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IN
CENTER FOR PROMOTION OF
COMPUTATIONAL SCIENCE AND ENGINEERING
FROM APRIL 1, 2003 TO MARCH 31, 2004

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Center for Promotion of Computational Science and Engineering

日本原子力研究所
Japan Atomic Energy Research Institute

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**Annual Report of R&D Activities in Center for Promotion of Computational Science
and Engineering
from April 1, 2003 to March 31, 2004**

Center for Promotion of Computational Science and Engineering

**Japan Atomic Energy Research Institute
Higashi-ueno, Taito-ku, Tokyo**

(Received February 24, 2005)

Major Research and development activities of Center for Promotion of Computational Science and Engineering (CCSE), JAERI, have focused on ITBL (IT Based Laboratory) project, computational material science and Quantum Bioinformatics. This report provides an overview of research and development activities in (CCSE) in the fiscal year 2003 (April 1, 2003 – March 31, 2004).

Keywords: JAERI, Annual Report Research and Development, Computational Science and Engineering, CCSE, ITBL Project, Computational Material Science, Quantum Bioinformatics.

JAERI-Review 2005-014

平成 15 年度 計算科学技術推進センター 研究開発年報

日本原子力研究所
計算科学技術推進センター

(2005 年 2 月 24 日受理)

日本原子力研究所 計算科学技術推進センターでは主に ITBL (IT Based Laboratory) 計画、材料計算科学、量子生命解析に関する研究開発活動を行っている。本報告書は、平成 15 年度の研究開発活動について報告するものである。

Contents

Foreword

1.	Introduction.....	1
2.	Overview of CCSE.....	2
3.	CCSE Research and Development Activities.....	3
3.1	ITBL Project.....	3
3.1.1	Overview.....	3
3.1.2	Research and Development of Parallel Basic Software System.....	8
3.1.3	Research and Development of Parallel Processing Tools.....	15
3.2	Computational Material Science.....	25
3.2.1	Macroscopic Quantum Dynamics in Superconductivity and Quantum Gas.....	26
3.2.2	Multiscale Simulations on the Irradiation Induced Property Changes and Fracture of Materials.....	27
3.3	Quantum Bioinformatics Research.....	35
3.3.1	Development of Protein Structural Information Databases And Analysis Tools.....	35
3.3.2	Development of DNA Repair Protein Databases.....	36
4.	Public Relations.....	40
4.1	Press Release.....	40
4.2	CCSE News.....	41
4.3	Workshops, Conferences and Events.....	43
4.4	Seminars.....	44
5.	Research Collaboration.....	50
6.	Research Achievements.....	54
6.1	Publications.....	54
6.2	Talks and Presentations.....	59
6.3	Awards.....	70

目次

前書き

1. 序論.....	1
2. CCSE の概要.....	2
3. CCSE 研究・開発活動.....	3
3.1 ITBL 計画.....	3
3.1.1 ITBL 計画の概要.....	3
3.1.2 並列処理基本ソフトウェアシステムの開発.....	8
3.1.3 並列処理ツールの開発.....	15
3.2 材料計算科学研究.....	25
3.2.1 超伝導と量子ガスにおける巨視的量子ダイナミクス.....	26
3.2.2 照射誘起による物性変化と材料破壊のマルチスケール・シミュレーション.....	27
3.3 量子生命解析研究.....	35
3.3.1 タンパク質構造情報データベースと解析ツールの開発.....	35
3.3.2 DNA 修復関連タンパク質データベースの開発.....	36
4. 広報活動.....	40
4.1 プレス発表.....	40
4.2 CCSE ニュース.....	41
4.3 ワークショップ、会議、イベント等.....	43
4.4 セミナー.....	44
5. 研究協力.....	50
6. 研究業績.....	54
6.1 研究論文.....	54
6.2 発表、講演等.....	59
6.3 受賞等.....	70

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Acronyms

ADVENTURE	ADVanced Engineering analysis Tool for Ultra large Real world
AESJ	Atomic Energy Society of Japan
API	Application Programming Interface
BAAQ	Bioinformatics: Ask Any Questions
BCC	Body Centered Cubic
BEC	Bose-Einstein condensate
CAE	Computer Aided Engineering
CCJJ	Capacitively-Coupled Josephson Junctions
CCSE	Center for Promotion of Computational Science and Engineering
CMD	Computational Material Design
CTRTx	CT Radiotherapy
EAM	Embedded Atom Method
ES	Earth Simulator
FCC	Face Centered Cubic
FEM	Finite Element Method
FLOPS	Floating Operations Per Second
FS	Free Surface
GB	Grain Boundary
GIF	Graphic Interchange Format
GUI	Graphical User Interface
HPC	High Performance Computer
IMRT	Intensity Modulated Radiation Therapy
IT	Information Technology
ITBL	IT Based Laboratory
JAERI	Japan Atomic Energy Research Institute
JAXA	Japan Aerospace Exploration Agency
JST	Japan Science and Technology Agency
LBM	Lattice Boltzmann Method
MpCC	Mesh-based parallel Code Coupling Interface
MPI	Message Passing Interface
NAREGI	National Research Grid Initiative
NDB	Nucleic Acid Database
NIED	National Institute for Earth Science and Disaster Prevention
NIMS	National Institute for Materials Science

PATRAS	PA rallel TR acking And S teering
PDB	P rotein D ata B ank
PST	P arallel S upport T oolkit
SCC	S tress C orrosion C racking
SFT	S tacking F ault T etrahedron
STA	S eamless T hinking A id
STAMPI	S eamless T hinking A id M essage P assing I nterface
STARPC	S eamless T hinking A id R emote P rocedure C all
TDGP	T ime- D ependent G ross- P itaevskii
TME	T ask M apping E ditor
VR	V irtual R eality

Foreword

The CCSE (Center for Promotion of Computational Science and Engineering) started in 1995 by renaming and reorganizing JAERI (Japan Atomic Energy Research Institute)'s computer center which had been organized in 1963. There are more than 60 members in the CCSE and its annual budget is more than 6 billion Japanese yen. It can be said that the CCSE is one of the oldest and biggest computational engineering research organizations in Japan. So far, the CCSE has conducted research and development activities such as development of a series of the parallel processing basic software for complex and large scale computational simulations in the science and engineering field. The CCSE has also made efforts to construct computational science and engineering related cooperative establishments in JAERI, in Japan and in the world.

One of the compiled fruits of years of efforts is ITBL (Information Technology Based Laboratory) project. The objective of ITBL project is to establish high-speed networking supercomputers to be distributed in different research organizations so that computational resources such as software, databases and computational power can be shared by all organization in Japan. ITBL can realize so called virtual research laboratory. The final goal of the CCSE is the COE in the world. In order to reach the goal, it is necessary to produce achievements as many as possible to the world. Then, we can get feedback to our outcomes and we can improve our research and development ability.

It is our pleasure to publish an annual report of our research and development activities in the fiscal year of 2003. We believe the research and development of in CCSE on a common technological basis of parallel processing for scientific computations through cooperative interactions with other research organizations under MEXT disseminates the fruits thereof in a proper fashion to the public domain as well as to other research and development activities in JAERI.

Genki Yagawa
Director
Center for Promotion of Computational
Science and Engineering,
JAERI

1. Introduction

Ministry of Education, Culture, Sports, Science and Technology (MEXT), Government of Japan (GOJ), is promoting computational science and engineering among the national and other semi-governmental research organization under its influence as one of the key factors for the coming new age of highly advanced technologies for scientific research and industrial applications.

The Center for Promotion of Computational Science and Engineering (CCSE) was established in Japan Atomic Energy Research Institute (JAERI) on October 1, 1995 based on and enhancing the mission of the former Computing and Information System Center of JAERI.

CCSE is expected to play a leading role in the research and development (R&D) of computational science and engineering in Japan. The major parts of its efforts were organized by the Science and Technology Agency of GOJ (STA), the former department of GOJ before restructured, as a national endeavor and entrusted to CCSE in accordance with STA's guidance.

CCSE puts special emphasis on the R&D activities of parallel computing technologies for the advanced computational science and engineering. As a step of this endeavor CCSE is developing a common technological basis of parallel processing for scientific computations through cooperative interactions with other research organizations under MEXT with a goal to disseminate the fruits thereof in a proper fashion to the public domain.

Since FY2000 (April 2000 – March 2001), as a link of the national project of “e-Japan” which promotes the spread and popularization of Information Technology (IT), CCSE has started ITBL project which aims to construct the virtual research environment which enables the innovative styled remote collaborations among research organizations all over Japan.

This report provides an overview of research and development activities in Center for Promotion of Computational Science and Engineering (CCSE), JAERI, in the fiscal year 2003 (April 1, 2003 – March 31, 2004).

2. Overview of CCSE

JAERI CCSE has its headquarters in Ueno, Tokyo and three branches in Tokai establishment, Naka establishment and Kansai establishment. At the end of FY2003 (March 31, 2004), the organization of CCSE is as follows;

R&D Activities

- (1) R&D Group for Parallel Basic Software
- (2) R&D Group for Parallel Algorithm
- (3) R&D Group for Parallel Processing Tools
- (4) R&D Group for Numerical Experiments
- (5) Quantum Bioinformatics Group

Promotion and Support Activities

- (6) Management Office for Parallel Processing Project
- (7) Office of Earth Simulator Use Support
- (8) Office of ITBL Promotion
- (9) Information Systems Operating Division
- (10) Office for OA Promotion

Group and Office (1) – (5) have R&D activities or promotions reported in this report, and R&D activities of CCSE in FY2003 described in Chapter 3 are as follows in order: ITBL Project, Computational Material Science and Quantum Bioinformatics Research.

3. CCSE Research and Development Activities

3.1 ITBL Project

3.1.1 Overview

ITBL (IT Based Laboratory) is a project started in 2001 whose objective is to realize, using information technology (IT), an environment for virtual joint research. ITBL aims to connect 100 or more supercomputers located in Japan over Super SINET so that they can be shared, and aims to build a comprehensive system enabling joint use over the Internet of large-scale experimental facilities and the like. ITBL will also develop and provide software for utilizing databases and supercomputers, thus promoting a variety of types of R&D and improving usage efficiency of various facilities, including supercomputers. Currently ITBL has six member institutions responsible for its development.

Background

Ever since the emergence of computers, performance measures such as computing capability and memory capacity have grown at a dramatic pace, even accompanying with reducing their prices. In particular, supercomputers, which are designed specifically for science and technology calculations, have achieved greater progress in performance than have other types of computers, and are recognized for having tremendously raised the level of R&D in science and technology. R&D is now accomplished much more rapidly and efficiently in many fields. However such benefits have only been obtainable in the limited fields due to a lack of application software designed for supercomputers. Moreover, high price of supercomputers limits their benefits to large research institutions, universities and large corporations.

Furthermore, supercomputers are still not popular among general researchers because there were only a few chances for them to get familiar with supercomputers and only a few specialists who help them to use supercomputers. When a supercomputer is installed in an institution, it is often used without any modification

for five or six years. It is fully occupied with jobs at the end of its service life, resulting in long wait times and inefficient usage. Besides supercomputers, a similar situation exists for extremely expensive experimental facilities, such as large-scale light-emitting facilities, accelerator facilities, large-scale electron microscopes, and large-scale optical and electromagnetic telescopes. These high price research and experimental facilities can now be remotely controlled, and measurement results can be obtained remotely using IT. Similar problems exist for large-scale databases, such as genomic and materials databases.

The objective of ITBL is to provide comprehensive systems that efficiently and effectively operate these valuable supercomputers, research and experimental facilities, and databases, enabling joint research by facilitating Internet access by researchers located in remote locations and belonging to different institutions.

Objectives

ITBL will enable researchers to use computer simulations as the means that conduct R&D in place of theory and experiment, and then improve R&D efficiency over a broad scope. In addition, ITBL will develop and provide systems facilitating joint research using large-scale databases and large-scale research and experimental facilities.

Specific measures include the following:

- (1) ITBL will provide an environment to use supercomputers and software, and also provide usage know-how, to corporations and research institutions that have not had access to supercomputers until now. ITBL will therefore help these organizations reduce dramatically cost and time required for product development and R&D.
- (2) ITBL will enable large-scale computations not possible before and will enable load sharing during congestion by connecting and sharing supercomputers located at different research institutions and universities. ITBL will also create an environment where different centers can use each other's unique

software, databases and hardware so that all resources can be operated and utilized efficiently, through which the centers can improve their capabilities.

- (3) ITBL will provide information (testing, development, and provision if necessary) on software and interfaces to enable networked use of large-scale research and experimental facilities belonging to different research institutions.
- (4) ITBL will develop and provide, over the Web, an environment needed by remotely located researchers for joint development (e.g., an environment enabling discussions, information presentations, and idea sharing by specific groups free of time and space constraints).

ITBL Project Targets

According to the e-Japan focus plan, ITBL is to be built for sharing the supercomputers of all research institutions in Japan by 2005. In order to achieve this, the following targets have been established:

- (1) Development and demonstration of technology that allows safe and simple sharing over a network of the computer resources of research institutions in Japan.
- (2) Preparation and sharing, over a high-speed network, of the computer resources of research institutions in Japan.
- (3) Making the technology and resources described above available to a wide range of researchers in Japan, so as to enable innovations in R&D technology in various leading-edge science and technology fields.

Specific means for achieving objectives

(1) Software and portal site preparations

- Preparation of existing software and databases and creation of libraries (including usage manuals, sample data, results, etc.)

- Assistance in new software development
- Consulting and assistance for users
- Development and operation of ITBL portal site serving as an access portal to ITBL.

This Website will not simply give information on ITBL; it will also serve as a portal for accessing ITBL applications and accessing ITBL shared computer resources. At the same time, this ITBL portal site will provide researchers with an environment enabling discussions, information presentations and idea sharing by specific groups free of time and space constraints. Also, a portal site will be realized that provides a wide range of information on computer simulations (e.g., High Performance Computing (HPC), Computer Aided Engineering (CAE)) and enables access to information at related academic societies, universities, research institutions, and corporations. Thus the portal site will be a central hub for accessing relevant information.

- Enabling remote control, monitoring, and data collection for experimental facilities over the Web (also doing new development work if required).

(2) Network preparations

ITBL will connect the supercomputers at various computing centers over a high-speed network to enable efficient operation, utilizing resource and so on.

- Enabling extremely large-scale computations that have not been possible until now.
- Enabling load sharing during (times of) congestion.
- Creation of an environment allowing different centers to use each other's unique software, databases, and hardware.

(3) Preparation of supercomputers to be jointly used

Since many computer centers have almost no extra capacity to accommodate the jobs of anyone besides current users, supercomputers that are to be jointly used by ITBL will be installed in 2001 at the Kansai

Research Establishment of JAERI

ITBL Member Institutions and Development Work Assignments

The ITBL project was started in April 2001. Six institutions have participated in the ITBL project since the first year:

- Japan Atomic Energy Research Institute (JAERI): Base soft./Application
- RIKEN: Base soft./Application
- National Institute for Materials Science (NIMS): Application
- National Aerospace Laboratory of Japan (NAL): Application
- National Research Institute for Earth Science and Disaster Prevention (NIED): Application
- Japan Science and Technology Corporation (JST): Application

Among these institutions, JAERI and RIKEN are handling the development of the common basic technology required for implementing the ITBL plan. Each of the six research institutions is handling different aspects of the development of application software that can be used through ITBL.

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

3.1.2 Research and Development of Parallel Basic Software System

The alpha prototype of the ITBL Infrastructure Software was released at the end of the last fiscal year. As soon as it was released, we began supporting the operation and maintenance of the latest version of software. We also carried out promotion activities to join various researchers and research groups on the ITBL network and supported them in various ways. The ITBL network has grown to 21 high-end computers from 12 organizations including 9 supercomputers, totaling to 7 TFLOPS of computing power and 6 Tera-byte memory capacities (Fig. 3.1-1). The ITBL has gathered over 500 registered users from 30 organizations to this date.

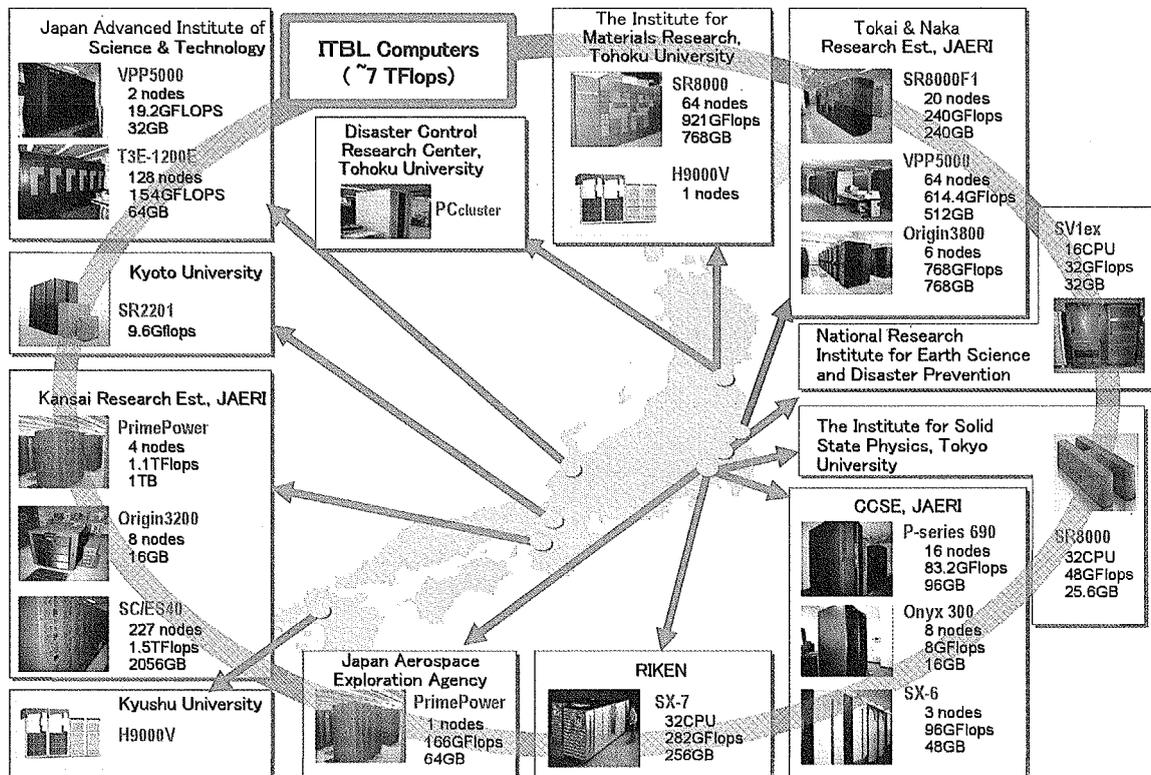


Fig. 3.1-1 Computational resources in ITBL

3.1.2.1 Research and Development of Parallel Processing Technology

3.1.2.1.1 Parallel Distributed Processing Technology for Application Software

During the 2003 fiscal year, in order to realize the heterogeneous computing environment with a Score PC cluster and other machines, Stampi (Seamless Thinking Aid Message Passing Interface) has been implemented on a Score cluster system to enable dynamic process creation defined in MPI-2 and MPI communication among multiple clusters [3.1-1]. In current implementation, Stampi uses a high performance vendor supplied communication mechanism and TCP/IP socket connections in intra-machine and inter-machine MPI communications, respectively. For the intra-machine MPI communication, the performance results via Gigabit Ethernet in Score-supplied and Stampi-supplied methods were 104.3 MB/s and 103.7 MB/s for 1 MByte message data, respectively. There was not significant performance degradation of intra-machine MPI communication in the Stampi-supplied method compared with that in the Score-supplied method. We also measured performance of inter-machine MPI communication in the dynamic and static mode and raw TCP socket connection, respectively. The results were almost the same as shown in Table 3.1-1, where “np” indicates the number of processors. Through performance measurement, effectiveness of Stampi flexible implementation has been confirmed.

