm/$s^2=10^{-2}m/s^2$

表10．国際単位に属さないその他の単位の例

名称	記号	SI 単位であらわされる数値
キュリー	Ci	1 Ci=3.7×10^{10}Bq
レントゲン	R	1 R = 2.58×10^{-4}C/kg
ラド	rad	1 rad=1cGy=10^{-2}Gy
レム	rem	1 rem=1 cSv=10^{-2}Sv
X線単位		1X unit=1.002×10^{-4}nm
ガンマ	γ	1γ=1 nT=10^{-9}T
ジャンスキー	Jy	1 Jy=$10^{-26}W \cdot m^{-2} \cdot Hz^{-1}$
フェルミ		1 fermi=1 fm=10^{-15}m
メートル系カラット		1 metric carat = 200 mg = 2×10^{-4}kg
トル	Torr	1 Torr = (101 325/760) Pa
標準大気圧	atm	1 atm = 101 325 Pa
カロリー	cal	
ミクロン	μ	1 μ =1μm=10^{-6}m

（第７版，1998年改訂）