Table 3.1-1 Inter-machine communication performance result (MB/s)

		np(Score)	np(Linux)	Latency	Message data size (Byte)				
					64K	1M	8M	64M	256M
Stampi	Dynamic	1	1	57.0 μ s	19.5	33.9	34.6	34.9	35.0
	Static	1	1	106.5 μ s	18.9	33.7	35.0	35.3	35.4
Raw TCP		1	1	61 μ s	30.1	37.2	37.3	36.9	36.8

3.1.2.1.2 High Performance Computing Technology in Nuclear Engineering

A tuning method for eigensolver of dense real symmetric matrices that are frequently used in the nuclear applications have been investigated [3.1-2]. The performance of various unrolled loops both in a rank-update operation and a matrix-vector multiplication have been examined, focusing on performance stability in vector/parallel processing. Particularly, Byte/Flop, which is defined as required data amounts per floating instruction, was used as a performance indicator in searching the best unrolling depth on a Hitachi SR8000F1 and on a Fujitsu VPP5000. In this implementation, the performance degradation caused by the cache architecture was removed, and local instability for performance was avoided. In other words, unrolling depth was determined under restraint condition that number of registers required for processing of an unrolled loop should be smaller than the number of registers of platform computer. We confirmed that the tuned routines for the Householder transform on a single processor of a SR8000F1 and a VPP5000 achieve 72.0% and 86.8% of their theoretical peak performance respectively.

3.1.2.2 ITBL Infrastructure Software

In the ITBL environment, it is required to handle the distributed resources and to support the design of distributed application on the supercomputer cluster. To meet these requirements, the ITBL infrastructure software has been developed such as security infrastructure, TME (Task Mapping Editor), Stampi (Seamless Thinking Aid Message Passing Interface), and so on. Security infrastructure is used to support community access. TME and Stampi are used for supporting component programming.

3.1.2.2.1 Security infrastructure

For construction of a grid system such as ITBL, it is crucial to realize securely access to the computational resources such as supercomputers of each organization and to realize single sign-on to supercomputers resulting in organic linkage of computational resources. We have designed ITBL security infrastructure so that computational resources are protected by a firewall installed for each local area network [3.1-3]. Only https was employed as communication protocol between sites in terms of a commonly used one because it is required that the system commonly works under the various kinds of security policy.

As for certification, ITBL employs a public key-based security mechanism with X.509 certification, where all kinds of information are encoded by secret key and decoded by public key in the ITBL system. This mechanism is implemented on ITBL server, which is established at each site. The server consists of three workstations (ITBL front server, ITBL relay server, ITBL data server) where security data and communication facilities are distributed on. Security is enhanced by separating physically data files and accessing those servers.

3.1.2.2.2 Task Mapping Editor (TME)

On the grid environment, geographically scattered resources, machines, databases and experiments should be linked organically and uniformly with higher abstraction. TME, the task mapping editor, has been developed for handling distributed resources, supporting the design of distributed application on the grid

environment ITBL and controlling job executions.

TME was intended to facilitate a framework in distributed computing focused on a local area network and to support a user-friendly graphical interface [3.1-4]. TME has been restructured by using security and communication infrastructures equipped on the ITBL. Due to the revisions made to run on the ITBL, it is now possible to couple the computer resources located apart in various institutes with the help of the authentication mechanism introduced in the ITBL system. Such a feasible extension to its usability makes TME a prominent Grid software or toolset. It has a function that allows users to register programs and data sets on remote machines as modules and to define relations among modules with graphical user interface (GUI). This enables the incorporation of multiple programs or data sets and executes them collectively as a batch processing. It also has a function to find a less busy computer automatically and to allocate a job to the computer. TME is designed to support visual programming with main feature of description by dataflow. TME facilitates a common frame or collaborative space between the developer and application users. On the TME window, a user can design a work flow diagram, just like a drawing tool, of the distributed applications. All resources are represented by icons on the TME naming space. All data-dependence is defined by a directed arrow linking icons. TME provides users with a higher level of schematic viewing for distributed application on the Grid-like environment as well as on the ITBL system.

In the fiscal year 2003, we have introduced a new control flow mechanism in the latest version of TME for the expert developers. This extension provides the structure of conditional branch and loop, and enables the development of more advanced applications. It can contribute to the development of an advanced PSE (Problem Solving Environment) on a distributed environment, which is one of the ultimate goals of Grid computing. The automatic submission and monitoring improved the efficiency of the jobs. Furthermore, the TME is equipped with an important mechanism allowing integration and sharing of user defined applets among the users who belong to a specific community. The current status of the TME is as follows: TME GUI is implemented as Java applets, and has been made available on a web browser such as Netscape Navigator 6 or later and Microsoft Internet Explorer 5.0 or later, on which JRE 1.3 or 1.4 has been plugged

in; TME main adapter and control layer programs have been ported to ten kinds of parallel computers, several kinds of WS serves, and WS/PC clusters.

3.1.2.2.3 Operation, Verification and Evaluation of ITBL Infrastructure

Various researchers and research groups are now operating the ITBL infrastructure software. Here we report several scientific applications that were successfully used on the ITBL in the fiscal year 2003.

(1) ITBL infrastructure software is applied for a numerical environment system in order to co-operate the different codes installed in the system, such as atmospheric code and air pollution code and execute them collectively [3.1-5]. A function of cooperating an atmospheric code and an air pollution code and that of cooperating an oceanic code and an oceanic pollution code have been implemented on ITBL.

The execution of the atmospheric code enables users to derive atmospheric information, such as wind velocity and temperature. The air pollution code 'GEARN-NEW' outputs information on dispersion of pollutants with acquisition of the results of the atmospheric code. The oceanic code 'POM' enables users to derive oceanic information. The oceanic pollution code 'SEA-GEARN' outputs information on dispersion of pollutants with acquisition of the results of oceanic code.

(2) The other application example is an atomistic simulation on ITBL, which demonstrates the usefulness of the container module [3.1-6]. A molecular-dynamics (MD) simulation is one way to study defect cluster formation and its interaction with dislocations in irradiated metals. The simulation is divided into a series of chunks for solving the problem of a longer CPU-time requirement. A pseudo-iteration structure of chunks is defined on the TME console, where a series of input and output files are set input and output containers, respectively. The user may simplify the whole process. Parallel computation of each MD simulation is executed by a portable parallel program called Parallel Molecular Dynamics Stencil (PMDS). The TME scheduler dynamically assigns these calculations to the free or less busy computer, realizing a high throughput computing. Consequently the users' mental work load is significantly mitigated by using TME

scheduling to control workflow. Fig. 3.1-2 shows illustration of the simulation. The integration of the applications and databases may further reduce the burden of carrying out analysis.

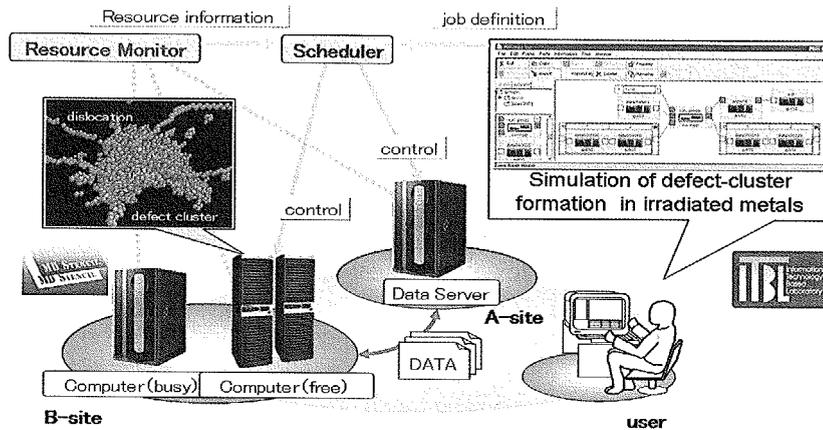


Fig. 3.1-2 Illustration of the atomistic simulation

(3) The last example of scientific applications on ITBL is a superconducting simulation [3.1-7]. Superconducting-device functions in complex configurations have been effectively studied on ITBL by sharing a visualized simulation results from geographically separated sites in real time. Coupled simulation has been also executed on the ITBL environment. In the simulation, a superconducting-device is divided into two regions, of which physical attributes are exchanged at every time step. In the production run, physical phenomena are simulated changing the mesh size of two regions independently. As for the vacuum region, Maxwell's equation is solved by linear partial differential equations. Though calculation is not suitable to vector processing, computational cost is low compared with the rest. As for super-conducting region, the Klein-Gordon equation is solved by a non-linear partial differential equation. Calculation is suitable to vector processing because the trigonometric functions are frequently used in the simulation. The computational cost is also high compared with the rest. In order to reduce the simulation time and to effectively use the computational resources, coupled simulation by vector and scalar processor should be employed.

3.1.3 Research and Development of Parallel Processing Tools

3.1.3.1 Scientific Application Tools: Integrated Simulation Technology

In order for the numerical simulation to reflect “real-world” phenomena, incorporation of multidisciplinary and multi-physics simulations considering various physical model and factors are becoming essential. The coupled simulation, tight or loose coupling, is recognized as one of the most important and effective strategy for studying multidisciplinary phenomena. Although loose coupled simulation system has significant advantages over strongly-coupled systems to analyze various physical phenomena, problems arise in the communication when trying to apply two independent parallel commercial codes initiated statically. We have been developing an “integrated numerical simulation system” to solve the communication error problem at the time of a dynamic process creation under meta-computing environments (Fig. 3.1-3) [3.1-8]. The aims of this study is to construct a competent coupler for carrying out multi-disciplinary simulations by allowing concurrent execution of arbitrary simulation codes on different computers in parallel. Two libraries make up the core of this system: Stampi and MpCCI (Mesh-based parallel Code Coupling Interface). The Stampi is a communications library based upon the MPI-2 specifications for the heterogeneous computing environment. MpCCI developed by the Fraunhofer SCAI (Institute for Algorithms and Scientific Computing) plays a role of the coupler to exchange and to interpolate the physical values between the simulation codes. As long as user subroutines may be added, even the commercial codes can be implemented to construct the integrated simulation systems.

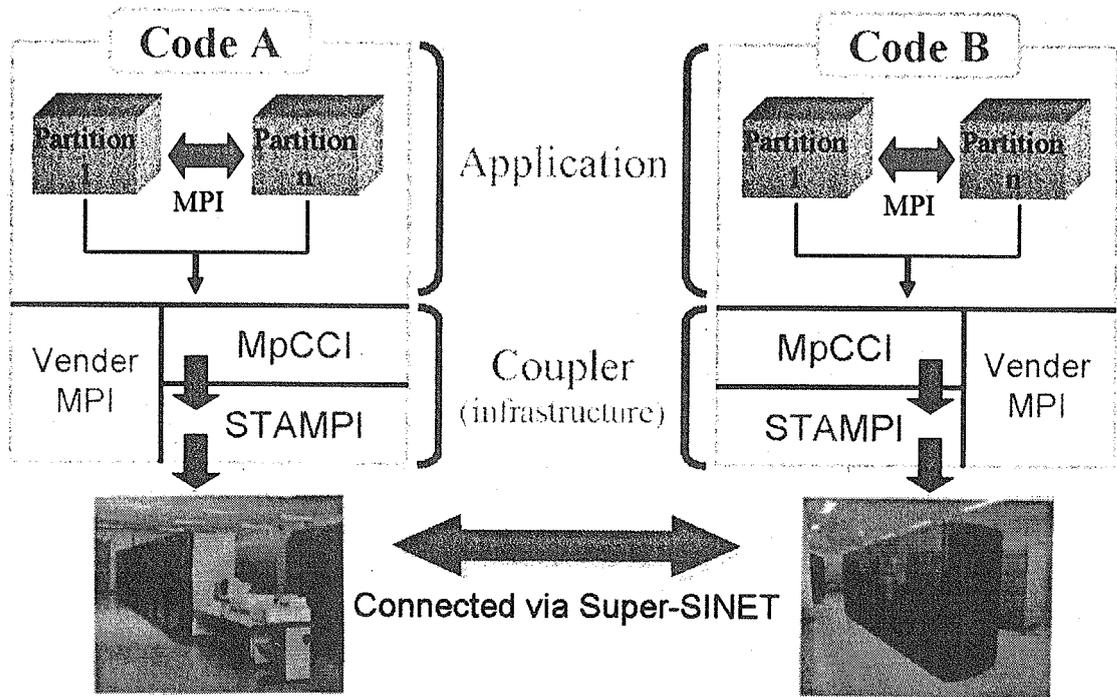


Fig. 3.1-3 Illustration of an integrated numerical simulation system for meta-computing

Fluid-structure coupled simulations for solving interactive problems have been implemented on a heterogeneous parallel computers environment using the proposed system [3.1-9]. During the 2003 fiscal year, we have applied the “integrated numerical simulation system” to the biomechanics field. In order to investigate the deformation behavior of the human artery resulting from transient blood flow, we have constructed an integrated simulation system by coupling STAR-CD and MECANO, both commercial software packages, on the ITBL [3.1-10]. It simulated the interaction between blood flow and a diseased blood vessel using an integrated simulation technique based on LC (Loose coupling) approach with Stampi and MpCCI.

3.1.3.2 Adaptive Visualization Technique in ITBL

The ITBL infrastructure possesses a powerful functionality to effectively connect any supercomputer (host) located in remote locations. In order for the visualization function to be useful in such an environment, efficient remote visualization functions become essential. In addition, since the ITBL enables users to communicate through a community function, a collaborative visualization, which refers to researchers in remote locations simultaneously accessing and monitoring the same visualized image, is an indispensable function. To meet this requirement, visualization tools, PATRAS/ITBL and AVS/ITBL, have been developed and applied to visualization and analysis of large-scale numerical simulation data. The PATRAS (PARallel TRACKing Steering) is a visualization tool developed by CCSE and NEC; AVS/Express is a commercial visualization tool.

3.1.3.2.1 PATRAS/ITBL

The PATRAS/ITBL visualization system aims at displaying the progress of the simulation in real time and collaborative visualization among sites [3.1-5, 11, 12]. The client/server system is adopted in the development of PATRAS/ITBL [3.1-5, 11]. The PATRAS serve-client remote visualization system carries out the visualization process on each processor on a supercomputer (server) and displays images on a user terminal (client). A client operates on the Web browser on a user terminal as a Java applet. A server consists of libraries and operates on a supercomputer. The servlet that operates on the ITBL server mediates the communication between the user terminal and the supercomputer. By this way, the user can track and steer simulation parameters and control the simulation procedure. Stampi libraries are used to gather the image data; the libraries execute visualization simultaneously on various remote hosts. Also, the PATRAS/ITBL is intended for carrying out message passing (communications) among heterogeneous parallel computer cluster (Fig. 3.1-5).

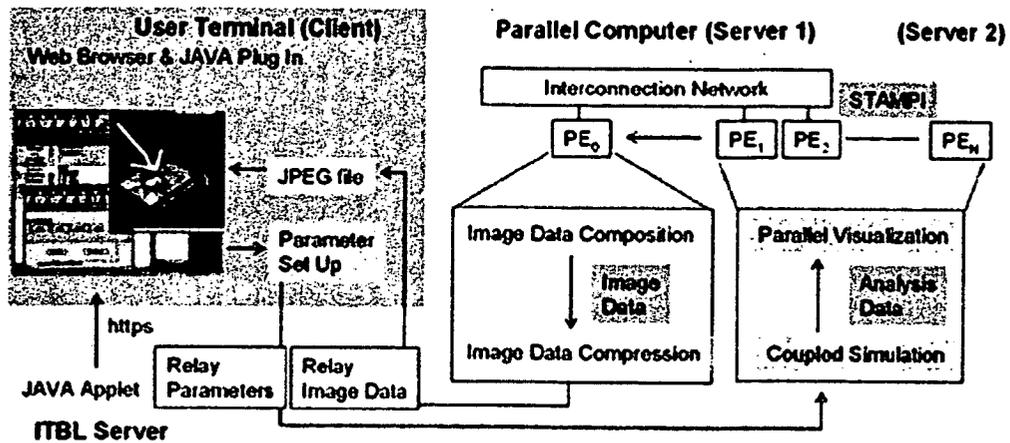


Fig. 3.1-5 PATRAS/ITBL - Configuration for visualization of coupled simulation results

A function for collaborative visualization has been developed in PATRAS/ITBL based on the original PATRAS software by storing image data in the common data area on the ITBL server (Fig. 3.1-6). By using this function, real-time visualization of data from numerical simulations is realized on supercomputers on the ITBL environment. Performance has been enhanced in several processes: image composition process, JPEG compression process, and smoothing process when generating iso-surface have been parallelized. In the fiscal year 2003, a new function has been added which enables TME (Task Mapping Editor) to control both the simulation and the PATRAS/ITBL visualization.

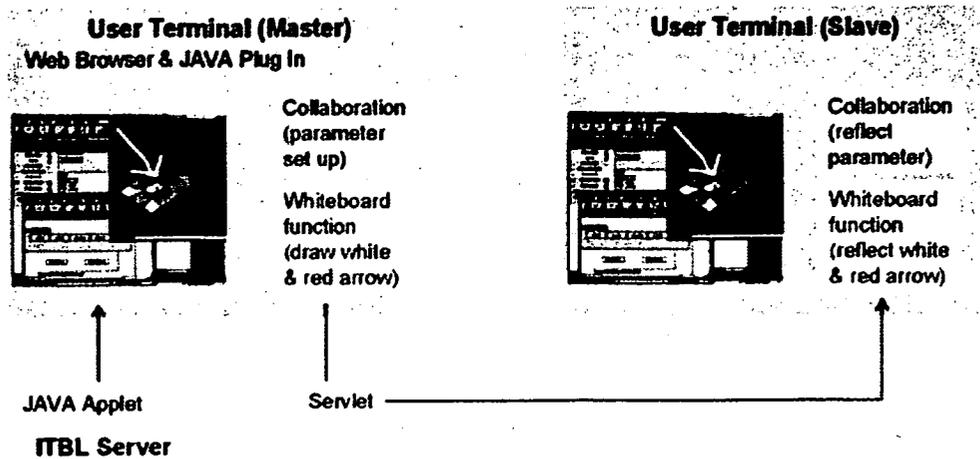


Fig. 3.1-6 PATRAS/ITBL - Configuration for collaborative visualization

3.1.3.2.2 AVS/ITBL

AVS/ITBL enables remote post-processing visualization of any data stored on any supercomputer located in the ITBL network through Web browsers. A collaborative visualization function has been developed in the AVS/ITBL. AVS/ITBL operates both on a graphics server (client visualization function) and on a user terminal (Web visualization function).

In AVS/ITBL, a function has been developed which enables to read data located on any ITBL host over a firewall. This function is realized by introducing a data-input remote module. The data files are temporarily copied from a remote computer to a local graphics server using STARPC (Seamless Thinking Aid Remote Procedure Call) API (Application Programming Interface). It is a remote-procedure-call based communication library for parallel computer clusters. It is used as a communication tool of the ITBL system infrastructure software. The module, together with the Tool Management process on the selected host (STARPC), acquires the file list. If a file is selected from the list, then it is transferred to the graphics server (STARPC) where it is read by the AVS/Express software. Finally, an image is displayed onto a graphics server terminal (Fig. 3.1-7).

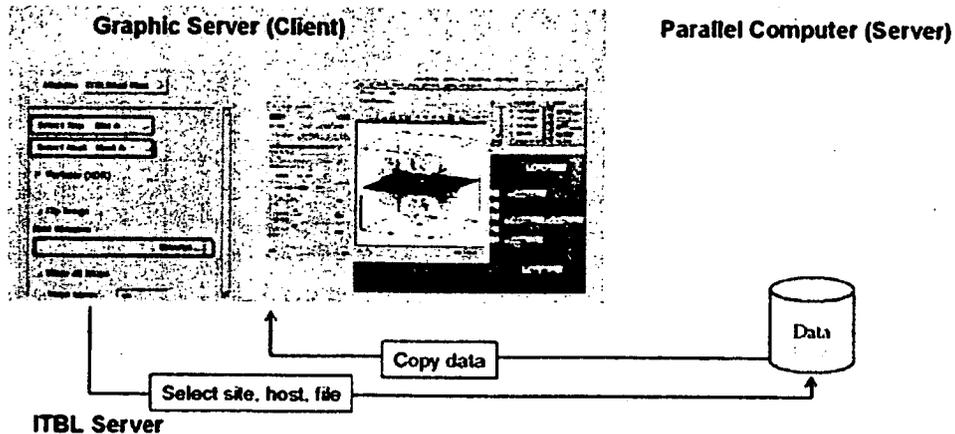


Fig. 3.1-7 AVS/ITBL - Configuration for client visualization

Another function has been also developed which can display the visualized image on a Web browser as well as controlling visualization parameters from a web browser. If the network file and the data file of AVS/Express have already been created by a user, it is possible for other joint users to execute the visualization easily even if they are not well-versed in the usage of AVS/Express. Users can display images with `showImage` or `showPolygon` functions supplied by AVS/ITBL (Fig.3.1-8). When "showImage" is selected, an image is displayed in 2D GIF images and when "showPolygo" is selected, it is displayed 3D GFA data (GFA is a file format for 3D data of AVS/Express). Users can operate those images such as rotation, scaling, and transportation of the objects interactively and change parameters for visualization. Users need to make network files including CGI relay module and image data generation module before visualization on the web. The CGI relay module is used for describing connections between parameters of AVS/Express and those appeared on the web. The AVS relay process was developed to enable data transportation between a graphic server and an ITBL server installed at users' site. Batch visualization function has been also developed. It enables TME job flow to invoke AVS/ITBL and enables performing a simulation and visualization collectively.

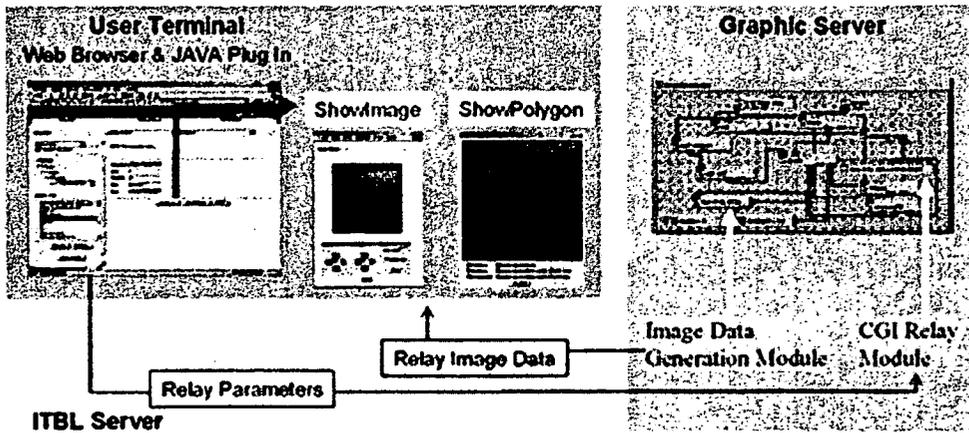


Fig. 3.1-8 AVS/ITBL - Configuration for web visualization

In the fiscal year 2003 developments were made to realize collaborative visualization and visualization of 3D animated graphics data using the AVS/ITBL. The collaborative visualization function is achieved by communication between visualization processes of AVS/ITBL, so that every user can monitor and control his/her image window. For example, viewpoints and parameters may be set independent of others in the group. The same image is shown only when the function is instructed to do so. As for the 3D animation, viewpoints may be changed while the animation is shown [3.1-13, 14].

Reference

- [3.1-1] Y. Tsujita, T. Imamura, N. Yamagishi, and H. Takemiya, "MPI-2 support in heterogeneous computing environment using a score cluster system.", Proc. of 2003 international symposium on parallel and distributed processing and applications.
- [3.1-2] T. Imamura, and K. Naono, "An evaluation towards an automatic tuning eigensolver with performance stability.", Proc. of 2003 international symposium on SACSIS.
- [3.1-3] K. Higuchi, T. Otani, Y. Hasegawa, Y. Suzuki, N. Yamagishi, K. Kimura, H. Maesako, M. Fukuda, and G. Yagawa, "Application of ITBL basic software for virtual organizations.", Proc. of the Conf. on Computational Engineering and Science, The Japan Society for Computational Engineering and Science, 8, 2, pp.797-800, (2003) [in Japanese].
- [3.1-4] T. Imamura, Y. Hasegawa, N. Yamagishi, and H. Takemiya, "Implementation of a resource handling environment for distributed applications on ITBL.", Proc. of the Conf. on Computational Engineering and Science, The Japan Society for Computational Engineering and Science, 8, 2, pp.793-796, (2003) [in Japanese].
- [3.1-5] Y. Suzuki and K. Sai, "Research and development of parallelized visualization system on Earth Simulator and grid-suited visualization system on ITBL.", All NEC C&C Systems Users Association Heisei year 15 collection of papers, pp.211-229, (2003) [in Japanese].
- [3.1-6] F. Shimizu, T. Kadoyoshi, H. Kaburaki, N. Yamagishi, Y. Hasegawa, and K. Higuchi, "Parallel molecular-dynamics simulation on ITBL.", Proc. of the Conf. on Computational Engineering and Science, The Japan Society for Computational Engineering and Science, 8, 2, pp.801-804, (2003) [in Japanese].
- [3.1-7] K. Higuchi, et al., "Grid computing supporting system on ITBL project.", Proc. Of ISHPC 2003, pp 245-257 (2003).
- [3.1-8] O. Hazama and Z. Guo, "Practical integrated simulation systems for coupled numerical simulations in parallel.", Proc. of the Int. Conf. on Supercomputing in Nuclear Applications (SNA2003), (2003).

CDROM

- [3.1-9] O. Hazama and Z. Guo, "Development of an integrated numerical simulation infrastructure for fluid-structure coupled problems.", Proc. of the Conf. on Computational Engineering and Science, The Japan Society for Computational Engineering and Science, 8, 2, pp.759-760, (2003) [in Japanese].
- [3.1-10] O. Hazama, Z. Guo, M. Yamagiwa, T. Hirayama, and T. Matsuzawa, "Proposal and implementation of a fluid-structure coupled simulation system with parallel commercial codes.", Proc. of the Int. Conf. on Computational & Experimental Engineering and Sciences (ICCES), (2003) [CDROM].
- [3.1-11] K. Sai, Y. Suzuki, F. Araki, H. Uehara, and H. Haginoya, "Utilization of PATRAS visualization software for large-scale data on Earth Simulator.", Proc. of the Conf. on Computational Engineering and Science, The Japan Society for Computational Engineering and Science, 8, 2, pp.761-764, (2003) [in Japanese].
- [3.1-12] Y. Suzuki, N. Matsumoto, and K. Sai, "Collaborative visualization for supporting joint researches in ITBL project.", Proc. of the Int. Conf. on Creating, Connecting and Collaborating through Computing, IEEE CS Press, pp. 187, (2004).
- [3.1-13] Y. Suzuki, and N. Matsumoto, "Development of remote visualization and collaborative visualization system in ITBL grid environment.", High Performance Computing, Veidenbaum et al. (Eds.) (ISHPC2003), LNCS2858, Springer-Verlag, pp.269-277, (2003).
- [3.1-14] Y. Suzuki, N. Matsumoto, N. Yamagishi, K. Higuchi, T. Otani, H. Nagai, H. Terada, A. Furuno, M. Chino, and T. Kobayashi, "Development of multiple job execution and visualization system on ITBL system infrastructure software and its utilization for parametric studies in environmental modeling.", Computational Science - ICCS 2003, Sloot et al. (Eds.), LNCS2659, Springer-Verlag, pp.120-129, (2003).

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3.2 Computational Material Science

Our group research two fields in material science: macroscopic quantum phenomena and fracture phenomena. The macroscopic quantum phenomena emerge under special situations such as superconductivity and Bose-Einstein condensation. Those phenomena are sensitive to external perturbations, and hence lead us to study device applications in atomic energy research. In addition, those phenomena are rich with fundamental quantum dynamics with intrinsic scientific importance. A model equation has been proposed that describes the dynamics of the superconducting phase in high-T_c superconductors. We have numerically studied their I-V characteristics, voltage responses under the current-biased situation, and clarified that the branching of the I-V characteristics, commonly seen in high-T_c superconductors, is originated from excitation of the localized rotating mode, which has been intensively investigated in nonlinear physics. In this year we succeeded in reproducing the rich variety of I-V characteristics in the high-T_c superconductors by varying the coupling strength in the model. This means that the physics of the I-V characteristics in high-T_c superconductors can be understood with the help of the concepts developed in nonlinear physics.

An ultra-cold atom gas under an optical lattice is known to exhibit macroscopic quantum phenomena: the Bose-Einstein condensate when the gas is bosonic, the superfluid state when it is fermionic. Here, the optical lattice is created by the interference effect of two laser beams. In order to study the Bose-Einstein condensate, we developed a simulation code and reproduced 3-dimensional dynamics of the rotating Bose-Einstein condensate. Whether the superfluidity appears or not in a strongly correlated fermion system is determined by the eigenstates of a huge matrix, called the Hubbard Hamiltonian matrix. We developed a parallelized code that diagonalizes the matrix by the Lanczos method on the Earth Simulator. The excellent performance of the code makes it possible to analyze theoretically the large strongly-correlated fermion systems that cannot be explored previously.

The research on fracture phenomena aims at deriving macroscopic properties of nuclear materials by computer simulations using atomistic and mesoscopic modeling methods. The final target of these simulations is to understand the mechanism of the fracture process in nuclear materials under irradiation and corrosive conditions, such as stress corrosion cracking phenomena of nuclear power plant components. In particular, we focus on understanding intergranular fractures of polycrystals using multi-scale approach. In the atomistic region, molecular dynamics (MD) method is employed to study the intergranular embrittlement due to hydrogen impurities and the emission of

dislocations from the crack-tip for the intergranular cracking. Also, a mesoscopic modeling method is devised to study the intergranular crack patterns, which are observed in nuclear power plants. Moreover, the behavior of the defects induced by irradiation is simulated by the MD method to assess the effects of irradiation on the strength of nuclear materials.

3.2.1 Macroscopic Quantum Dynamics in Superconductivity and Quantum Gas

3.2.1.1 Observation of Localized Excitation and I-V Characteristics in High-Tc Superconductors

Layered High-Tc superconductors are naturally-stacked Josephson junctions (intrinsic Josephson junctions). The superconducting layer in the intrinsic Josephson junction is so extremely thin that the charge neutrality breaks down inside the layers. A model equation for the phase dynamics in the junctions has been proposed including this feature. We revealed in 1998 that the model equation describes two types of dynamics: the plane-wave like propagating mode called the longitudinal Josephson plasma and the localized rotating-mode peculiar to the discrete nonlinear systems. Both modes have been detected in high-Tc superconductors; the longitudinal Josephson plasma has been observed in the microwave absorption experiments; the localized rotating-mode has been identified to be the origin of the multiple-branch structure in the I-V characteristics. These results allow us to interpret the intrinsic Josephson junctions as the reality of the discrete nonlinear system that currently gets attention in nonlinear physics. In this year we investigated in more details the dynamics of the nonlinear localized modes and demonstrated that this dynamics can systematically explain the rich variety of c-axis I-V characteristics observed in various high-Tc superconductors [3.4-1]. These indicate that high-Tc superconductors are quite unique systems where the dynamics of the nonlinear localized mode play an essential role rather than that of the linear plasma mode.

3.2.1.2 Exact Diagonalization for Trapped Fermi Atom Gas Loaded on an Optical Lattice

We numerically studied the fermionic atom gas under an optical lattice created by two laser beams. We adopted the Hubbard model with the trap potential, and investigated a broad range of interaction from attractive to repulsive since the broad range can be experimentally covered by the use of Feshbach resonance. The Hamiltonian matrix of

the Hubbard model is mathematically described as

$$H_{Hubbard} = I \otimes A + A \otimes I + D \quad (1)$$

where I , A and D are the identity matrix, a sparse matrix due to the hopping between neighboring sites and a diagonal matrix originated from the presence of the one-site repulsion, respectively. In order to numerically diagonalize the Hubbard Hamiltonian matrix (1), the Lanczos method has been previously used. However, the number of Fermi particles that we can compute is severely limited since the Hamiltonian matrix size almost exponentially grows with increasing the particles. We developed therefore parallelization techniques [3.2-2] to diagonalize Hamiltonian matrices on the Earth Simulator which make it possible to examine a system that was too large to be explored. According to the memory architecture of Earth Simulator, we devised two techniques for parallelization: one is for the distributed memory and uses the message passing; the other is for shared memory and uses the multitasking. Especially in the multitasking, we developed a parallel strategy in order to overcome low floating-operation efficiency caused by massive communications due to large-scale matrix operations. The strategy is that a CPU inside a node unit is assigned only for the communication. By utilizing the technique based on the strategy, we achieved 2.7 TFlops (33% peak ratio) by using 128 nodes (1024 processors) and succeeded in obtaining the smallest eigenvalue and its eigenvector of a matrix with about 18-billion dimension [3.2-2]. This technique will be applied to research for the collective quantum phenomena of many body systems. We are now studying the possibility of superfluidity on a system composed of 20 sites and 16 fermions, the maximum one among the previous exact diagonalization studies to our knowledge.

3.2.2 Multiscale simulations on the irradiation induced property changes and fracture of materials

3.2.2.1 First-principles calculations for energetics of segregation and embrittling potency of all non-transition elements in Ni Σ 5(012) symmetrical tilt grain boundary

We performed first-principles calculations to investigate energetics of segregation and embrittling potency energies for almost all non-transition elements from H to Rn when these elements are in Ni Σ 5(012) symmetrical tilt grain boundary[3.4-3]. We used WIEN2k code, which is based on full-potential linearized augmented plane wave method. This method is the most accurate among various methods to calculate the

electronic structure of condensed matters (solid).

Figure 3.2.2-1 shows the calculated surface and grain-boundary segregation energies from H to Ar. The figure indicates that almost all elements have a tendency to segregate to grain-boundary region. In particular, the grain-boundary segregation energies of B, S and P are large, which agree well with experimental facts that these elements have a high potency to segregate to grain boundaries. Figure 3.2.2-2 shows the difference of surface segregation energy and grain-boundary segregation energy. This is called “embrittling potency energy” according to the Rice-Wang model. From this figure, we find that most elements have a positive embrittling potency energy, which means that those elements have a potency of embrittling Ni. There are a few exceptions, however, for light elements like boron and carbon. These trends are in good agreement with experimental facts. Furthermore, rare gas like He, Ne, and Ar has very large embrittling potency energies, which is also consistent with the experimental fact that there is a phenomenon called “fission gas swelling.”

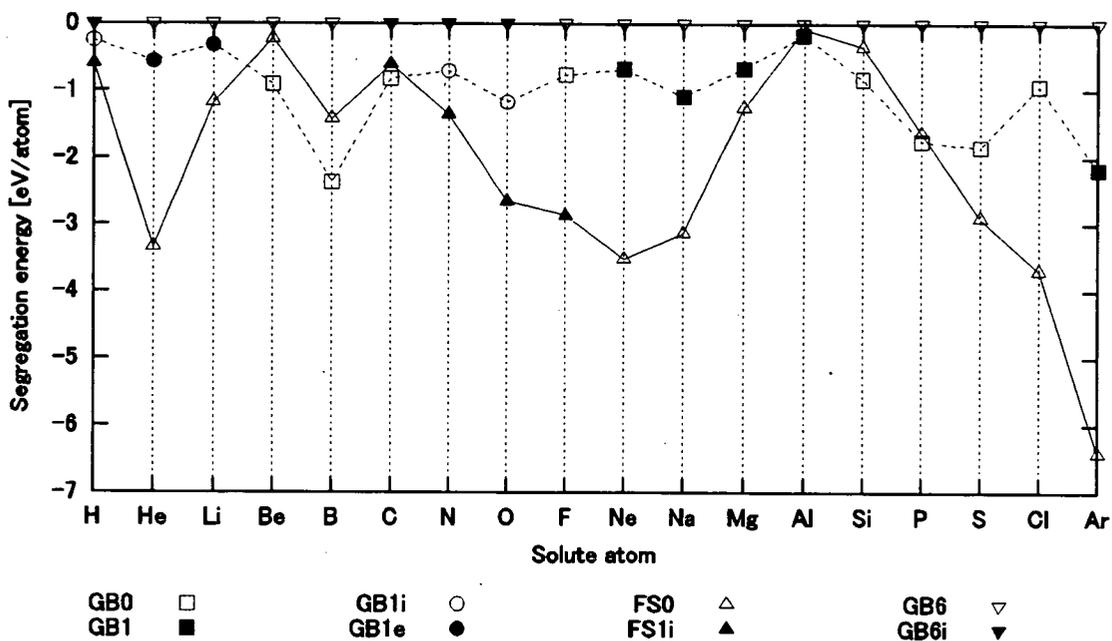


Fig.3.2.2-1 Calculated surface and grain-boundary segregation energies. The symbols indicate segregation sites on surface and in grain-boundary. FS means free surface and GB grain boundary. GB6 indicates inner bulk site, the energy of which is set to zero.

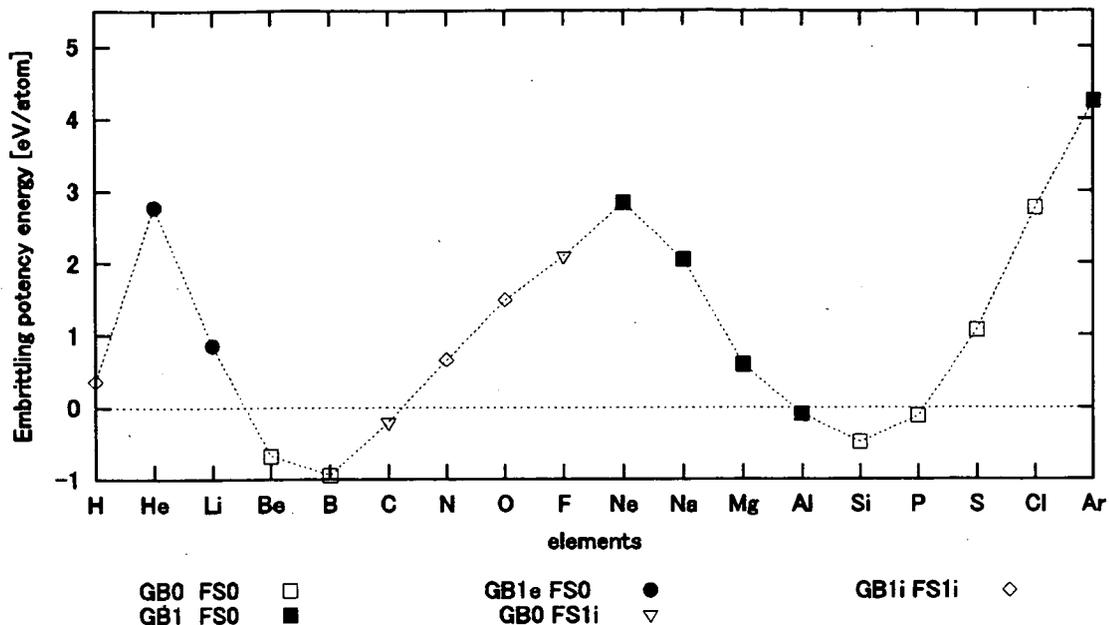


Fig.3.2.2-2 Embrittling potency energies that are the difference of surface and segregation energies as shown in Fig.3.2.2-1.

3.2.2.2 Atomistic simulation study of geometries and energetics of Ni grain boundaries with and without hydrogen impurity

It has long been known that small concentrations of hydrogen impurity can substantially reduce the mechanical strength of transition metals; this phenomenon is called "hydrogen embrittlement." But its microscopic origin has not been well understood. A theoretical model is proposed by Rice and Wang in 1989 based on the thermodynamic framework of intergranular decohesion. This theory describes the competition between the brittle boundary separation and the plastic crack blunting processes in the presence of impurity segregation at the grain boundaries. For the former process, the resistance to brittle fracture is characterized by the thermodynamic work corresponding to the energy difference of the grain boundary (GB) and the free surface (FS). This means that if hydrogen impurities favor energetically at the grain boundaries than at the surfaces, hydrogen segregation to the grain boundaries may lower the energy necessary to cause intergranular fracture.

Useful and currently feasible tools to assess this mechanism are ab initio and atomistic simulation techniques. We employed these techniques with the embedded atom method (EAM) in the framework of the Rice-Wang model, and investigated the hydrogen embrittlement of Ni for a series of symmetrical tilt grain boundaries. We

calculated the binding energy of hydrogen in various sites of both grain boundaries and free surfaces. To confirm the quantitative aspect of the EAM results, we have carefully compared several quantities from the ab initio studies with the existing data from experiments; they are surface energies, multilayer relaxation of FS/GB, the binding energy and binding sites of hydrogen, and so on. Our calculation gave the hydrogen binding energies in the range of 2.7-2.9 eV at the surface sites while 2.1-2.6 eV at the grain boundary sites; both are larger than that at the face-centered-cubic (FCC) crystal interior site, 2.1 eV [3.2-4]. These data therefore imply that, to all the types of GB's we have investigated, hydrogen segregates and causes the embrittlement.

3.2.2.3 Molecular dynamics study on the pinning of an edge dislocation by interstitial clusters in FCC metals

Radiation hardening of metals has been studied experimentally and theoretically since the early days of the development of nuclear reactors. Hardening of irradiated materials mainly occurs as a result of pinning of dislocations by irradiation induced defects, such as interstitial clusters. With the development of transmission electron microscopy, the resolution of a minimum defect comes down to a few nanometers, and detailed microstructures formed by irradiation have been identified. However hardening mechanisms have not been clearly understood. An atomistic method is employed to predict a pinning structure since a short range interaction of atoms near a dislocation core should be taken into consideration.

We use the molecular dynamics method to study the pinning structure formed by the interaction of an edge dislocation with an irradiation induced interstitial cluster in fcc crystals of Cu and Al. The embedded atom method (EAM) potential is employed in the simulation. The size of the simulation cell is $200 \times 170 \times 120 \text{ \AA}$ in the x, y, and z directions, and the number of atoms used is 3.8×10^5 . The x, y, and z directions are [110], $[\bar{1}12]$, and $[1\bar{1}1]$. The boundary conditions are periodic in the x and y directions and mixed free for the z direction. A hexagonal interstitial cluster is inserted under an edge dislocation as an initial condition, and we found that various types of jog structures are formed depending on the size of a hexagonal interstitial cluster. The number of interstitial cluster site ranges from 7 to 721, the maximum width of which corresponds to 5.1 \AA to $2.1 \mu\text{m}$. It is found [3.2-5] that a small cluster with sites of 7 is absorbed into one of the partial dislocations. A medium size cluster of sites of 19 and 37 forms a superjog with a dislocation. Here, one side is constricted and the other side is extended, as shown in Fig.3.2.2-3(a). With increasing the size, a cluster attracts a dislocation

elastically, but the formation of a jog is not observed as shown in Fig.3.2.2-3(b).

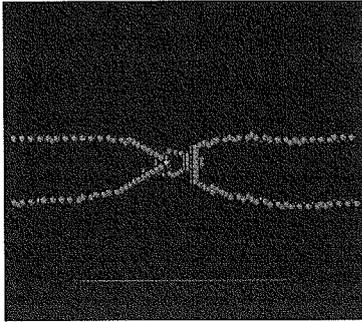
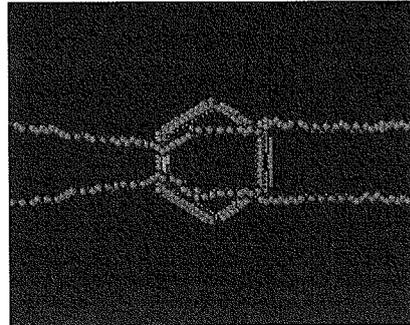


Fig.3.2.2-3(a) A superjog formed due to an interaction of an extended edge dislocation with an interstitial cluster consisting of 37 sites



(b) An extended dislocation trapped by an interstitial cluster consisting of 331 sites

3.2.2.4 Molecular dynamics study on the formation of stacking fault tetrahedra and unfauling of Frank loops in fcc metals

Irradiation of face centered cubic (fcc) metals by neutron or charged particles induces atomic collision cascades, where varieties of defect clusters nucleate from the migration and coalescence of self-interstitial atoms and vacancies. Typical clusters formed by this displacement cascade process are hexagonal dislocation loops called Frank loops containing the stacking fault with the Burgers vector $1/3\langle 111 \rangle$. These defects are well observed by transmission electron microscopy and are considered to cause significant effects of irradiation hardening and fracture due to dislocation channeling. It is predicted that unfauling of Frank loops may lead to the formation of dislocation channeling through the absorption of these unfaulted loops by gliding dislocations. Detailed mechanistic processes of these Frank loops, however, are not well known since there is the resolution limit in electron microscopy in the range less than 1-5 nm and the elasticity theory becomes invalid for that range. We therefore study these processes by the molecular dynamics method (Fig 3.2.2-4).

With increasing the size of the faulted cluster, there is some point that the energy of the faulted dislocation loop becomes larger compared with the unfaulted perfect dislocation loop. This means that the unfaulted dislocation loop is energetically favorable with increasing size. However, many large-sized faulted Frank loops are observed by the transmission electron microscopy, and unfauling condition is not clearly known. There seems to be some energy barrier for this transformation. We determine this

energy barrier by applying the external shear stress and raising the temperature of the system. In particular, we focused on the intrinsic Frank loop of the diagonal length ranging from 4 to 14 nm and proposed the mechanism that lowers the critical unfaulting stress[3.2-5].

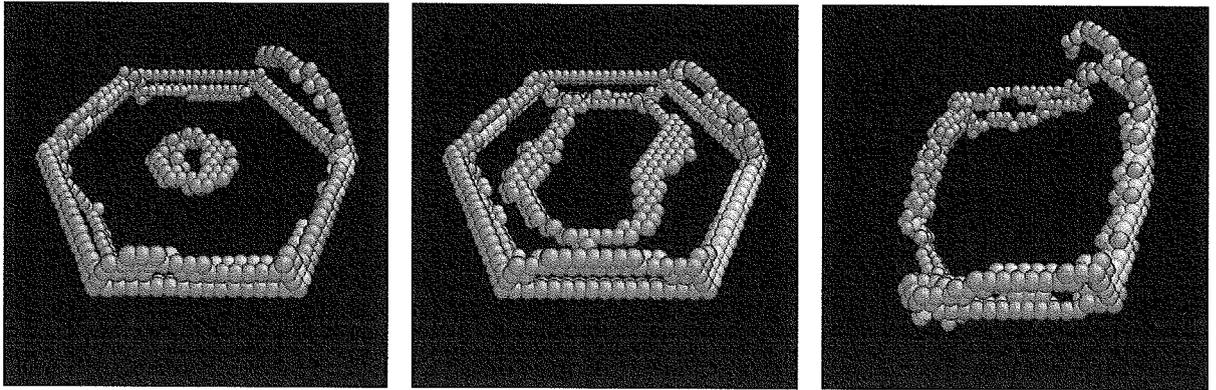


Fig.3.2.2-4 Unfaulting of Frank loop

References

- [3.2-1] M. Machida and T. Koyama, "Localized Rotating-modes in Capacitively-Coupled Intrinsic Josephson Junctions: Systematic Study of Branching Structures and Collective Dynamical Instability," *Phys. Rev. B*, **70**, 024523 (2004).
- [3.2-2] S. Yamada, M. Machida and T. Imamura, "Parallel Computation of Large-Scale Eigenvalue Problems of Strongly Correlated Electrons on the Earth Simulator," *IPSJ Transactions on Advanced Computing Systems*, No. *SIG6(ACS6)*, **45**, 161 (2004), [in Japanese].
- [3.2-3] M. Yamaguchi, M. Shiga and H. Kaburaki, "Energetics of segregation and embrittling potency for non-transition elements in the Ni Σ 5(012) symmetrical tilt grain boundary: a first-principles study," *J. Phys.: Condens. Matter*, **16**, 3933 (2004).
- [3.2-4] M. Shiga, M. Yamaguchi and H. Kaburaki, "Structure and energetics of clean and hydrogenated Ni surfaces and symmetric tilt grain boundaries using embedded-atom method," *Phys. Rev. B*, **63**, 245402 (2003).
- [3.2-5] H. Kaburaki, T. Kadoyoshi, F. Shimizu, H. Kimizuka and S. Jitsukawa, "Molecular dynamics study on the interaction of a dislocation and radiation induced defect clusters in FCC crystals," *Proc. Supercomputing in Nuclear Applications (SNA'2003)*, Paris, France, Sept. (2003).

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3.3 Quantum Bioinformatics Research

The group covers wide range of computational biology, including bioinformatics and macromolecular simulation. Bioinformatics is the field to analyze huge amount of data emerging out of genome sequencing and structural genomics projects. Macromolecular simulation deals with large size biomolecules, such as protein complexes binding to DNA/RNA. It is not common to find a single group working in these two fields of computational biology. The difficulty in forming a group like ours lies in the fact that each member is required to have wide knowledge in some of the following fields: biology, physics, chemistry, mathematics, evolution, statistics, and computation. The research in this group is a basic science and aims to expand knowledge on biology developing new ideas and techniques. The knowledge we will gain will easily be applied to pharmaceutical science for development of new drugs to cure diseases, and to agricultural science. The followings are one of the cross-sections of our research activity.

3.3.1 Development of protein structural information databases and analysis tools

Emergence of whole genome sequences of more than 200 species from different kingdoms of life has laid an enormous impact on our view toward life. In addition, three-dimensional (3D) structures of the representative proteins are being obtained. Those pieces of information must be converted so that they are understandable. There is lots of software available on the Internet to retrieve meaningful information from the genome sequences and proteome structures. However, the variety in methods and data formats precludes us from deep analyses. The obstacles are as follows;

- 1) There exists no overviews for the state-of-the-art software for bioinformatics,
- 2) There are so many software to handle a single data that no one can tell which software should be used to meet the end, and
- 3) There are so many data formats for input and output that conversion between different formats is getting a most time consuming job.

We have initiated, in 2002, developing a system named BAAQ (Bioinformatics: Ask

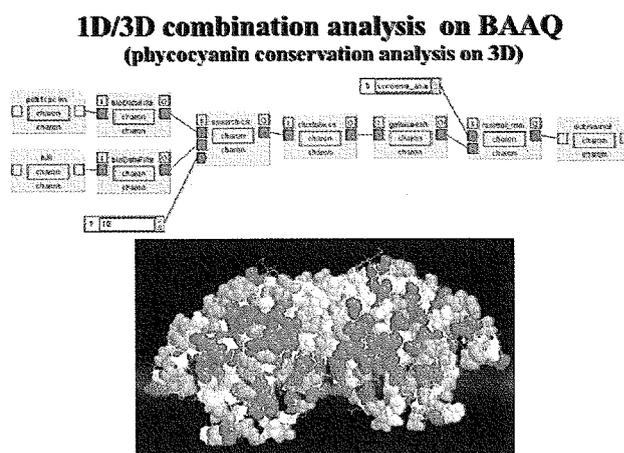


Fig.3.3.1-1: Structural bioinformatics analysis on BAAQ. The conserved residues on the surface of phycoerythrin are colored in red.

Any Questions) that realize easy analyses of these data. BAAQ works on GUI named TME (Task Mapping Editor) developed by CCSE. On TME any data and software are visualized as icons, and data flow as lines connecting icons. In 2003, we have finished standardization of data formats used on BAAQ to XML. With this standardization, the addition of new software into BAAQ has become easy. We are adding software for automatic protein three-dimensional structure superposition, for multiple amino acid sequence alignment and visualization, for protein torsion angle analysis, for secondary structure prediction, for DNA binding motif search, for molecular phylogeny drawing [3.3-1], for protein-protein interaction prediction and so forth. Along with the process of development of those tools, we have developed databases [3.3-2] and have found new proteins out of genome sequences [3.3-3] at the collaboration with other researchers and those results contributed to the progress of genome annotations [3.3-4].

3.3.2 Development of DNA repair protein databases

DNA molecules carry genetic information. If they are damaged by radiation, the organisms repair the damages. Without the DNA repair, DNA sequence would change frequently and genetic information would not be delivered from generation to generation. DNA repair is one of the essential mechanisms for any organisms and is carried out by proteins called DNA repair proteins through a series of chemical reactions. To understand the mechanism of DNA repair, we are integrating information about amino acid sequences, three-dimensional structures and functions of proteins related to DNA repair and developing a new database. Along with this project, we have started analyzing DNA repair mechanism of a specific bacterium named *Deinococcus radiodurans*, which are known to survive under high bombardment of radiation. By irradiation, the DNA strand breaks, and the

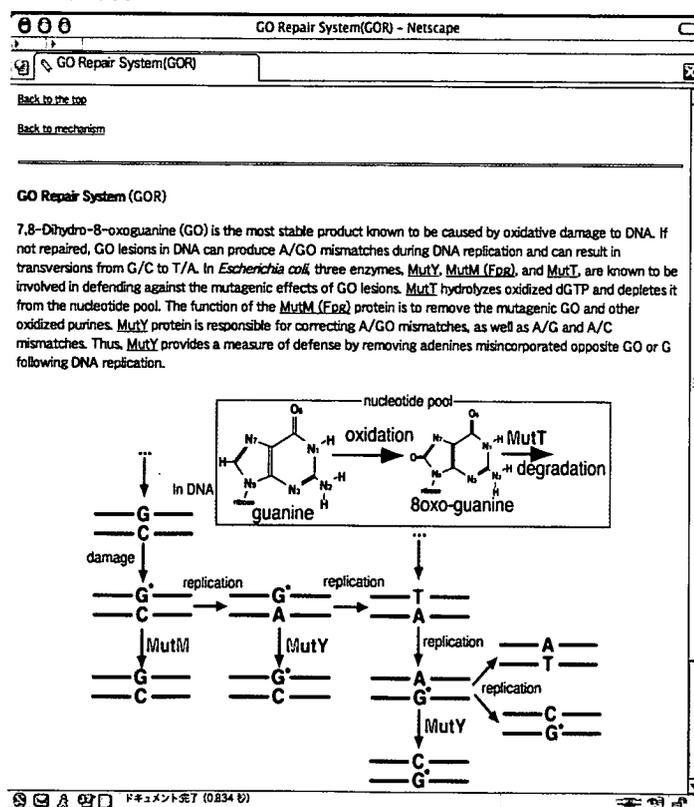


Fig.3.3.2-1: A database of DNA repair related proteins. The explanation of MutT, one of the well-studied DNA repair related proteins, is on the display.

organism repairs the broken DNA very efficiently. This efficient DNA repair gives this organism the ability to survive in such a severe environment. The molecular mechanism of the repair, however, is still unknown. To understand the molecular mechanism, we have computationally analyzed the genome sequence of *D. radiodurans* using the resources in ITBL and stored

the result in a database named *DeinoBase*. The database is now available on the Internet. With the database and our newly developed method to predict protein function from genome sequences, we have started an analysis to find new proteins that work as guardians of genome in *D. radiodurans*. Considering the highly efficient DNA repair, it is very likely that the organism has unknown proteins that repair DNA. This analysis is carried out in strong collaboration with Department of Ion-Beam-Applied Biology at Takasaki Establishment. The discovery of the proteins will bring us better understanding of the DNA repair mechanism of *D. radiodurans* and provide valuable information to other field of science, such as medicine[3.3-5, 3.3-6].

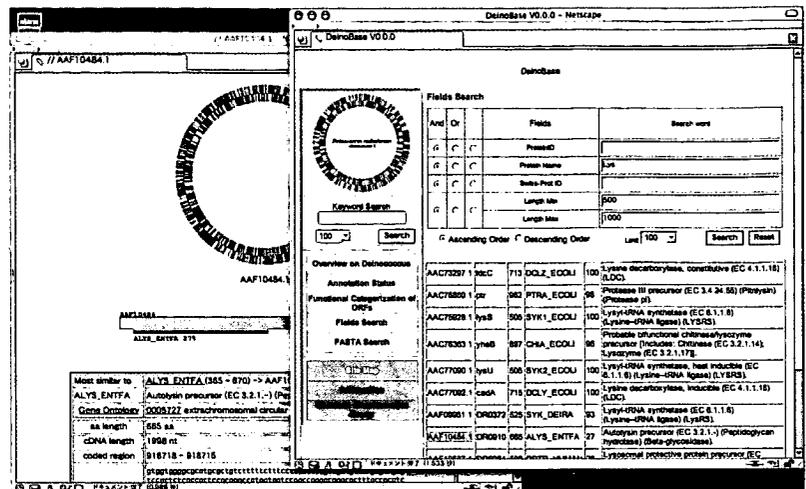


Fig.3.3.2-2: *DeinoBase*, a database of *Deinococcus radiodurans* genome annotation.

References

- [3.3-1] T. P. O. Kim, K. Yura, N. Go and T. Harumoto, "Divergent Actins from Karyorelictean, Heterotrich, Litostome Ciliates," *J. Euk. Microbiol.*, **51**, 227 (2004).
- [3.3-2] A. Yamaguchi, K. Iida, N. Matsui, S. Tomoda, K. Yura and M. Go, "Het-PDB Navi.: A database for protein-small molecule interactions," *J. Biochem (Tokyo)*, **135**, 79 (2004).
- [3.3-3] K. Nakamura, T. Kawabata, K. Yura and N. Go, "Novel types of two-domain multi-copper oxidizes: Possible missing links in the evolution," *FEBS Letters*, **553**, 239 (2003).
- [3.3-4] K. Matsuda, T. Nishioka, K. Kinoshita, T. Kawabata and N. Go, "Finding evolutionary relations beyond superfamilies: Fold-based superfamilies," *Protein Science*, **12**, 2239 (2003).
- [3.3-5] K. Yura, H. Kono and N. Go, "Molecular in silico biology of DNA repair enzymes: A trial of genome function prediction through gene positional information," *The 15th Annual Meeting of the Korean Society for Molecular and Cellular Biology*, Seoul, Korea, Oct. 9-10, 2003, p.115 (2003).
- [3.3-6] K. Yura, H. Kono and N. Go, "A trial of genome function prediction through gene positional information in the case of DNA repair proteins," *4th East Asian Biophysics Symposium*, Taipei, Taiwan, Nov. 3-6, 2003, p. 69 (2003).

Staff List

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Principal Scientist: Kimiaki SAITO

Research Scientist: Hidetoshi KONO

Hisashi ISHIDA

Invited Researcher: Akio KITAO

4. Public Relations

4.1 Press Release

- 2003/03/21 Science News, "Anyone can use Bioinformatics"
- 2003/03/26 Kyoto Shimbun, "Interested in protein – Middle & High School students study BSE.—"
- 2003/04/17 Nikkan Kogyo Shimbun, "Earth Simulator got a Prime Minister Award"
- 2003/05/02 Nihon Keizai Shimbun, Technology, "3-D Blood Flow Simulation in the Blood Vessel"
- 2003/05/12 Nihon Keizai Shimbun, Industries, "Remote Handling of Large Scale Experimental Facility, JAERI & Fujitsu · Proceeding Research Cooperation by Preventing Information Leak –"
- 2003/05/29 Nihon Keizai Shimbun, Industries, "High Power Laser ---- Research Cooperation with Private Companies ----"
- 2003/08/30 Yomiuri Shimbun, Kyoto, "Come on! Future Novel Award Scientists!"
- 2003/10/15 Nihon Keizai Shimbun, Industries, "Demonstration of "IT Laboratory"
- 2003/12/18 Nikkan Kogyo Shimbun, and Other two News Papers, "Development of Storage Grid"

4.2 CCSE News

No.23, January 2003

- Shinji Hioki, "Computational Science and Bring up Human Resources"
- Yoshio Suzuki, "Development of Visualization Tool for ITBL Basic Software"
- "Topic by Young Scientist (Susumu Yamada)"
- Yoshihiko Orita, "Outputs from Public Invitation System for R&D of Computational Science and Engineering Software"
- Hideo Kaburaki, "2nd CCSE Workshop"
- Kenji Higuchi, "3rd CCSE Workshop"
- Masahiko Machida and Masayuki Okano, "CCSE Seminar"
- Yutaka Ueshima, "Report of Presentation in the Open School of Science Council of Japan"
- Futoshi Shimizu, "Report of Poster Session in SC2002"
- Naoki Inoue, "High Level Evaluation of Earth Simulator in Foreign Countries – Won Gordon Bell Awards and Selected as the Best Invented Product by the "Time"'"

No.24, March 2003

- Norihisa Doi, "For the Promotion of Computational Science and Technology."
- Kenji Higuchi, "Success of the Connection Experiment with Outside Super-computers by using ITBL Basic Software"
- Yutaka Ueshima, "Report of Winning the MEXT Minister Awards for the Idea Contest in the 7th Science Exhibition and Experiment Show"
- "Topic by Young Scientist (Nobuaki Hatano)"
- Kei Yura, "4th CCSE Workshop"
- Takayuki Ohtani, "3th ITBL Symposium"
- Masahiko Machida and Masayuki Okano, "CCSE Seminar"

No.25 June 2003

- "Topic by Young Scientist (Hidetoshi Kohno)"
- Tetsuya Kuno, "Report of Winning the 35th(FY2002) AESJ Technology Awards"
- Futoshi Shimizu, "Report of Winning the FY2002 JSES Report Awards"
- Kentaro Isogai, "Introduction of S-cube"
- "5th CCSE Workshop"
- Masahiko Machida and Masayuki Okano, "CCSE Seminar"

No.26 January 2004

- Rebzo Takeda, "Computational Science Shoulders COE."
- Yoshio Suzuki, "Report Won the invitation report contest by NEC C&C System User Association"
- Osamu Hazama, "Report of Winning the SNA2003 "Best Poster Award""
- "Topic by Young Scientist (Nobuaki Ohno)"
- Naoki Inoue, "6th CCSE Workshop"
- Mitsuhiro Itakura, "7th CCSE Workshop"
- Nobuhiro Yamamoto, "Report of Poster Session in SC2003"
- Takayuki Ohtani, "4th ITBL Symposium"
- Masahiko Machida and Masahiro Okano, "CCSE Seminar"

No.27 March 2004

- Nobuyuki Satohuka, "Views of Computational Fluid Dynamics"
- Yoshiyuki Hoshi, "Report Won the Awards in the Visual Science Fiesta 2003"
- Osamu Hazama, "Report of Winning the SNA2003 "Best Poster Award"
- Yoshihiko Orita, "Outputs from Public Invitation System for R&D of Computational Science and Engineering Software"
- Kazuo Gorai and Yasuhiro Idomura, "Development of the Shared File System for Wide Area and Wide Band"
- "Comprehensive Symposium on the Wide use of ITBL Technologies"
- "Topic by Young Scientist (Atsuhiko Itakura)"
- Office of ITBL Promotion, "Report of Holding the International Symposium "Frontiers in Bioinformatics: Structure, Interaction and Function""
- Masahiko Machida and Masahiro Okano, "CCSE Seminar"

4.3 Workshops, Conferences and Events

Workshops

- 5th CCSE Workshop concerning the Collaboration between ITBL and ADVENTURE (May 28, 2003)
- 6th CCSE Workshop “Programs and Results of Large Scale Numerical Simulations in the Atomic Energy research field using Earth Simulator,” (July 2, 2003)
- 3rd Computational Materials Design workshop (Sep. 10-13, 2003)
- 2nd Open Workshop about DNA Repair Enzyme, JAERI, Kizu, Kyoto, October 22, 2003
- 7th CCSE Workshop “Numerical Modeling and Simulation of SCC” (October 23, 2003)
- 2nd Open Workshop about Sequence, Structural Database, JAERI, Kizu, Kyoto, February 9, 2004
- 2nd Open Workshop about Biomolecular Simulation, JAERI, Kizu, Kyoto, February 9, 2004
-

Symposium

- The 4th ITBL symposium (October 20, 2003)
- Frontiers in Bioinformatics: Structure, Interaction and Function, Kyoto, Kyoto, February 10, 2004 (in collaboration with Bioinformatics Unit at Nara Institute of Science and Technology)
- Special session “Programmes and Results of Large Scale Numerical Simulations with Earth Simulator in the Atomic Energy research field” at 2003 Fall Meeting of the AESJ (Sept. 15-17, 2003, Shizuoka)

4.4 Seminars

- **Finite Element Method (FEM) code seminar**

As a finite element method code for the ITBL environment, we have worked to install ADVENTURE codes developed by Prof. Yoshimura of Tokyo University and other colleagues. Besides the R&D works, we held the seminar for the usage of the codes.

1st FEM –Adventure- seminar, on Oct. 28, 2004, instructor: Yoshimura, S. (Graduate School of Frontier Sciences, the University of Tokyo), Kawai, H. (Intelligent Modeling Laboratory, the University of Tokyo), Mimura, Y. (Graduate School of Frontier Sciences, the University of Tokyo), Miyoshi, A. (INSITE corporation)

- **Computational Material Design (CMD) workshop**

In cooperation with Osaka University, Japan Science and Technology Agency, and International Institute for Advanced Studies, we have held CMD workshops twice in every year. Each workshop was scheduled in 5 days from Tuesday to Saturday. It was composed of 2 or 3 courses corresponding to the expertise grade of participants. The lecturers are all top-end researchers in Japan. The participants were 30-40 persons, increasing in every year.

- **Gaussian seminar**

Gaussian, a well known program of a molecular orbital method, has been used in the various scientific fields of material design, bio-chemical reaction simulation, and medicine designing etc... The seminar was prepared in order to manage a big code of Gaussian easily and variously according to the purpose of the usage. The lecturers were Prof. Yamabe of Nara University of Education and Prof. Minato of Nara University. Both are top experts of Gaussian in Japan. The participants were 15 persons in enterprises, universities and research organizations.

2nd Gaussian seminar, on Feb. 2-3, 2004, instructor: Minato, T. (Information Processing Center, the University of Nara), Yamabe, S. (Department of Education, Nara University of Education)

- **Bio-informatics seminars**

We have held 3 seminars in accord with the following research theme, "DNA recovery enzyme", "Sequence/Structure database", and "Bio-molecular simulation" in cooperation with Osaka Science and Technology Center. The participants were totally 105 persons of universities, research organizations, and enterprises.

• **Plasma/photon/fluids, Material properties, Computational chemistry, Information/mathematics seminars and the integrated symposium**

In order to enlarge the link of the user community in those fields, we have held the seminars in the application fields in cooperation with Osaka Science and Technology Center. The participants of each seminar were 44, 24, 34, and 25 researchers of universities, research organizations, and enterprises respectively. The integrated symposium of the above-mentioned fields was held and the participants were totally 63 persons.

• **Super Science Seminar(S-cube)**

For high school students, we have opened the educational seminar every Wednesday. The theme and lecturers are selected in the various fields of top-end scientific researches in Japan. In FY 2003, we held 43 times and participants reached to 603 persons totally.

24th on Apr. 16, 2003

“Building a Hydrogen Energy -based society from theoretical condensed matter physics design-”, instructor: Kasai, H. , Nakanishi, H.(Department of Applied Physics, Graduate School of Engineering, Osaka University)

25th on Apr. 23, 2003

“The World of Nano-Science”, instructor: Akai, H. (Department of Physics, Graduate School of Science, Osaka University)

26th on May. 7, 2003

“You can enjoy Cosmical Hydrodynamic Simulations”, instructor: Shibata, K. , Tanuma, S. (Kwasan and Hida Observatories, Kyoto University)

27th on May. 14, 2003

“Lens Antenna Experiment”, instructor: Toyomasu, S. (Misato Observatory)

28th on May. 28, 2003

“Welcome to the International Space Station!”, instructor: Tabuchi, T. (KIBO Utilization Promotion Office, Space Utilization Research Center, Office of Space Utilization Systems, National Space Development Agency)

29th on Jun. 4, 2003.

“Dream of Super Computers”, instructor: Joe, K. (Department of Advanced Information & Computer Science, Graduate School of Human Culture & Science, Nara Woman’s University)

30th on Jun. 11, 2003

“The first hundred year of Relativity”, instructor: Sato, H. (Konan University)

31st on Jun. 18, 2003

“Environment of Three-dimensional Visualization and its Application to Science”,
instructor: Ido, S. (Department of Computer Science, Faculty of Engineering,
Saitama Institute of Engineering)

32nd on Jun. 25, 2003

“Introduction to Utilize Information –we produce knowledge from data-”, instructor:
Teramoto, T. (Department of Electronics and Computer Engineering, Tsuyama
National College of Technology)

33rd on July 16, 2003

“Natural Energy can be from Biomass –car moves by waste oil and fat-”, instructor:
Saka, S. (Department of Socio-Environmental Energy Science, Graduate School of
Energy Science, Kyoto University)

34th on Jul. 23, 2003

“What is a mechanism of intelligent systems, and how do we realize it”, instructor:
Miki, M. (Department of Knowledge Engineering and Computer Sciences, Faculty
of Engineering, Doshisha University)

35th on Jul. 30, 2003

“Visualization of Biological Sample’s Internal Structure”, instructor: Yokota, H.
(Advanced Computing Center, RIKEN)

36th on Aug. 7, 2003

“The visualization of the air flow around a paper plane with a portable wind tunnel”,
instructor: Takama, N. (Center for International Research on MicroMechatronics,
Institute of Industrial Science, the University of Tokyo)

37th on Aug. 20, 2003

“Life of the Star and Synthesis of Elements –human being allowed to live by the
nature-”, instructor: Baba, H. (Osaka University)

38th on Aug. 26, 2003

“A recipe for making an original 3D-garden using the 3D-Network World Simulator,
“3D-NWS””, instructor: Wada, K. (UNTROD, Inc.)

39th on Aug. 27, 2003

“Virtual Tour in Human Body”, instructor: Chihara, K. (Graduate School of
Information Science, Nara Institute of Science and Technology)

40th on Aug. 28, 2003

“How can we look inside the human body?”, instructor: Masaki, S. (Brain Activity
Imaging Center, Advanced Telecommunications Research Institute International)

41st on Sep. 17, 2003

“How’s the Internet working? –the communication infrastructure for changing our

daily life-”, instructor: Yamaguchi, S. (Graduate School of Information Science, Nara Institute of Science and Technology)

42nd on Sep. 24, 2003

“An Astronomical Observatory on the Internet –toward Japanese virtual observatory-”, instructor: Mizumoto, Y. (National Astronomical Observatory of Japan)

43rd on Oct. 8, 2003

“Discover radiations around you”, instructor: Kanno, I. (Quantum Science and Engineering Center, Graduate School of Engineering, Kyoto University), Izumi, Y. (Department of Nuclear Engineering, Graduate School of Engineering, Osaka University), Horiguchi, T. (Atomic Energy Research Institute, Kinki University)

44th on Oct. 15, 2003.

“Secret of Magic Balls”, instructor: Himeno, R. (Advanced Center for Computing and Communication, RIKEN)

45th on Oct. 29, 2003

“Let’s create video animation!”, instructor: Jouma, A. (Studio False co.,Ltd.)

46th on Nov. 5, 2003.

“The Law of Light Found in Manga?! –from an angel’s halo to freely bending light-”, instructor: Makino, K. (Comic Art Department, Faculty of Art, Kyoto Seika University)

47th on Nov, 12, 2003

“Computer Simulation Technology in Aerospace –technology for design and development of aircraft and spacecraft-”, instructor: Fujii, K. (Institute of Space and Astronautical Science, Japan Aerospace Exploration Agency)

48th on Nov. 19, 2003

”Sound” What is it? –audible sounds & ultrasonics-”, instructor: Watanabe, Y. (Faculty of Engineering, Doshisha University)

49th on Nov. 26, 2003

“Dream Vehicles with Water and Laser”, instructor: Kajiwara, I. (Department of Mechanical and Aerospace Engineering, Tokyo Institute of Technology)

50th on Dec. 17, 2003

“The Predictive Powers of Present-day Scientific Knowledge –the Biohistory for 4 thousand million years-”, instructor: Sezaki, K. (Japan Synchrotron Radiation Research Institute)

51st on Dec. 25, 2003

“Let’s challenge operating of a nuclear reactor on computer!”, instructor: Okumura,

K. (Department of Nuclear Energy System, Japan Atomic Energy Research Institute), Nakano, M. (Kobe Shipyard & Machinery Works, Mitsubishi Heavy Industries, Ltd.)

52nd on Dec. 25, 2003

“The Sensuous Science Experiments of the Natural Disaster Phenomena”, instructor: Nohguchi, Y. (National Research Institute for Earth Science and Disaster Prevention)

53rd on Dec. 25, 2003

“Biological Evolution and Protein –Hemoglobin as an example-”, instructor: Go, N. (Center for Promotion of Computational Science and Engineering, Japan Atomic Energy Research Institute)

54th on Dec. 26, 2003

“CAMP Cricket Workshop –Toy Box of Lights-”, instructor: CAMP staff (CSK CORPORATION, Social Contribution Planning Office, OKAWA Center)

55th on Dec. 27, 2003

“Look! What a amazing radiation power!”, instructor: Nishimura, A. (Advanced Photon Research Center, Japan Atomic Energy Research Institute)

56th on Dec. 27, 2003

“Wonderful Shapes of Biomolecules –DNA, Prion, SARS, Ion Channel-”, instructor: Honma, Y. (Niigata Woman’s Junior College)

57th on Dec. 27, 2003

“The Earthquake Shakes our Building”, instructor: Yamashita, T. (Earthquake Disaster Mitigation Research Center, National Research Institute for Earth Science and Disaster Prevention)

58th on Jan. 21, 2004

“Let’s learn what the radioactivity or radioactive ray is, and let’s know what the nuclear power is”, instructor: Nakagome, Y. (Research Reactor Institute, Kyoto University)

59th on Jan. 28, 2004

“Practical Robots becoming familiar”, instructor: Kanda, S. (Peripheral Systems Laboratories, Fujitsu Laboratories, Ltd.)

60th on Feb. 18, 2004

“The Mathematical Theory of Kaleidocycle”, instructor: Onishi, T. (Nara Woman’s University Secondary School)

61st on Feb. 25, 2004

“Let’s Experience a Virtualized 360-degree Panoramic World”, instructor: Yokoya,

N. (Nara Institute of Science and Technology)

62nd on Mar. 17, 2004

“What causes an earthquake? What happens when it occurs?”, instructor: Hashimoto, M. (Research Center for Earthquake Prediction, Disaster Prevention Research Institute, Kyoto University)

63rd on Mar. 24, 2004

“Let’s make CM with 3D-CG”, instructor: Nirazuka, N. (SystemEXE corporation)

64-66th on Mar. 29-31, 2004

“Learning by experience of making an original 3D-garden”, instructor: Wada, K. (UNTROD, Inc.)

5. Research Collaboration

The CCSE has cooperated research and development activities with other organizations both domestically and internationally.

5.1 International Cooperation

- (1) Research cooperation between JAERI and Fraunhofer Institute (Germany) concerning research and development in computational science and engineering
- (2) Research cooperation between JAERI and Stuttgart University

5.2 Domestic Cooperation

- (1) Study on Super Computer Network Formation (with National Institute of Informatics)
- (2) Study on Molecular Dynamics Simulation technique (with Toshiba, Ltd.)
- (3) Study on spin dynamics of magnetic multi-layer film by using parallel computing (with Hitachi, Ltd.)
- (4) Study on practical application of turbulence model to numerical fluid dynamics (with IHI, Ltd.)
- (5) Study on development of parallelization support tool for AVS/Express (with KGT, Ltd.)
- (6) Research and development on enhancement of mesh generator, visualization system and simulation for land foundation analysis (with RIKEN)
- (7) Study on Molecular Dynamics Simulation of destruction by using numerical experiment environment (with the Japan Research Institute, Ltd.)
- (8) Study on hydrogen assisted corrosion cracking mechanism by using Molecular Dynamics (with National Institute of Advanced Industrial Science and Technology)
- (9) Development of super parallel simulation system for enhancement of radiation medical treatment (with Japan Science and Technology Agency)
- (10) Research on the open source visualization platform in the ITBL environment (Fujitsu Tokushima Engineering Inc.)
- (11) R&D works of e-learning system using grid computer (KGT Inc.)
- (12) The environmental research and evaluation on the IPv6-Globus in the ITBL

- environment (Osaka University)
- (13)R&D works on the HPC-middle ware in the ITBL environment (Tokyo University)
- (14)R&D works on the inductive mechanism in the collaboration of the researchers belonging to different research fields and on its supporting human interfaces (Kyoto Seika University)
- (15)Research on the incompressible fluids analysis in the ITBL environment (Kyoto Institute of Technology)
- (16)Research on the micro-macro integrated fluid simulation in the ITBL environment (Kyoto Institute of Technology)
- (17)Research on the mass parallel large scale simulation on the nonlinear behavior (Osaka City University)
- (18)Educational collaboration with Super Science High school (Nishiyamato-gakuen high school)
- (19)Construction of remote support system of radiation therapy (Tokyo Metropolitan University of Health Science and other organizations)
- (20)Study on bioinformatic analysis by using ITBL (A) (with Molecular chemistry research institute, Okazaki National Cooperative Utilization Research Organization)
- (21)Study on bioinformatic analysis by using ITBL (B) (with Institute of Molecular and Cellular Biosciences , the University of Tokyo)
- (22)Study on bioinformatic analysis by using ITBL (C) (with National Institute of Genetics)
- (23)Study on bioinformatic analysis by using ITBL (D) (with Nagahama Institute of Bio-Science and Technology)
- (24)Study on bioinformatic analysis by using ITBL (E) (with Nagoya University)
- (25)Study on bioinformatic analysis by using ITBL (F) (with Nagaoka University of Technology)
- (26)Study on bioinformatic analysis by using ITBL (G) (with Nara Institute of Science and Technology)
- (27)Simulation of biomolecular phenomena (A) (with Yokohama City University)
- (28)Simulation of biomolecular phenomena (B) (with Dokkyo University School of Medicine)
- (29)Study on Structure and Dynamics of protein considering water contribution (with Nagaoka University of Technology)
- (30)Development of grid computing front end using rata base and rule base (with

Computing and Communication Center, Kyushu University)

- (31) Construction of nano-technology simulation environment by using multiple super computers (1) (with Institute For Materials Research, Tohoku University)
- (32) Study on Integrated Tsunami information analysis system (with Disaster Control Research Center, Tohoku University)
- (33) Conceptual design of optimum user interface for network computing (with Kyoto University)
- (34) Study on application of eigen-value problem to principle and practical problems under dispersed computing environment (with University of Electro-Communications)
- (35) Validation of application applicability to network computing environment (with University of Tokyo)
- (36) Study on parallelization and performance evaluation of Magnetohydrodynamics (MHD) code (with Solar-Terrestrial Environment Laboratory, Nagoya University)
- (37) Study on numerical calculation algorithm of wall turbulent flow and turbulent flow model (with Nagoya University)
- (38) Study on performance evaluation and enhancement of parallel numerical calculation library PARCEL (A) (with Tsukuba University)
- (39) Study on performance evaluation and enhancement of parallel numerical calculation library PARCEL (B) (with Computing and Communication Center, Kyushu University)
- (40) Study on performance evaluation and enhancement of parallel numerical calculation library PARCEL (C) (with Tsukuba University)
- (41) Study on parallel programming method by message passing in application region (with University of Tokyo)
- (42) Study on super parallelization, vectorization of numerical fluid dynamics (with University of Tokyo)
- (43) Development of numerical simulation technique for super-conduction novel order condition (A) (with Osaka Prefecture University)
- (44) Development of numerical simulation technique for super-conduction novel order condition (B) (with Institute For Materials Research, Tohoku University)
- (45) Study on living body simulation by using integrated simulation technology under ITBL environment (with Japan Advanced Institute of Science and Technology)
- (46) Study on development of research community system on ITBL by using

ADVENTURE (with University of Tokyo)

- (47) Study on parallel finite element analysis by using KAERI-MESH and its application to HPC education (with University of Tokyo)
- (48) Study on application of Parallel Molecular Dynamics Stencil (A) (with Kanazawa University)
- (49) Study on application of Parallel Molecular Dynamics Stencil (B) (with University of Tokyo)
- (50) Study on crack progress analysis by using free mesh method (with University of Tokyo)
- (51) Study on plastic phenomena by using Molecular Dynamics (with Teikyo University of Science and Technology)
- (52) Study on two phase flow by using particle method (with Tsukuba University)
- (53) Study on finite element analysis of in silico Human Hip Joint for the purpose of use of ITBL environment (with Osaka University)
- (54) Study on development of HPC middleware using ITBL environment (with University of Tokyo)
- (55) Study on deformation technology of visualization information process for support of collaboration among researchers in different field under ITBL environment (with Kyoto Seika University)
- (56) Study on non-compressive fluid analysis methodology under ITBL environment (with Kyoto Institute of Technology)
- (57) Study on micro-macro integrated fluid simulation technology under ITBL environment (with Kyoto Institute of Technology)
- (58) Study on super parallel large scale non-linear behavior analysis using ITBL environment (with Osaka City University)

6. Research Achievements

6.1 Publications

Journal Reports

- 1) Aikawa, H., "Activity in Super Science Seminar (S-cube)", Journal of Human Interface Society, Vol.5, No.2, 61 (2003).
- 2) Ako M., Machida M., Koyama T., Ishida T., Kato M., "Vortex state of nano-scaled superconducting complex structures (d-dot)", Physica C, 412-414, 544(2004).
- 3) Calhoun J. R., Kono H., Wang W., DeGrado W. F., and Saven J. G.: Computational design and characterization of a monomeric helical dinuclear metalloprotein., J. Mol. Biol., 334, 1101 (2003).
- 4) Ebihara, K. and Watanabe, T., "Evaluation of Influence of Pipe Width on Interfacial Growth of Horizontal Stratified Two-Phase Flow in Rectangular Pipe by Lattice Boltzmann Method", Trans. Jpn. Soc. Mech. Eng. B, 70, 1393 (2004) [in Japanese].
- 5) Ebihara, K. and Watanabe, T., "The lattice Boltzmann Simulation of the droplet creation in the horizontal stratified two-phase flow", Nagare 23, 253(2004) [in Japanese].
- 6) Fu X., Kono H., and Saven J. G.: Probabilistic approach to the design of oligomeric proteins., Protein Eng., 16, 971 (2003).
- 7) Gromiha M. M., Siebers J. G., Selvaraj S., Kono H. and Sarai A.: Intermolecular and Intramolecular Readout Mechanisms in Protein-DNA Recognition., J. Mol. Biol., 337, 285 (2004).
- 8) Itakura M., "Frozen Quasi Long Range Order in the Random Anisotropy Heisenberg Magnet", Physical Review B 68 (2003) 100405 (R).
- 9) Kato M., Ako M., Machida M., Koyama T., Ishida T., "Structure of Magnetic Flux in Nano-scaled Superconductors", J. Mag. Mag. Mat., 272-276, 171(2003).
- 10) Kato M., Ako M., Machida M., Koyama T., Ishida T., "Ginzburg-Landau calculations of d-wave superconducting dot in s-wave superconducting matrix (d-dot) ", Physica C, 412-414, 352(2004).
- 11) Kim T. P. O., Yura K., Go N. and Harumoto T.: Divergent Actins from Karyorelictean, Heterotrich, Litostome Ciliates., J. Euk. Microbiol., 51, 227 (2004).
- 12) Kono H. and Saven J. G.: Combinatorial protein design., Biophysics, 43, 186 (2003) [in Japanese].
- 13) Koyama T., Machida M., Kato M., and Ishida T., "Phase Dynamics in a d-dot

- Embedded in an s-wave Superconductor," *Physica C*, 412-414, 358(2004).
- 14) Machida M., Koyama T., Kato M., and Ishida T., "Vortex Dynamics in d-dot arrays Embedded in Conventional Superconductors", *Physica C*, 408-410, 587 (2004).
 - 15) Machida M., Koyama T., Kato M., and Ishida T., "Electronic Structure of a Half Quantized Vortex", *Physica C*, 412-414, 367(2004).
 - 16) Machida M. and Koyama T., "Localized Rotating Modes in Capacitively Coupled Intrinsic Josephson Junctions: Systematic Study of Branching Structure and Collective Dynamical Instability", *Phys. Rev. B*, 70, 024523(2004).
 - 17) Machida M. and Sakai S., "Unified Theory for Magnetic and Electric Field Coupling in Multi-stacked Josephson Junctions", *Phys. Rev. B*, 70, 144508(2004).
 - 18) Machida M., Koyama T., Kato M., and Ishida T., "Direct Numerical Experiments for Neutron Detection using Superconductor MgB₂", *Nucl. Inst. and Methods in Physics Research A*, 529, 409(2004).
 - 19) Matsuda K., Nishioka T., Kinoshita K., Kawabata T. and Go N.: Finding evolutionary relations beyond super families: Fold-based superfamilies., *Protein Science*, 12, 2239 (2003).
 - 20) Nakamura K., Kawabata T., Yura K., and Go N.: Novel types of two-domain multi-copper oxidizes: Possible missing links in the evolution., *FEBS Letters*, 553, 239 (2003).
 - 21) Oobatake M., Kono H., Wang Y. and Sarai A.: PROTEINS: Anatomy of specific interactions between lambda repressor and operator DNA by energy-component analysis., *Struct. Funct. Genet.*, 53, 33 (2003).
 - 22) Shiga M., Yamaguchi M., and Kaburaki H., "Structure and energetics of clean and hydrogenated Ni surfaces and symmetric tilt grain boundaries using embedded-atom method", *Physical Review B* vol.68, 245402 (2003).
 - 23) Shiga M., Takayanagi T., "Quantum path-integral molecular dynamics calculations of the dipole-bound state of the water dimer anion", *Chemical Physics Letters* vol.378, pp.539-547 (2003).
 - 24) Shiga M, Tachikawa M., "Ab initio path integral study of hydronium ion", *Chemical Physics Letters* vol.374, pp.229-234 (2003).
 - 25) Shinoda W., Shiga M., and Mikami M., "Rapid estimation of the elastic constants by molecular dynamics simulation under constant stress", *Physical Review B*, vol.69 134103 (2004).
 - 26) Suematsu H., Machida M., Koyama T., Ishida T., Kato M., "Finite Element Method for Bogoliubov-de Gennes equation: Application to nano-structure superconductors", *Physica C*, 412-414, 548(2004).

- 27) Takayanagi T., Shiga M., "Photodissociation of Cl₂ in helium clusters: an application of hybrid method of quantum wavepacket dynamics and path integral centroid molecular dynamics", *Chemical Physics Letters* **372**, 90 (2003).
- 28) Wada A., Takayanagi T., Shiga M., "Theoretical simulations on photoexcitation dynamics of the silver atoms embedded in helium clusters", *J. Chemical Physics*, **119**, 5478(2003).
- 29) Watanabe T., "Flow pattern and heat transfer rate in Rayleigh-Benard convection", *Physics of Fluids*, **16**, 972 (2004).
- 30) Watanabe T., "Numerical evidence for coexistence of roll and square patterns in Rayleigh-Benard convection", *Physics Letters A*, **321/3**, 185 (2004).
- 31) Yamaguchi A., Iida K., Matsui N., Tomoda S., Yura K., and Go M.: Het-PDB Navi. : A database for protein-small molecule interactions., *J. Biochem (Tokyo)*, **135**, 79 (2004).
- 32) Yamaguchi A., Iwadata M., Suzuki E., Yura K., Kawakita S., Umeyama H., and Go M.: Enlarged FAMSBASE: 3D protein structure models of genome sequences for 41 species., *Nucleic Acids Research*, **31**, 463 (2003).
- 33) Yamguchi M., Shiga M., and Kaburaki H., "First-Principles Study on Segregation Energy and Embrittling Potency of Hydrogen in Ni Sigma 5 (012) Tilt Grain Boundary", *J. Phys. Soc. Japan*, **73**, 441(2004).
- 34) Yamaguchi M., Shiga M., and Kaburaki H., "Energetics of segregation and embrittling potency for non-transition elements in the Ni Sigma 5 (012) symmetrical tilt grain boundary: a first-principles study ", *J. Phys.: Condens. Matter*, **16**, 3933 (2004).

Reports published by JAERI

- 1) Isogai, K., "Distributed computing system; Development of a control server", JAERI-Data/Code 2003-010 (2003).
- 2) Isogai, K., Yasuhara, Y., "Report and analysis of S-cube(Super Science Seminar)", JAERI-Tech 2004-039 (2003).
- 3) Kimura, H., Sakai, T., "Bioinformatics; Data base and application execution Web system", JAERI-Data/Code 2004-001 (2003).
- 4) Kimura, H., Sakai, T., "Bioinformatics; Construction of protein 3D structure prediction system", JAERI-Data/Code 2004-008 (2003).
- 5) Miyazaki, M., "Equipment of visualization environment of a large-scale structural analysis system", JAERI-Tech 2004-038 (2003).
- 6) Yamasaki, I., "Equipment of educational teaching material for FEM", JAERI-Tech

2004-040 (2003).

- 7) Yasuhara, Y., "Visualization environment and its utilization of ITBL building", JAERI-Data/Code 2004-009 (2003).

Proceedings

- 1) Slovic A. M., Kono H., Lear J. D., Saven J. G, and DeGrado W. F.: Computational design of WSK, a water-soluble analogue of the potassium channel KcsA., Proc. Natl. Acad. Sci. USA, 101, 1828 (2004).
- 2) Yamada S., Machida M. and Imamura T., "Parallel Computation of Large-Scale Eigenvalue Problems of Strongly Correlated Electrons on the Earth Simulator" (in Japanese), Proc. of HPCS2004, IPSJ Symposium Series, Vol. 2004, No.1, pp103-110, 2004.
- 3) Yamada S. and Imamura T., "PARCEL: Eigenvalue Problem Solver" (in Japanese), Proc. of the Conference on Computational Engineering and Science, Vol. 8, No.2, pp.753-756, 2003.

Books

- 1) Go N.: ("Biophysics in the world" in) "What is biophysics?", Kyoritsu Shuppan, Tokyo, 171 (2004) [in Japanese].
- 2) Kono H and Sarai A.: ("Structure-Specificity Relationship in Protein-DNA Recognition" in) "Bioinformatics of Genome Regulation and Structure", Kluwer Academic Pub, Boston, 155 (2004).

Others : Followings are publications written by scientists outside CCSE whose research activities were supported by the Earth Simulator Use Support division in CCSE.

- 1) Guo J.-H. *et al.*, "Molecular Structure of Alcohol-Water Mixtures", Phys. Rev. Lett., 91, 157401 (2003).
- 2) Boero M. *et al.*, "First principles molecular dynamics simulations of a hydrated electron in normal and supercritical water", Phys. Rev. Lett., 90, 226403 (2003).
- 3) T.Ishihara, Y. Kaneda, M. Yokokawa, K. Itakura, and A. Uno, "Spectra of energy dissipation, enstrophy and pressure by high-resolution direct numerical simulation of turbulence in a periodic box", J. Phys. Soc. Jpn. 72, 983 (2003).
- 4) Tsuji Yoshiyuki and Ishihara Takashi, "Similarity scaling of pressure fluctuation in

- turbulence”, *Phys. Rev. E*, **68** 02630968 (2003).
- 5) Idomura Y., Tokuda S., and Kishimoto Y., *Nucl. Fusion* **43**, 234 (2003).
 - 6) Ishikura S., Kogawa H., Furakawa M., Kikuchi K., Hino R., Arakawa C., “Bubble dynamics in the thermal shock, problem of the liquid metal target”, *J. Nucl. Mater.* **318**, 113 (2003).
 - 7) Imai R., Ishikura S., Kogawa H., Hino R., Arakawa C., “Development of a fluid-structure interaction code for a mercury target”, *Trans. JSCES*, Paper No. 20030014, (2003).

6.2 Talks and Presentations

Poster:

- 1) Gong X.J., Yura K., and Go N.: A bioinformatics integration framework based on task mapping editor (TME), *Frontiers in Bioinformatics: Structure, Interaction and Function*, Kyoto, (2004).
- 2) Hazama, O. and Guo, Z. : “Practical integrated simulation systems for coupled numerical simulations in parallel”, *Proc. of the Int. Conf. on Supercomputing in Nuclear Applications (SNA2003)*, (2003) [CDROM].
- 3) Higuchi M., Ishida H., Kitao A., Yamagata Y. and Go N.: Molecular dynamics simulation study of 8-oxo-dGMP recognition mechanism of MutT, *The 41st Annual meeting of biophysical society of Japan*, Niigata, Japan, (2003) [in Japanese].
- 4) Higuchi M., Ishida H., Kitao A., Yamagata Y. and Go N.: Molecular dynamics simulation study of recognition mechanism of MutT, *Institute for Molecular Science Symposium*, Okazaki, Japan, (2003) [in Japanese].
- 5) Higuchi M., Ishida H., Kitao A., Yamagata Y., and Go N.: Study of recognition mechanism of MutT by molecular dynamics simulation, *Frontiers in Bioinformatics: Structure, Interaction and Function*, Kyoto, Japan (2004).
- 6) Ishida H. and Go N.: Molecular dynamics simulation of branch migration in RuvA tetramer – Holliday, *The Eighth Annual International Conference on Research in Molecular Biology*, San Diego, U.S.A., (2004).
- 7) Ishida H. and Go N.: Molecular Dynamics Simulation of Damaged DNA and 8oxoGuanine DNA Glycosylase Complex, *The 3rd Annual meeting of protein science society of Japan*, Sapporo, Japan, (2003) [in Japanese].
- 8) Ishida H. and Go N.: Molecular Dynamics Simulation of RuvA - Holliday junction Complex, *Frontiers in Bioinformatics: Structure, Interaction and Function*, Kyoto, Japan, (2004).
- 9) Ishida H. and Go N.: Molecular Dynamics Simulation of RuvA-Holliday junction Complex, *The 41st Annual meeting of biophysical society of Japan*, Niigata, Japan, (2003) [in Japanese].
- 10) Ishida H. and Go N.: Molecular Dynamics Simulation of RuvA-Holliday junction Complex, *The 9th Keihanna Conference on Molecular Biophysics*, Keihanna, Japan, (2004).
- 11) Kato M., Ako M., Machida M., Koyama T., Ishida T., “Structure of Magnetic Flux in Nano-scaled Superconductors”, *ICM2003 Rome, Italy* (July 2003).

- 12) Kim O.T.P., Yura K., and Go N.: Analyses of RNA-binding site properties and development of a method to predict RNA interfaces on proteins, *Frontiers in Bioinformatics: Structure, Interaction and Function*, Kyoto, Japan, (2004).
- 13) Kono H., Gromiha M.M., Siebers J.G., Selvaraj S. and Sarai A.: Direct or Indirect Readout in Protein-DNA Recognition?, *The 48th Biophysical Society*, Baltimore, USA, (2004).
- 14) Kono H., Yura K., Go N. and Sarai A.: Finding Genes in Yeast Genome Regulated by the Same Transcription Factors Using Empirical Potentials Derived 3D Protein-DNA Complex Structures, *Keystone Symposia: Frontiers in Structural Biology*, Utah, USA, (2004).
- 15) Kono H.: Contributions of Direct and Indirect Readouts to Protein-DNA Recognition, *The 9th Keihanna Conference on Molecular Biophysics (KCMB 2004): Physical aspects of protein folding and function*, Kyoto, Japan, (2004).
- 16) Machida M., Koyama T., Kato M., and Ishida T., "Vortex Dynamics in d-dot arrays Embedded in Conventional Superconductors", *M2S Rio*, Brasil (May 2003).
- 17) Machida M., and Itakura M., "Phase and Amplitude Fluctuations above the Upper Critical Field in Type II Superconductors with Short Coherence Length", *ISS2003 Tsukuba*, Japan (Nov. 2003).
- 18) Machida M., Koyama T., Kato M., and Ishida T., "Direct Numerical Experiments for Neutron Detection using Superconductor MgB₂", *NOP2004 & PSND2004* (Jan. 2004).
- 19) Machida M., Sasa N., Matsumoto H., "Coexistence of Vortex Liquid and Solid in Rotating Bose-Einstein Condensate", *QFS 2004*, Trento, Italy (Jul. 2004).
- 20) Metsugi S., Kitao A. and Go N.: Trajectory length of Protein MD necessary for calculation of various physical amounts with high accuracy, *The 41st Annual meeting of biophysical society of Japan*, Niigata, Japan, (2003) [in Japanese].
- 21) Metsugi S., Kono H., Yura K. and Go N.: The structure and function of proteins that have many Under Wrapped Hydrogen Bonds, *The 3rd Annual meeting of protein science society of Japan*, Sapporo, Japan, (2003) [in Japanese].
- 22) Nakamura K., Kawabata T., Yura K., and Go N.: Novel types of two-domain multi-copper oxidases: Possible missing links in the evolution, *Frontiers in Bioinformatics: Structure, Interaction and Function*, Kyoto, Japan, (2004).
- 23) Narumi I., Yura K., Saito K. and Kikuchi M.: Search for a new DNA repair genes out of function unknown genes, *The 25th Annual Meeting of the Molecular Biology Society of Japan*, Kobe, Japan, (2003) [in Japanese].
- 24) Sarai A., Ahmad S., Gromiha M.M., Kumar M.D.S., Bava A. and Kono H.:

- Developing Genome-Scale Prediction System for Transcription Factors and their Targets, The 14th International Conference on Genome Informatics, Yokohama, Japan, (2003).
- 25) Sarai A., Prabakaran P., Siebers J. G., Ahmad S., Gromiha M.M. and Kono H.: QSAR analysis of protein-DNA complexes, The 41st The annual meeting of the Biophysical Society of Japan, Niigata, Japan, (2003) [in Japanese].
- 26) Uedaira H., Kono H., Prabakaran P., Kitajima K. and Sarai A.: Heat Capacity Changes upon Binding of Proteins to DNA, The Japan Society of Calorimetry and Thermal Analysis, Hiroshima, Japan, (2003) [in Japanese].
- 27) Uedaira H., Kono H., Prabakaran P., Kitajima K. and Sarai A.: Structure-Thermodynamic Relationship in Protein-DNA Binding: Heat Capacity Changes, The 14th International Conference on Genome Informatics, Yokohama, Japan, (2003).
- 28) Yura K. and Go M.: Prediction of enzyme specificity determinant residues - a case study on fungal peroxidases, The 41st Annual meeting of the Biophysical Society of Japan, Niigata, Japan, (2003) [in Japanese].
- 29) Yura K., Kono H. and Go N.: A trial of genome function prediction through gene positional information, The 3rd Annual Meeting of the Protein Science Society of Japan, Sapporo, Japan, (2003) [in Japanese].
- 30) Yura K., Kono H. and Go N.: DNA repair related protein prediction through gene positional information, The 6th Meeting on Frontiers of Microbial Genome Research. Kazusa, (2004) [in Japanese].

Oral:

- 1) Ebihara, K. and Watanabe, T., "Evaluation of Influence of Pipe Width on Interfacial Growth of Horizontal Stratified Two-Phase Flow in Rectangular Pipe by Lattice Boltzmann Method", *Trans. Jpn. Soc. Mech. Eng. B*, 70, 1393 (2004).
- 2) Ebihara, K. and Watanabe, T., "The lattice Boltzmann simulation of the droplet creation in the horizontal stratified two-phase flow", *Proc. 17th Symp. CFD*, 63 (2003).
- 3) Guo, Z., Hazama, O., Yamagiwa, M., Hirayama, T. and Matsuzawa, T. : "Proposal and implementation of a fluid-structure coupled simulation system with parallel commercial codes", *Proc. of the Int. Conf. on Computational & Experimental Engineering and Sciences (ICCES)*, (2003) [CDROM].
- 4) Hazama, O. and Guo, Z. : "Development of an integrated numerical simulation infrastructure for fluid-structure coupled problems", *Proc. of the Conf. on Computational Engineering and Science, The Japan Society for Computational Engineering and Science*, 8(2), pp.759-760, (2003) [in Japanese].
- 5) Higuchi, K., Otani, T., Hasegawa, Y., Suzuki, Y., Yamagishi, N., Kimura, K., Aoyagi, T., Nakajima, N., Fukuda, M., Imamura, T. and Yagawa, G. : "Development of a virtual research environment in ITBL project", *Proc. of the Int. Conf. on Supercomputing in Nuclear Applications (SNA2003)*, (2003) [CDROM].
- 6) Higuchi, K., Imamura, T., Suzuki, Y., Shimizu, F., Machida, M., Otani, T., Hasegawa, Y., Yamagishi, N., Kimura, K., Aoyagi, T., Nakajima, N., Fukuda M. and Yagawa G. : "Grid computing supporting system on ITBL project", *High Performance Computing, Veidenbaum et al. (Eds.) (ISHPC2003), LNCS2858, Springer-Verlag*, pp.245-257, (2003).
- 7) Higuchi, K., Otani, T., Hasegawa, Y., Suzuki, Y., Yamagishi, N., Kimura, K., Maesako, H., Fukuda, M. and Yagawa, G. : "Application of ITBL basic software for virtual organizations", *Proc. of the 8th Conf. On Computational Engineering and Science, The Japan Society for Computational Engineering and Science*, 8(2), pp.797-800, (2003) [in Japanese].
- 8) Imamura, T., Yamagishi, N., Takemiya, H., Hasegawa, Y., Higuchi K. and Nakajima, N. : "A visual resource integration environment for distributed applications on the ITBL system", *High Performance Computing, Veidenbaum et al. (Eds.) (ISHPC2003), LNCS2858, Springer-Verlag*, pp.258-268, (2003).
- 9) Imamura, T., Hasegawa, Y., Yamagishi, N. and Takemiya, H. : "Implementation of a resource handling environment for distributed applications on ITBL (IT-Based Laboratory)", *Proc. of the 8th Conf. On Computational Engineering and Science, The*

- Japan Society for Computational Engineering and Science, 8(2), pp.793-796, (2003) [in Japanese].
- 10) Kaburaki H., Kadoyoshi T., Shimizu F., Kimizuka H., Jitsukawa S.: "Molecular dynamics study on the interaction of a dislocation and radiation induced defect clusters in FCC crystals", Supercomputing in Nuclear Applications(SNA'2003), Sept.2003, Paris(France).
 - 11) Kaburaki H., Kadoyoshi T., Shimizu F., Kimizuka H.: "Development of parallel molecular dynamics stencil and its application to defect simulations in materials science", 6th International Seminar on Science and Computing, Sept.2003, Moscow(Russia).
 - 12) Kaburaki H., Kadoyoshi T., Shimizu F., Kimizuka H., Jitsukawa S.: "Molecular dynamics simulation on the irradiation induced dislocation loops in FCC metals", The 8th IUMRS International Conference on Advanced Materials, Oct.2003, Yokohama(Japan).
 - 13) Kadoyoshi T., Kaburaki H., Shimizu F., and Kimizuka H., "Molecular dynamics study on the dislocation loops in FCC metals", Annual APS March Meeting 2004, Montreal, Canada (March, 2003).
 - 14) Kadoyoshi T., Kaburaki H., Shimizu F., Kimizuka H., Jitsukawa S.: "Molecular dynamics simulation of radiation induced point defects in FCC metals", 11th International Conference on Fusion Reactor Materials, Dec.2003, Kyoto(Japan).
 - 15) Kadoyoshi T., Kaburaki H., Shimizu F., Kimizuka H., Jitsukawa S., Li J.: "Molecular dynamics simulation on the morphological transformation of dislocation loops in FCC metals", Materials Research Society(MRS) Fall Meeting, Dec.2003, Boston(U.S.A.).
 - 16) Kato M., Ako M., Machida M., Koyama T., Ishida T., "Ginzburg-Landau calculations of d-wave superconducting dot in s-wave superconducting matrix (d-dot)", ISS2003 Tsukuba, Japan (Nov. 2003).
 - 17) Kimizuka H., Kaburaki H., Kadoyoshi T., Shimizu F.: "Molecular dynamics study on the behavior of emitted dislocations from a crack-tip in the fracture process of FCC metals", American Physical Society March Meeting, March,2004, Montreal(Canada).
 - 18) Kimura, H., "Introduction for ITBL project", High-Performance Networking and Computing (SC 2003), Phoenix, on Nov. 2003.
 - 19) Kono H. and Saven J. G.: Ab initio Profile for a given backbone structure-application for protein design and detection functionally important residues, 224th American Chemical Society Annual Meeting (ACS), New York,

- USA, (2003).
- 20) Kono H., Yura K. and Go N.: Genome function prediction based on transcription systems, The 41st annual meeting of the Biophysical Society of Japan, Niigata, Japan, (2003).
 - 21) Kono H., Yura K. and Go N.: Genome function prediction based on transcription systems, The 59th Annual meeting of the Physical Society of Japan, Kyushu Univ., Japan, (2004) [in Japanese].
 - 22) Koyama T., Machida M., Kato M., and Ishida T., "Phase Dynamics in a d-dot Embedded in a s-wave Superconductor", ISS2003 Tsukuba, Japan (Nov. 2003).
 - 23) Machida M., Koyama T., Kato M., Ishida T., "Electronic Structure of a Half Quantized Vortex", ISS2003 Tsukuba, Japan (Nov. 2003).
 - 24) Machida M., Koyama T., Kato M., and Ishida T., "Non-equilibrium Superconductivity and Vortex Fluctuations in MgB₂ Thin Films", NSF2003(CREST Nano-fab International Workshop), Kyoto, Japan (Nov. 2003).
 - 25) Machida M., Koyama T., Kato M., and Ishida T., "Creation of Frustrated System by D-dot Array", 2004 Annual Meeting of American Physical Society, Montreal, Canada (Mar. 2004).
 - 26) Machida M., Yamada S., Koyama T., Kato M., Ishida T., "Numerical Studies for Novel Superconducting Properties and Neutron Detector Applications by Superconductor Nano-fabrication Techniques", Autumn Meeting of Atomic Energy Society of Japan, Shizuoka (September, 2003).
 - 27) Machida M., "Superconducting Fluctuation and Nernst Effect", Autumn Meeting of Physical Society of Japan, Okayama (September, 2003).
 - 28) Machida M., Itakura M., "Superconducting Fluctuation and Formation of Local Superconducting Order", Autumn Meeting of Physical Society of Japan, Okayama (September, 2003).
 - 29) Machida M., Yamada S., Kano T., "Current Status of Tera-flops Parallel Simulations for Superconducting States", JSME 16th Computational Mechanics Conference, Kobe (October, 2003).
 - 30) Machida M., Sasa N., Matsumoto H., "Vortex States in Rotating Bose-Einstein Condensate", Workshop at Research Institute for Mathematical Sciences (Nonlinear Wave Phenomena and their Application) Kyoto (September, 2003).
 - 31) Machida M., Koyama T., Kato M., Ishida T., "Spin Ice Created by D-dot : Creation of Frustrated Systems by using Superconducting Nano-fabrication Techniques", Workshop of the Institute for Solid State Physics (Novel Material Properties Created by Frustration) Kashiwa (December, 2003).

- 32) Machida M., Sasa N., Matsumoto H., "Vortex Dynamics in Bose-Einstein Condensate of Dilute Atomic Gas: Vortex Creation and Energy Dissipation", Workshop at Research Institute for Mathematical Sciences (Gauge Structure of Fluid Vortex Field and Variation Principle), Kyoto (January, 2004).
- 33) Machida M., Sasa N., Matsumoto H., "Vortex Penetration and Lattice Formation in Rotating Bose-Einstein Condensate", Workshop of the Institute for Solid State Physics (New Research Frontier of Quantum Condensate) Kashiwa (January 2004).
- 34) Machida M., Itakura M., "Vortex Excitation in Nano-scale High-Tc Superconductors", Spring Meeting of Physical Society of Japan, Fukuoka (March, 2004).
- 35) Ohno, N., Suzuki Y. and Kureta, M. : "Parallel volume rendering on immersive projection technology", 16th Lecture meeting of the Institute of Electrical Engineers of Japan, (2004) [in Japanese].
- 36) Sai, K., Suzuki, Y., Araki, F., Uehara, H. and Haginoya, H. : "Utilization of PATRAS visualization software for large-scale data on Earth Simulator", Proc. of the Conf. on Computational Engineering and Science, The Japan Society for Computational Engineering and Science, 8(2), pp.761-764, (2003) [in Japanese].
- 37) Sarai A., Selvaraj S., Gromiha M. M. and Kono H.: Structure-Function Relationship in DNA Sequence Recognition by Transcription Factors, Bioinformatics (2004), Second Asia Pacific Bioinformatics Conference (APBC2004), NZ, (2004)
- 38) Sasa, N., "Numerical Simulation of Ginzburg-Landau Equation by Splitting Method", The Annual Meeting of the Japan Society for Industrial and Applied Mathematics, Kyoto (2003).
- 39) Sasa N., "Numerical Simulation of Nonlinear Schrodinger Equation by Splitting Method", The Annual Meeting of the Japan Physical Society of Japan, Okayama (2003).
- 40) Sasa N, Machida M, Matsumoto H., "Numerical Simulation of 3-dimensional Nonlinear Schrodinger Equation for Bose-Einstein Condensation", Workshop of Nonlinear Wave Phenomena and Applications, Kyoto (2003).
- 41) Sasa N, Machida M, Matsumoto H., "Numerical Simulation of 3-dimensional GP Equation for Bose-Einstein Condensation", Workshop of Mathematical Theories and Applications of Nonlinear Wave and Nonlinear Dynamics, Fukuoka (2003).
- 42) Sasa N, Machida M, Matsumoto H., "Vortex Nucleation and Lattice Formation in a Rotating Bose-Einstein Condensation", Workshop of New development of Research in Quantum Condensed Matter, Tokyo (2004).

- 43) Sasa N, Machida M, Matsumoto H., "Vortex Dynamics in Dilute Atomic Gas Bose-Einstein Condensate: Nucleation and Annihilation, Process of Energy Dissipation", Workshop of Gauge Structure and Variational Principle in Fluid Vortex Field, Kyoto (2004).
- 44) Sasa N, Machida M, Matsumoto H., "Numerical Simulation of 3-dimensional Dynamics for Bose-Einstein Condensation", The Annual Meeting of the Japan Society for Industrial and Applied Mathematics, Fukuoka (2004).
- 45) Shiga M., Shinoda W., Yamaguchi M., Mikami M., and Kaburaki H., "Molecular dynamics and hybrid Monte Carlo methods for isothermal-isostress ensemble", International Conference on Molecular Simulation", International Conference on Molecular Simulation 2004, Tsukuba (January, 2004).
- 46) Shiga M., Shinoda W., Mikami M., Kaburaki H., "Molecular dynamics method to control temperature and stress and its applications", Conference on Molecular Structure 2003, Kyoto (September 2003).
- 47) Shimizu F., Kaburaki, F., Yamagishi N., Hasegawa Y., Yamada S., Sasa N., Machida M., Kimura K., and Arakawa C., "R&D on Parallel Algorithms in JAERI", SC2003: High Performance Computing and Communications, Pheonix, USA (November, 2003).
- 48) Shimizu F., Itakura M., Kaburaki H., and Kimizuka H., "Molecular dynamics simulation on the three dimensional grain boundary fracture patterns in the FCC nanocrystals", Annual APS March Meeting 2004, Montreal, Canada (March, 2003).
- 49) Shimizu F., Kadoyoshi T., Kaburaki H., Yamagishi N., "Parallel Molecular-Dynamics Simulation on ITBL", Proceedings of the Conference on Computational Engineering and Science, 8, 801, Tokyo, May 2003.
- 50) Shimizu F., Kaburaki H., "Radiation induced property change and fracture of materials using atomistic simulation methods", 2003 Fall Meeting of the Atomic Energy Society of Japan, Shizuoka, September 2003.
- 51) Sluiter, M.H.F., Belosludov, R.V., Jain, A., Belosludov, V.R., Adachi, H., Kawazoe, Y., Higuchi, K. and Otani, T. : "Ab initio study of hydrogen hydrate clathrates for hydrogen storage within the ITBL environment", High Performance Computing, Veidenbaum et al. (Eds.) (ISHPC2003), LNCS2858, Springer-Verlag, pp.330-341, (2003).
- 52) Suzuki, Y. and Sai, K. : "Research and development of parallelized visualization system on Earth Simulator and grid-suited visualization system on ITBL", All NEC C&C Systems Users Association Heisei year 15 collection of papers, pp.211-229, (2003) [in Japanese].

- 53) Suzuki, Y., Matsumoto, N., Yamagishi, N., Higuchi, K., Otani, T., Nagai, H., Terada, H., Furuno, A., Chino M. and Kobayashi, T. : "Development of multiple job execution and visualization system on ITBL system infrastructure software and its utilization for parametric studies in environmental modeling", Computational Science - ICCS 2003, Sloot et al. (Eds.), LNCS2659, Springer-Verlag, pp.120-129, (2003).
- 54) Suzuki Y., and Matsumoto, N. : "Development of remote visualization and collaborative visualization system in ITBL grid environment", High Performance Computing, Veidenbaum et al. (Eds.) (ISHPC2003), LNCS2858, Springer-Verlag, pp.269-277, (2003).
- 55) Suzuki, Y., Matsumoto, N. and Sai, K. : "Collaborative visualization for supporting joint researches in ITBL project", Proc. of the Int. Conf. on Creating, Connecting and Collaborating through Computing, IEEE CS Press, pg. 187, (2004).
- 56) Tsujita, Y., Imamura, T., Yamagishi, N. and Takemiya, H. : "MPI-2 support in heterogeneous computing environment using an SCore cluster system", Parallel and Distributed Processing and Applications (ISPA2003), LNCS2745, Springer-Verlag, pp.139-144, (2003).
- 57) Ueshima, Y.: "Education on science technology and an exhibit in science museum using portable VR", 8th Japan Calculation Engineering, Tokyo, on May. 2003.
- 58) Ueshima, Y., Yamasaki, I., Isogai, K., Miyazaki, M., Kimura, H., Aikawa, H.: "Let's use friendly virtual reality!", Business & Technology fair 2003 Kansai, Osaka, on May. 2003.
- 59) Watanabe T., "Flow pattern and heat transfer rate in three-dimensional Rayleigh-Benard convection," 10th European PVM/MPI User's Group Meeting, September 29, 2003, Venice, Italy.
- 60) Yamada S., Imamura T., and Machida M., Development of a Parallel Solver for Large-Scale Eigenvalue Problems ICIAM 2003 - 5th International Congress on Industrial Applied Mathematics, Sydney, Australia (July, 2003).
- 61) Yamada S., Imamura T., "PARCEL: Eigenvalue Problem Solver", The 8-th Conference on Computational Engineering and Science, Tokyo (2003).
- 62) Yamada S., M. Machida M. and Imamura T., "Parallel Solver for Large-Scale Eigenvalue Problems of Hubbard Model on the Earth Simulator", Numerical Analysis and New Information Technology, Kyoto, (2003).
- 63) Yamada S., Machida M., and Imamura T., "Parallel Computation of Large-Scale Eigenvalue Problems of Strongly Correlated Electrons on the Earth Simulator", High Performance Computing Systems 2004, Tokyo, (2004).

- 64) Yamamoto, K., Isogai, K.: "An Attempt to share educational contents", PSE Workshop 2003, Sapporo, 161 (2003.7).
- 65) Yamamoto N., Shimizu F., Yokokawa M., Sekiguchi S., Kaburaki H., Himeno R., Kurokawa M., Takei T., Matsumoto H., "Construction of a Portal Site for MD Stencil on the Grid", IPSJ SIG Technical Reports, 2003-HPC-96, 55, Tokyo, October 2003.
- 66) Yasuhara, Y., Yamasaki, I.: "ITBL utility dissemination using portable VR system & 3D AVS Player", International Industrial Fair 2003, Kobe, on Nov. 2003.
- 67) Yura K., Gong X.J. and Go N.: Development of an Integrated Bioinformatics System for Protein Sequence and Structure Computational Analyses, International Workshop: Integrated Databases and DataGrid for Structural Biology and Molecular Biology, Institute for Protein Research, Osaka University, Japan, (2004).
- 68) Yura K., Kono H., and Go N.: A trial of genome function prediction through gene positional information in the case of DNA repair proteins, 4th East Asian Biophysics Symposium. Taipei, (2003).
- 69) Yura K., Kono H., and Go N.: A trial of genome function prediction through gene positional information in the case of DNA repair proteins, Frontiers in Bioinformatics: Structure, Interaction and Function, Kyoto, Japan, (2004).
- 70) Yura K., Kono H., and Go N.: DNA repair related protein prediction through gene positional information, The 2nd Workshop on DNA Repair Proteins, Kizu, Japan, (2003) [in Japanese].
- 71) Yura K., Kono H., and Go N.: Molecular in silico biology of DNA repair enzymes: A trial of genome function prediction through gene positional information, The 15th Annual Meeting of the Korean Society for Molecular and Cellular Biology, Seoul, Korea, (2003).
- 72) Yura K., Shionyu M. and Go M.: Information reduction protein 3D structures to genome sequences with 3D-keynote. GenProC2004: Open Workshop on What research will be promoted by protein 3D structures, Tokyo Garden Palace, Japan, (2004) [in Japanese].

Others : Followings are presentations made by scientists outside CCSE whose research activities were supported by the Earth Simulator Use Support division in CCSE.

- 1) Fleig O., C. Arakawa, "Large Eddy Simulation of Tip Vortex Flow at High Reynolds number", AIAA 2004_0263, 42nd AIAA Aerospace Sciences Meeting and Exhibit, Reno, USA, Jan. 2004.
- 2) Satake S., et al.: Large Scale Structures of Turbulent Shear Flow via DNS, A.

Veidenbaum et al. (Eds.), Lecture Notes in Computer Science 2858, High Performance Computing, pp.468-475, 2003.

- 3) Takase K., et al., "Large-Scale Numerical Simulations on Two-Phase Flow Behavior in a Fuel Bundle of RMWR with the Earth Simulator," Proc. International Conference on Supercomputing in Nuclear Applications (SNA2003), Paris, France, 2003.
- 4) Yoshida, et al., "Numerical Simulation of Liquid Film around Grid Spacer with Interface Tracking Method," Proc. International Conference on Advanced Nuclear Power Plants and Global Environment (GENES4/ANP2003), Kyoto, Japan (2003).

6.3 Awards

1) Best Paper Award

All NEC C&C Systems Users Association

Suzuki, Y. and Sai, K.: "Research and development of parallelized visualization system on Earth Simulator and grid-suited visualization system on ITBL."

2) Best Poster Award

International Conference on Supercomputing in Nuclear Engineering (SNA'2003)

Hazama, O. and Guo, Z.: "Practical integrated simulation systems for coupled numerical simulations in parallel."

3) The HPC Challenge Award for the Most Geographically Distributed Application:

"Global Analysis of Arthropod Evolution," (Together with the University of Stuttgart), the HPC Challenge Award was given for showing the effectiveness of Grid infrastructure technologies ranging over 5 continents through database searching schemes at SC2003.

国際単位系 (SI) と換算表

表1 SI基本単位および補助単位

量	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
物質質量	モル	mol
光度	カンデラ	cd
平面角	ラジアン	rad
立体角	ステラジアン	sr

表3 固有の名称をもつSI組立単位

量	名称	記号	他のSI単位による表現
周波数	ヘルツ	Hz	s ⁻¹
力	ニュートン	N	m·kg/s ²
圧力、応力	パスカル	Pa	N/m ²
エネルギー、仕事、熱量	ジュール	J	N·m
工率、放射束	ワット	W	J/s
電気量、電荷	クーロン	C	A·s
電位、電圧、起電力	ボルト	V	W/A
静電容量	ファラド	F	C/V
電気抵抗	オーム	Ω	V/A
コンダクタンス	ジーメンズ	S	A/V
磁束	ウェーバ	Wb	V·s
磁束密度	テスラ	T	Wb/m ²
インダクタンス	ヘンリー	H	Wb/A
セルシウス温度	セルシウス度	°C	
光束	ルーメン	lm	cd·sr
照度	ルクス	lx	lm/m ²
放射能	ベクレル	Bq	s ⁻¹
吸収線量	グレイ	Gy	J/kg
線量当量	シーベルト	Sv	J/kg

表2 SIと併用される単位

名称	記号
分、時、日	min, h, d
度、分、秒	°, ', "
リットル	l, L
トン	t
電子ボルト	eV
原子質量単位	u

1 eV = 1.60218 × 10⁻¹⁹ J
1 u = 1.66054 × 10⁻²⁷ kg

表4 SIと共に暫定的に維持される単位

名称	記号
オングストローム	Å
バ	b
バル	bar
ガリ	Gal
キュリー	Ci
レントゲン	R
ラド	rad
レム	rem

1 Å = 0.1 nm = 10⁻¹⁰ m
1 b = 100 fm² = 10⁻²⁸ m²
1 bar = 0.1 MPa = 10⁵ Pa
1 Gal = 1 cm/s² = 10⁻² m/s²
1 Ci = 3.7 × 10¹⁰ Bq
1 R = 2.58 × 10⁻⁴ C/kg
1 rad = 1 cGy = 10⁻² Gy
1 rem = 1 cSv = 10⁻² Sv

表5 SI接頭語

倍数	接頭語	記号
10 ¹⁸	エクサ	E
10 ¹⁵	ペタ	P
10 ¹²	テラ	T
10 ⁹	ギガ	G
10 ⁶	メガ	M
10 ³	キロ	k
10 ²	ヘクト	h
10 ¹	デカ	da
10 ⁻¹	デシ	d
10 ⁻²	センチ	c
10 ⁻³	ミリ	m
10 ⁻⁶	マイクロ	μ
10 ⁻⁹	ナノ	n
10 ⁻¹²	ピコ	p
10 ⁻¹⁵	フェムト	f
10 ⁻¹⁸	アト	a

(注)

- 表1-5は「国際単位系」第5版、国際度量衡局 1985年刊行による。ただし、1 eV および 1 uの値はCODATAの1986年推奨値によった。
- 表4には海里、ノット、アール、ヘクタールも含まれているが日常の単位なのでここでは省略した。
- barは、JISでは流体の圧力を表わす場合に限り表2のカテゴリーに分類されている。
- EC閣僚理事会指令では bar, barn および「血圧の単位」mmHgを表2のカテゴリーに入れている。

換算表

力	N (=10 ⁵ dyn)	kgf	lbf
	1	0.101972	0.224809
	9.80665	1	2.20462
	4.44822	0.453592	1

粘度 1 Pa·s (=N·s/m²) = 10 P (ポアズ) (g/(cm·s))

動粘度 1 m²/s = 10⁶ St (ストークス) (cm²/s)

圧	MPa (=10 bar)	kgf/cm ²	atm	mmHg (Torr)	lbf/in ² (psi)
	1	10.1972	9.86923	7.50062 × 10 ³	145.038
力	0.0980665	1	0.967841	735.559	14.2233
	0.101325	1.03323	1	760	14.6959
	1.33322 × 10 ⁻⁴	1.35951 × 10 ⁻³	1.31579 × 10 ⁻³	1	1.93368 × 10 ⁻²
	6.89476 × 10 ⁻³	7.03070 × 10 ⁻²	6.80460 × 10 ⁻²	51.7149	1

エネルギー・仕事・熱量	J (=10 ⁷ erg)	kgf·m	kW·h	cal (計量法)	Btu	ft·lbf	eV
	1	0.101972	2.77778 × 10 ⁻⁷	0.238889	9.47813 × 10 ⁻⁴	0.737562	6.24150 × 10 ¹⁸
	9.80665	1	2.72407 × 10 ⁻⁶	2.34270	9.29487 × 10 ⁻³	7.23301	6.12082 × 10 ¹⁹
	3.6 × 10 ⁶	3.67098 × 10 ⁵	1	8.59999 × 10 ⁵	3412.13	2.65522 × 10 ⁶	2.24694 × 10 ²⁵
	4.18605	0.426858	1.16279 × 10 ⁻⁶	1	3.96759 × 10 ⁻³	3.08747	2.61272 × 10 ¹⁹
	1055.06	107.586	2.93072 × 10 ⁻⁴	252.042	1	778.172	6.58515 × 10 ²¹
	1.35582	0.138255	3.76616 × 10 ⁻⁷	0.323890	1.28506 × 10 ⁻³	1	8.46233 × 10 ¹⁸
	1.60218 × 10 ⁻¹⁹	1.63377 × 10 ⁻²⁰	4.45050 × 10 ⁻²⁶	3.82743 × 10 ⁻²⁰	1.51857 × 10 ⁻²²	1.18171 × 10 ⁻¹⁹	1

1 cal = 4.18605 J (計量法)
= 4.184 J (熱化学)
= 4.1855 J (15 °C)
= 4.1868 J (国際蒸気表)
仕事率 1 PS (仏馬力)
= 75 kgf·m/s
= 735.499 W

放射能	Bq	Ci
	1	2.70270 × 10 ⁻¹¹
	3.7 × 10 ¹⁰	1

吸収線量	Gy	rad
	1	100
	0.01	1

照射線量	C/kg	R
	1	3876
	2.58 × 10 ⁻⁴	1

線量当量	Sv	rem
	1	100
	0.01	1



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